Guide to Using WVASE®
Spectroscopic Ellipsometry Data Acquisition and Analysis Software

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PREFACE

WVASE® is the most sophisticated and complete software available for optical data analysis. It is also the integrated data acquisition software for J.A. Woollam Co., Inc. spectroscopic ellipsometers. WVASE® contains many features and functions that are important for ellipsometric applications in virtually all thin film and surface science areas, both in situ and ex situ. Written for the Microsoft Windows® operating system (32-bit, enhanced mode), WVASE® is user-friendly and very fast.

Ellipsometry is an extremely sensitive characterization technique which can be used to determine thin film layer thicknesses and/or optical constants. However, the sensitivity of ellipsometry has, in the past, been difficult to realize as characterization power because ellipsometry is an indirect measurement technique requiring the computational power of modern computers. In other words, the experimental data must be fit to a model, with the fit parameters providing the desired information. WVASE® is designed to handle data modeling and fitting from simple single film problems to extremely complex multi-sample, multi-layer problems. Additionally, the analysis features of WVASE® are not limited to ellipsometric data as WVASE® can work simultaneously with any combination of reflection, transmission, and ellipsometric data.

Our general experience is that ellipsometric measurement and analysis problems span a very wide range of difficulties, and there are no general optimal procedures which apply to all samples and structures. The approach which is best for a given sample structure is dictated not only by the sample structure, but also by the information which you intend to determine about the sample. As a result, some care is required to ensure that accurate and precise results are obtained. In this regard, there is no substitute for hands-on experience; however, we have endeavored to help you build this experience to the necessary level as fast as possible with a variety of data analysis examples.

We are dedicated to helping our customers solve their particular problems when possible, and we enjoy sharing our extensive knowledge base with our customers. We have tried to address in this manual many of the difficulties that we and other J.A. Woollam Co., Inc. customers have reported to us. We would appreciate your comments on this manual and your suggestions for improving its usability in future editions, as well as any suggestions you may have for improvements to our software and our ellipsometers.

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Glossary of Terms

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Chapter 1 Introduction

1.1 WVASE® as a Windows® application

Do not run Windows® in standard mode if you wish to run WVASE™!

WVASE® is a Windows® application that will run on Windows® 95, Windows® 98, Windows® NT, Windows® XP, Windows® XP-64bit (as a 32bit application), Windows Vista™, Windows 7™, Windows Vista™-64bit and Windows 7™-64bit (as a 32bit application). As Windows® and WVASE® continue to evolve, updates on system requirements may supersede the requirements described here.

WVASE® makes use of the standard graphical user interface features: pull down menus, resizable windows, copying to the clipboard, scroll wheel, short cut keys, etc. If you are not familiar with the basics of Windows® (using a mouse, menus, etc.) we have included a short introduction in chapter 3 - Navigating WVASE®. This chapter is not comprehensive, however, and you might still need to read the Windows® user guide or ask a knowledgeable person to give you a quick lesson.

1.2 Organization of this manual

This document is organized in a modular form to facilitate later revisions and expansions. New documentation will become available as new analysis features are added, as new hardware options become available, or as new versions of Windows® are released. The following is a complete list of the chapters and appendices in this manual, with a short description of each.

Tutorial

A Short Course in Ellipsometry A general review of ellipsometry, covering the theory and implementation of ellipsometers, optical data analysis, and the optical properties of materials and thin films. This is a good place to begin.

Navigating WVASE®: A discussion of the window structure and menubar organization within WVASE®, along with a basic tutorial on the use of Windows®. The commands for moving between windows, controlling the global settings (including memory management), and exiting the program are also reviewed.

Reference

Hardware Window: VASE®: A complete reference to all commands and options available from the Hardware window of WVASE® for VASE® systems. This window is used for all data acquisition and control of the VASE® instrument.
Reference

**Hardware Window:** *M-Series:* A complete reference to all commands and options available from the Hardware window of WVASE® for *M-XX* systems, both in situ and ex situ. *M-XX* instruments are controlled from this window.

Reference

**The Experimental Data Window:** A complete reference to all commands and options available from the WVASE® Experimental Data window, including loading, saving, merging, and appending data files, changing data types, and selecting data ranges for fitting.

Reference

**The Model Window:** A complete reference to all commands and options available from the WVASE® Model window, which is used to construct optical models for data analysis. Included is a comprehensive list of WVASE®-supported layer types.

Reference

General Oscillator Layer: A complete reference for the WVASE®’s powerful and flexible Generalized Oscillator layer. Included are tips for using the layer.

Reference

**The Generated Data Window:** A complete reference to all commands and options available from the WVASE® Generated data window. This window is used to store and manipulate data calculated from the optical model in the Model window.

Reference

**The Graph Window:** A complete reference to all commands and options available from the WVASE® Graph window, which is used to plot experimental and calculated data, optical constants, depth profiles, and many other quantities. A discussion of how to move these figures within the *Windows*® environment and how to export plots and/or data to other applications is also included.

Reference

**The Fit Window:** A complete reference to all commands and options available from the Fit window in WVASE®. This window is used to fit the optical model in the Model window to experimental data contained in the Experimental Data window.

Tutorial

**Data Acquisition Procedures and Strategies:** How to acquire ellipsometric data, as well as the many other optical data types which can be measured with a J.A. Woollam Co. ellipsometer. Strategies for the acquisition of ellipsometry data from various types of samples are reviewed, as well as tips for optimizing the hardware and scan settings to get the best possible data.

Tutorial and Reference

**Ex Situ Data Analysis:** A comprehensive discussion of data analysis strategies for a very broad range of materials and sample structures. Strategies in this section are applicable to static optical data (ellipsometric, reflectance, or transmission), acquired with all J.A. Woolam Co. ellipsometers, or with any instruments that acquire one or more of the optical data types supported by WVASE®.

Tutorial and Reference

**Ex Situ Data Analysis Examples:** A collection of examples of the analysis of ellipsometry, reflectance, and transmittance data, ranging from very basic to very advanced. The examples in this chapter cover many of the analysis strategies discussed in the previous chapter. These examples may be worked in sequence for educational purposes, or may be consulted as a reference for a particular sample type or structure.

Tutorial

**In Situ Dynamic Data Analysis and Examples:** A comprehensive discussion of data analysis strategies for data acquired as a function of time, *in situ* or *ex situ*, with examples. Strategies in this section are applicable to dynamic data acquired specifically with the *M-Series* instruments.

Reference

**Appendices:** Appendices A-C cover the file format specifications for the various file types used by WVASE®.
1.3 How to use this manual

Even experienced ellipsometer users will gain from reading the tutorial chapters!

This manual contains both a complete reference on all options and procedures available within WVASE® and a thorough review of ellipsometry in general and ellipsometric data acquisition and analysis procedures. We recommend reading the following chapters in order, then consulting the reference chapters (chapters 4-10) as necessary for specific operational procedures.

All users

- Chapter 2 - ‘A Short Course in Ellipsometry’.
- Chapter 3 - ‘Navigating WVASE®’.

After reading these chapters, proceed through the chapters listed below for the ellipsometer that you are using.

Ex situ users

- Chapter 12 – ‘Data Acquisition Procedures and Strategies’
- Chapter 13 - ‘Ex Situ Data Analysis’. This is a very long and thorough chapter, and you may wish to skim over most of the material, concentrating on sample structures and materials of particular interest to you.
- Chapter 14 - ‘Ex Situ Data Analysis Examples’. It is essential that you try working the examples as you go through this chapter.

In situ users

- Chapter 15 - ‘In Situ Dynamic Data Analysis and Examples’
Chapter 2 A Short Course in Ellipsometry

[Revised November 11, 2008 (version 3.690)]

2.1 Short course overview

The short course will benefit novices and experts alike!

This chapter contains a general overview of ellipsometry, starting from the assumption that the reader has no familiarity with the subject. To fully utilize the measurement power of ellipsometry there are certain concepts that the user should be familiar with. These concepts are presented here for the novice, but the experienced user of ellipsometry will also benefit from the detailed discussion of many of the topics in this chapter. Some sections may be skipped by the novice, and have been marked as ‘Advanced’ in the left margin.

In this chapter you will learn

Ellipsometry Basics
- What ellipsometry measures and what information can be obtained.
- Advantages of variable angle and spectroscopic measurements.
- Discussion of accuracy and precision

General Procedure Overview
- Determining material properties from the data measurements via a model-dependent analysis.

*Following sections discuss each step in detail.

Measurement
- Polarized light and use of Jones vectors to conveniently described.
- Optical components used in ellipsometers.
- Primary ellipsometer configurations (advantages and disadvantages).
- Detailed descriptions: Rotating Analyzer Ellipsometer.
- Optics calibration.

Model
- Description of Optical Constants (metals, dielectrics, semiconductors).
• How polarized light reflects from layered structures.
• Calculating psi and delta from the model.

**Fit and Results**

• How regression analysis is used to fit variable parameters in the optical model for a sample to the experimental optical data.
• How to evaluate the results of regression fits.

This short course is a fairly general treatment and the precise details of running WVASE™ are presented in the remaining chapters. In addition, a review of general references on ellipsometry is provided at the end of this chapter.

### 2.2 What is ellipsometry?

Ellipsometry is a very sensitive measurement technique that uses polarized light to characterize thin films, surfaces, and material microstructure. It derives its sensitivity from the determination of the relative phase change in a beam of reflected polarized light, exceeding the sensitivity of an intensity reflectance measurement. Also, ellipsometry is more accurate than intensity reflectance because the absolute intensity of the reflected light does not have to be measured, thus no special reference samples need to be maintained.

**What does an ellipsometer measure?**

Ellipsometry measures the change in polarization state of light reflected from (or transmitted through) the surface of a sample. Fundamentally, ellipsometry refers only to the measurement of the polarization state of a light beam. However, ellipsometric measurements are usually performed in order to describe an "optical system" that modifies the polarization state of a beam of light. For thin film sample analysis, the "optical system" is simply the sample.

The measured values are expressed as psi (Ψ) and delta (Δ). These values are related to the ratio of Fresnel reflection coefficients \( \tilde{R}_p \) and \( \tilde{R}_s \) for p- and s-polarized light, respectively.

\[
\rho = \frac{\tilde{R}_p}{\tilde{R}_s} = \tan(\Psi)e^{i\Delta}
\]  

(2.1)

Because ellipsometry measures the ratio of two values it can be highly accurate and very reproducible. Because the ratio is a complex number, it also contains "phase" information (Δ), which makes the measurement very sensitive.

**What parameters can be determined?**

Ellipsometry can determine optical constants, layer thicknesses, and many physical quantities which affect the optical constants.

Ellipsometry is commonly used to characterize both thin films and bulk materials. The most common application is measurement of thin film thickness and optical constants. For many samples, ellipsometry is sensitive to film thickness on a sub-monolayer level. It has also proven to be the primary technique for determining optical constants in the UV, visible, and IR wavelength ranges. Ellipsometry is very flexible and is sensitive to many microstructural material properties.

Ellipsometry has been used to determine:
Optical constants (n, k or $\varepsilon_1, \varepsilon_2$)

Thin film thickness (single or multiple layers)

Doping concentration

Surface and interfacial roughness

Alloy ratio

Crystallinity

Optical anisotropy

Depth profile of material properties

Growth or Etch rate (in-situ)

Temperature (in-situ)

Spectroscopic ellipsometry combined with variable angle of incidence is an extremely powerful measurement technique. It has many advantages over similar optical characterization tools (e.g. reflectometry, single-wavelength ellipsometry). In the last decade, two things have greatly increased the usefulness of ellipsometry for routine sample analysis.

1. The development of automated spectroscopic data acquisition systems such as diode array detector and rotating element ellipsometers.

2. The development of fast digital microcomputers to run the measurement system and to analyze data.

**Why variable angle spectroscopic ellipsometry (VASE®)?**

*Variable vs. fixed angle of incidence.*

The combination of variable angle of incidence and spectroscopic measurements allows the user to acquire large amounts of data from a given sample. More importantly, the spectral acquisition range and angles of incidence may be optimized for the determination of certain sample parameters such as a layer thickness or the optical constants of one of the films. As a result the variable angle of incidence spectroscopic ellipsometer has the flexibility necessary to handle a very broad range of sample materials and structures, and has the power to characterize many complex structures which single angle and/or single wavelength ellipsometers cannot.

*Spectroscopic vs. single wavelength measurements.*

Many simple samples may be characterized by ellipsometric measurements at a single wavelength, and indeed there are a large number of commercial instruments available for this purpose. Spectroscopic measurements provide much more information about the sample, and also provide the ability to acquire data in spectral regions where the measured data are most sensitive to the model parameters which are to be determined. In many cases the dispersion (variation with wavelength) of the optical constants of a given material is known, or the optical constants may be parameterized in such a way as to enforce some type of dispersion on the optical constants (Cauchy, Lorentz, and parametric semiconductor models for example). In this case the acquisition of spectroscopic data allows the user to take advantage of this knowledge to obtain more information from the analysis of the ellipsometric data than would be possible when analyzing data from a single wavelength.
Comparison to Reflectance Measurements

VASE vs. intensity reflectance

Variable angle spectroscopic ellipsometry acquires two pieces of information at every wavelength/angle combination. Reflectance measurements are generally confined to normal incidence, which provides a single term at each wavelength. More measured parameters increase the possible material properties that can be determined by VASE®.

In addition, ellipsometry measurements can be both highly accurate and sensitive. It derives its sensitivity, which is greater than a simple reflection measurement, from the relative phase change that is measured (the quantity \( \Delta \)). The phase information has been shown to greatly increase sensitivity to the surface condition, which allows ellipsometry to study ultra-thin films on a sub-monolayer level.

Also, ellipsometry is more accurate than intensity reflectance because the absolute intensity of the reflected light does not have to be measured. For rotating element ellipsometers like those made by the J.A. Woollam Co., Inc., the detectors only need to have a linear intensity response. They do not need to be calibrated in an absolute sense, such that no special reference samples need to be maintained. There is also less concern with factors that can affect the absolute intensity measurement, such as fluctuations in light intensity at the source, partial-scattering from the surface, or the measurement beam being larger than the sample.

What are the regimes of applicability?

There are several factors that determine the limits on the information about a given sample that may be determined by ellipsometry. Most of these factors are related to the length scale of the probe used in ellipsometry, i.e. the wavelength of the incident light beam. Spectroscopic ellipsometers are now available covering a wide wavelength range; therefore the choice of ellipsometer is often determined by the best wavelength range to meet a given application.

Ellipsometry works best for film characterization when the film thickness is not too much smaller or larger than the wavelength of the light used for the measurement. It is relatively difficult to use a probe of 500 nm wavelength to characterize a 0.5 nm or 1000 nm thick films, whereas films from about 5 nm to 1000 nm are much simpler to characterize with this wavelength. In general, an infrared ellipsometer is best for thick films (100 nm – 50 microns), while the visible and ultra-violet wavelengths are best for thinner films (1Å – 1 microns).

Also, roughness features on the sample surface or at film interfaces should be less than ~ 10% of the probe beam wavelength for the ellipsometric analysis to be valid. Larger features can cause non-specular scattering of the incident beam and depolarization of the specularly reflected beam. Again, the preferred wavelength range will depend on the application. Mirror-like surfaces are typically measured with ultraviolet and visible ellipsometry; however, industrial-rolled aluminum surfaces have been measured with the longer wavelengths of an IR ellipsometer.

Finally, the uniformity of a film within the measured spot is a critical factor. It is best if the thickness of films under study varies by no more than about 10% over the width of the spot on the sample surface, or the assumption of parallel interfaces of the film will not be valid, and the calculated data cannot be expected to match the experimental data. Measurement of the ‘% depolarization’ can help model the extreme non-idealities of patterned or non-uniform samples. However, this measurement is only possible with a rotating compensator or AutoRetarder® enhanced VASE®.

Ellipsometry best for smooth surfaces.
Accuracy and precision of SE experiments

Ellipsometry is very precise, but its accuracy is difficult to determine.

Ellipsometric measurements are, by nature, very precise. Also, if the model used to fit the ellipsometric data is unique (i.e. does not contain any strongly correlated parameters), the results of the modeling of the ellipsometric data will be very precise as well, meaning that many measurements of the same quantity (a layer thickness, for example) will yield the same result to a very high degree of precision.

It is almost impossible to specify the accuracy of an ellipsometer to the level of its precision. To do so would require another measurement technique with accuracy comparable to the extreme (sub-monolayer) precision of the ellipsometer. We can only hope that by making the ellipsometer and model as accurate as possible the results will be accurate as well. We constantly check our results against any technique that can provide similar information on samples, and routinely find very good agreement with other legitimate metrology techniques. In all cases, when a questionable result is obtained from ellipsometric modeling, it is advisable to corroborate the ellipsometric results with data from other experiments such as Rutherford back-scattering, transmission electron microscopy, and atomic force microscopy.

2.3 General procedure for optical experiments

All optical experiments follow the same general procedure as outlined in this section. Optical experiments never directly measure the sample parameters of interest (thicknesses, optical constants, etc.); rather they measure some quantity that is a function of the parameters of interest. It is then necessary to solve the inverse problem of modeling the measured data to estimate the values of the sample parameters that yield data predicted from the model which best match the measured data. This procedure may be divided into the following four steps, as illustrated in Figure 2.1 below.

Figure 2.1. Basic procedure used in ellipsometry measurements to determine material properties from experimental data.
Measurement

First, the sample is measured. Contrary to most advertising, no optical experiment directly measures layer thickness, optical constants, or any other useful structural or optical parameter of a sample. Rather, optical experiments measure things like reflected or transmitted beam intensities or polarization states. Hopefully, these quantities are affected by the physical sample parameters we are interested in (layer thicknesses, etc.) such that by measuring these uninteresting optical quantities (R, T, Ψ, Δ) we can somehow infer the values of the physical parameters we are actually interested in. Thus, we build an optical experiment and measure beam intensities (reflectance and transmittance) or polarization states (ellipsometric Ψ and Δ), usually as functions of the light beam wavelength, angle of incidence, and/or polarization state.

This chapter details the measurement of ellipsometry data. First, a description of polarized light and Jones vectors are presented. Optical components used to construct an ellipsometer are discussed with detailed descriptions of the different ellipsometer configurations that are available. Special attention is given to rotating analyzer and rotating compensator ellipsometers, because of their applicability to Woollam ellipsometer models. Finally, the calibration of the optical elements is discussed.

Development of a model

Having obtained optical measurements, we must now construct a model from which we can accurately predict what we should measure from a sample of known properties. This model should contain some known parameters, such as the wavelength of the incident light, the incident beam polarization state, and the angle of incidence. The model should also contain some unknown physical parameters, such as layer thicknesses and optical constants.

In this chapter, we give a brief discussion of optical constants, as they are a key component to any model. Next, a description is given of how polarized light reflects from layered structures. This description includes how to calculate the ellipsometry parameters, Ψ and Δ, for a given sample structure.

Fit model to measured data

After we develop a model, we can vary the unknown physical parameters and generate data until we find a set of optimized parameters that yield calculated data that closely match our measured optical data. It is our hope that these parameters then accurately represent the true physical structure of the sample under study. The Levenberg-Marquardt multivariate regression algorithm is employed for the fitting process.

This chapter contains a description of how regression analysis is used to fit variable parameters in the optical model. This includes a review of the Levenberg-Marquardt regression algorithm used by the Woollam Co.

Evaluate the best-fit model

Having found a set of physical parameters yielding calculated data which closely match the experimental optical data, we must now establish that the best-fit set of parameters is unique, physically reasonable, and not strongly correlated. If these criteria are met, we can conclude that the best-fit model probably represents the
physical reality of the sample. We may also calculate a number of statistical quantities that help to evaluate the accuracy and precision of the fit results.

The model can be modified if we are unsatisfied with the results; either because statistics show the results are not unique or because the features in the experimental data are not adequately described by the current model. Later in this chapter, we discuss in greater detail how to evaluate the results of a regression fit.

2.4 Polarized light

Ellipsometry uses polarized light for measurements. The first step in understanding polarized light is to understand an electromagnetic plane wave, which is a solution of Maxwell’s equations for electromagnetic fields. In this section we review the properties of the plane wave, the Jones matrix calculus for describing polarization states, and the various types of light polarization states encountered in ellipsometric experiments.

Maxwell’s equations and the electromagnetic plane wave

Maxwell’s equations for a non-conducting, non-dispersive medium appear as follows:

Maxwell’s equations.

\[ \nabla \cdot \vec{E} = 0 \]
\[ \nabla \cdot \vec{B} = 0 \]
\[ \nabla \times \vec{E} + \frac{1}{c} \frac{\partial \vec{B}}{\partial t} = 0 \]
\[ \nabla \times \vec{B} - \frac{\mu \varepsilon}{c} \frac{\partial \vec{E}}{\partial t} = 0 \]

(2.2)

where \( \vec{E} \) and \( \vec{B} \) are the electric and magnetic fields, \( c \) is the speed of light, and \( \mu \) and \( \varepsilon \) are the permeability and dielectric function, respectively (assuming the medium of propagation to be isotropic). Any propagating light beam must obey these equations.

These equations can be combined to yield the wave equation for the electric field:

The wave equation.

\[ \nabla^2 \vec{E} - \frac{1}{\nu^2} \frac{\partial^2 \vec{E}}{\partial t^2} = 0, \]

(2.3)

where the optical impedance \( \nu \) is defined as

Optical impedance.

\[ \nu = \frac{c}{\sqrt{\mu \varepsilon}}. \]

(2.4)

A solution of the electric field wave equation is the electromagnetic plane wave:

A plane wave, mathematically speaking.

\[ \vec{E}(\vec{r}, t) = \vec{E}_0 \exp \left( -\frac{i2\pi}{\lambda} \vec{q} \cdot \vec{r} \right) \exp(i\omega t), \]

(2.5)
where \( \vec{q} \) is a unit vector along the direction of wave propagation, \( \vec{n} \) is the complex index of refraction \( n - ik \) (as per Azzam and Bashara\(^1\)), \( \lambda \) is the wavelength of the light in vacuum, \( \omega \) is the angular frequency of the wave, and \( \vec{E}_0 \) is a complex vector constant specifying the amplitude and polarization state of the wave. Such a wave propagating in a medium with no absorption (\( k=0 \)) is shown in Figure 2.2. If the time-dependent term is defined as \( \exp(i\omega t) \) as per Azzam and Bashara\(^1\).

![A linearly polarized plane wave.](image)

**Figure 2.2. An electromagnetic plane wave.**

The \( E \)-field, \( B \)-field, and the direction of propagation are all orthogonal with respect to each other. Because of the relationship between the fields, only the \( E \)-field and the direction of propagation are required to completely define a plane wave.

Polarization states are usually defined in terms of the direction and phase of the \( E \)-field vector, only.

Note that the complex index of refraction appears in the expression for the plane wave. If the imaginary part of the complex index (the extinction coefficient) is non-zero, the amplitude of the wave will decay exponentially as it propagates, according to the following expression (assuming propagation along the \( z \)-direction):

\[
E \propto \exp \left( -\frac{2\pi k z}{\lambda} \right),
\]

where \( k \) is the extinction coefficient, \( z \) is the distance of propagation in length units, and \( \lambda \) is the wavelength, in the same length units as the distance of propagation. The wave will then decay to \( 1/e \) of its original amplitude after propagating a distance, \( D_P \), known as the penetration depth, given by

\[
D_P = \frac{\lambda}{2\pi k}
\]

This is an important concept, as many materials exhibit large values of the extinction coefficient such that the light beam may penetrate a few tens of nm or less into the material. We cannot expect to gain any information from a film or interface unless the light beam used in the ellipsometric experiment penetrates to the film or interface we are studying, and is also able to propagate back out of the sample after reflection from the interface. For this reason it is usually not possible to measure the thickness of metal films more than 50 nm (or so) in thickness, as very little of the incident light beam reaches the bottom of the metal film and gets back out to reach the detector.

Jones vectors and matrices

One of Maxwell’s equations states that the divergence of the displacement field must equal $4\pi \rho$ times the local charge density:

$$\nabla \cdot \vec{D} = 4\pi \rho.$$  \hspace{1cm} (2.8)

where $\vec{D}$ is the displacement field and $\rho$ is the charge density. In the absence of space charges, $\rho$ is zero and if we assume the material to be isotropic the above equation reduces to

$$\nabla \cdot \vec{E} = 0,$$  \hspace{1cm} (2.9)

where $\vec{E}$ is the electric field. This requires that the components of the polarization vector $\vec{E}_0$ must lie in the plane perpendicular to the direction of beam propagation, again assuming the material in which the beam is propagating is isotropic. In this case, we can describe the polarization state of any beam by specifying its components along any two orthogonal axes in the plane perpendicular to the direction of beam propagation.

In ellipsometric experiments it is common to use the so-called p- and s-directions as the two orthogonal basis vectors used to express beam polarization states, as shown below. The p-direction is defined as lying in the plane of incidence. The plane of incidence contains the incident and reflected beams and the vector normal to the sample surface. The s- direction (from Senkrecht, German for perpendicular) lies perpendicular to the p-direction such that the p-direction, s-direction, and direction of propagation (in that order) define a right-handed Cartesian coordinate system.

1. linearly polarized light ...

2. reflect off sample ...

3. elliptically polarized light !

![Figure 2.3. Geometry of an ellipsometric experiment, showing the p- and s-directions.](image)

We can now express any totally polarized beam by specifying the components of the electric field of the beam along the p- and s-directions. These components are complex numbers, which may be conveniently written as a two-component vector, known as a Jones vector.

$$\vec{E} = \begin{bmatrix} E_p \\ E_s \end{bmatrix}.$$  \hspace{1cm} (2.10)
We may now express the action of any optical component or sample upon the polarization state of the propagating beam very simply, by means of a 2 x 2 transfer matrix, known as a Jones matrix. The diagonal elements of the Jones matrix represent the change of amplitude and phase of the p- and s- components of the beam, while the off-diagonal elements describe the transfer of energy from the p-component to the s-component, and vice versa.

The Jones matrix calculus provides a very convenient and powerful means of describing optical systems, such as ellipsometers, and will be used throughout the remainder of this section.

**Light Polarization States**

The polarization state of a light beam refers to the path its Electric field traces as it propagates through space and time. There are three classifications of polarization used to describe a plane wave: linear, circular, and elliptical. Details are presented in the following sections.

**Linear Polarization**

If one looks at the E-field vector of linearly polarized light in a plane perpendicular to the direction of propagation (x-y plane), one sees that the E-field is lies in one line at all times. Hence the name linearly polarized light. The tip of the E-field vector traces out a line segment as function of time.

![Linearly polarized light, looking into the beam.](image)

This general linear polarization can be described as two component waves propagating in phase, in the same direction, but with orthogonal E-fields in the x and y directions. The polarization state is defined with respect to some physical frame of reference. The orientation of the total E-field with respect to the coordinate system is defined by the relative amplitudes of the $E_x$ and $E_y$-fields. The Jones vector representation of linearly polarized light is

$$
\begin{bmatrix}
E_x e^{i\phi} \\
E_y e^{i\phi}
\end{bmatrix}
$$

where $\phi$ is a phase angle, which must be identical for both components. For the special case of p- or s-polarized light, the (normalized) Jones vectors have the particularly simple forms (up
to an arbitrary multiplicative complex constant) \( \begin{bmatrix} 1 \\ 0 \end{bmatrix} \) (p-polarized) and \( \begin{bmatrix} 0 \\ 1 \end{bmatrix} \) (s-polarized).

If the \( E_x \) and \( E_y \)-fields are equal in magnitude but 90° out of phase, then the polarization state is called circular because in the x-y plane, the tip of the total \( E \)-field vector traces out a circle as a function of time.

There are two types of circular polarizations. If, looking into the propagating beam, the electric field vector is precessing counterclockwise around the circle, the beam is left-circularly polarized, and the normalized Jones vector for the beam (up to an arbitrary multiplicative constant) is \( \frac{1}{\sqrt{2}} \begin{bmatrix} i \\ 1 \end{bmatrix} \). If the electric field vector is precessing clockwise around the circle the beam is right-circularly polarized, and the corresponding normalized Jones vector for the beam is \( \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -i \end{bmatrix} \).

In general the \( E_x \) and \( E_y \)-fields do not have to be equal in magnitude, and they could have any phase relationship. For a general polarization state, the tip of the total \( E \)-field vector traces out an ellipse as a function of time.
Linear and circular polarizations are just special types of elliptically polarized light. Ellipsometry measures $\Psi$ and $\Delta$ by determining the polarization ellipse of the probe beam after interaction with the sample, hence its name.

**Unpolarized (randomly polarized) light**

A beam of light usually consists of a very large number of individual photons, and it may be the case that the individual photons exhibit random polarization states. In other words, while each photon will always have a well-defined polarization state, the resulting beam does not exhibit a well-defined polarization state. In this case we say that the beam is randomly polarized. Unpolarized light cannot be represented in the Jones vector formalism, and the more sophisticated four-component Stokes vector calculus is required. Note that unpolarized light entering the detector of a rotating analyzer ellipsometer is indistinguishable from circularly polarized light.

**Partially polarized light**

A light beam may consist of two or more components with well-defined polarization states, yet the resultant total beam does not exhibit a single well-defined polarization state. Such is the case when a polarized beam is reflected from a non-uniform film, or a transparent substrate exhibiting back surface reflection effects. This is referred to as partially polarized light. Means for calculating these effects are discussed later in this section. As was the case for unpolarized light, partially polarized beams cannot be represented with a single Jones vector, but may be represented as a sum of Jones vectors or as a single four-component Stokes vector.

### 2.5 Optical components used in ellipsometers

In this section we describe several optical components commonly used in ellipsometers.

**Light sources**

Unlike single-wavelength ellipsometers, which can utilize laser sources, spectroscopic ellipsometers require a broad spectral output to match the desired range of measurements. To cover wavelengths from the vacuum ultraviolet to the infrared, the following sources are utilized:

- **Deuterium ($D_2$) lamp**: 140 nm – 300 nm
- **Xenon (Xe) lamp**: 190 nm – 2 $\mu$m
- **Quartz Tungsten Halogen (QTH) lamp**: 350 nm – 2 $\mu$m
- **Silicon carbide globar**: 1.5 $\mu$m – 40 $\mu$m

Ideally the light source would be very stable (constant intensity vs. time) and exhibit roughly constant output as a function of wavelength over the necessary spectral range, but no such source exists. The Xe arc lamp can be used from 190 nm in the deep ultraviolet to over 2 $\mu$m in the infrared. However, they exhibit low intensity below about 260 nm and have very strong atomic emission lines from about 880 nm to 1010 nm, which can overload the silicon detector used in the ellipsometer.
Optical fibers

The use of fibers makes it very simple to align the ellipsometer.

Optical fibers are used in the J. A. Woollam Co., Inc. ellipsometers in order to couple the light beam between optical elements. These fibers typically have a 200-400 micron core diameter. Two types of fibers are used. The UV transmitting fibers exhibit good transmission deep into the UV end of the spectrum, but have a strong absorption band around 1340-1450 nm such that they cannot be used in this spectral region. The IR fibers do not transmit much light below ~300 nm, but are transmitting throughout the NIR region.

Beam modulators

Two types of devices are commonly used for beam modulation. The first is the simple mechanical chopper, used in the J. A. Woollam Co., Inc. systems to harmonically modulate the intensity of the light beam, for subsequent synchronous detection. Electro-optic or magneto-optic modulators are also commonly used to harmonically perturb either the beam intensity or polarization state for subsequent synchronous detection. These types of modulators can be very difficult to calibrate and maintain, may be very sensitive to temperature, and are rather expensive.

Polarizers

A polarizer converts any polarization to linear.

The most important optical element for making ellipsometric measurements is the polarizer. An ideal polarizer will transmit light polarized in one direction, but will not transmit any light polarized along the perpendicular direction. A polarizer converts any light beam into linearly polarized light oriented along the transmitting axis.

Nearly ideal optical polarizers are commercially available, but must be matched to the wavelength range of the spectroscopic ellipsometer. For instance, light exiting a calcite Glan-Taylor polarizer is linearly polarized to 1 part in 10$^6$, and is useful (transmits sufficient light) from 230 nm to 2200 nm.

Jones matrices for a polarizer.

The Jones matrix for an ideal polarizer will depend on the orientation of the axis of the polarizer. Normalized Jones matrices for several polarizer orientations are shown below.

\[
\begin{bmatrix}
1 & 0 \\
0 & 0
\end{bmatrix}
\]

Axis along p-direction

\[
\begin{bmatrix}
0 & 0 \\
0 & 1
\end{bmatrix}
\]

Axis along s-direction

\[
\begin{bmatrix}
1 & 1 \\
2 & 1
\end{bmatrix}
\]

Axis 45° between p- and s-directions

The best way to describe a polarizer of arbitrary orientation is to rotate the coordinate system to match the axis of the polarizer, use the p-direction polarizer matrix shown above, and then rotate the coordinate axes back to the normal p- and s-directions. This will be demonstrated in the subsequent sections when we use the Jones matrix approach to calculate $\Psi$ and $\Delta$ for the rotating analyzer ellipsometer.
Retarders

A retarder introduces a phase delay between perpendicular linear polarizations (the perpendicular components of the electric field of the beam). They can be constructed from thin plates of birefringent material or from polished crystal rhombs. However, the exact retardation of such elements is a strong function of optical alignment and of the light wavelength being used. Retarders are useful but they are harder to work with than polarizers.

Some ellipsometric measurement schemes use a compensator, which can convert linearly polarized light to circularly polarized light. An ideal compensator is an optical retarder that has a retardation of exactly 90° (or 1/4 wave). A rotatable compensator combined with a rotatable polarizer can convert unpolarized light into any elliptical polarization.

Detectors

Three types of detectors are commonly used for ellipsometry: photodiodes, ccd-arrays, and photomultiplier tubes. The VASE® currently employs silicon and InGaAs photodiode detectors; which are inexpensive, polarization state insensitive, and linear over a broad range of beam intensities. This technology is supplemented in the VUV-VASE® with a photomultiplier tube for detection at short wavelengths. These devices are more expensive, exhibit polarization sensitivity, and do not exhibit linear response to the incident beam intensity. However, they have superior sensitivity necessary in the ultraviolet spectral region.

Silicon-diode detector arrays are used in the M-44® and M-88® systems. The array of diodes allows simultaneous monitoring of multiple spectral components (44 or 88), which are dispersed onto the diode array. Similarly, the M-2000® spectroscopic ellipsometers are able to measure hundreds of wavelengths simultaneously when the light beam disperses across a charge-coupled device (CCD) array. Silicon arrays can be used up to 1100 nm, but are replaced with InGaAs to cover the near infrared (to 1700 nm).
2.6 Ellipsometer configurations

In this section we discuss the principles of ellipsometer design, and a number of possible configurations for ellipsometric experiments. Particular attention is paid to the configuration of the J. A. Woollam Co., Inc. instruments.

Principles of ellipsometer design

All ellipsometers have many things in common. All ellipsometer arrangements start with a light source and end with a detector. It is the arrangement of optical components between the source and detector that defines the type of ellipsometer being used. In the following discussion, the term ‘analyzer’ is used to describe a polarizer placed just prior to the detector in the optical path. There are three primary types of ellipsometers - null, polarization modulation, and rotating element ellipsometers.

Null ellipsometry

The null ellipsometer configuration is constructed as follows:

Source ⇒ Polarizer ⇒ Compensator ⇒ Sample ⇒ Analyzer ⇒ Detector

To perform a measurement, the orientation of the polarizer, compensator, and analyzer are adjusted to "null" (extinguish) the light hitting the detector. Usually performed manually, this measurement technique is slow and it is very difficult to make spectroscopic measurements. Assuming quality optical elements and four zone nulling are used; the null configuration is accurate and has low systematic errors.

Polarization modulation ellipsometers

The polarization modulation configuration:

Source ⇒ Polarizer ⇒ Modulator ⇒ Sample ⇒ Analyzer ⇒ Detector

A PME ellipsometer may acquire data at a very rapid rate. The modulator is typically a time dependent retarder which can run at very high speeds, ~50 kHz. Theoretically, the high modulation rate allows for very fast data acquisition (10 milliseconds per point). However, to achieve satisfactory signal to noise levels; either a very intense source, like a laser, or longer integration times are required. (The signal to noise is directly related to how many photons are collected during the measurement.) To perform spectroscopic measurements, the amplitude of the modulation needs to be adjusted at each wavelength. Constructing an ellipsometer of this type with stable calibration characteristics is difficult, and stable calibrations are necessary for high accuracy measurements. Also, polarization modulators tend to exhibit strong sensitivity to the ambient temperature.

Rotating polarizer/analyzer ellipsometers

The null and polarization modulation ellipsometer configurations included a retarding element after the polarizer. However, it is possible to construct ellipsometers that use just the two polarizers (polarizer and analyzer). The are several advantages to using only polarizers:

- Polarizers can be made with nearly ideal optical behavior.
- Polarizers are achromatic over wide spectral ranges.
- Polarizers are relatively easy to construct.
• Polarizers are relatively easy to align within a system.

There are, however, disadvantages of a system without a retarder:

• Sensitivity is lost when $\Delta$ is near 0° or 180°. (The polarization modulation ellipsometer arrangement loses sensitivity for $\psi$ near 45°.)

• One of the elements must be rotated at a speed that is typically limited from 10 to 60 Hz. The time required to make one measurement with adequate signal to noise is not fundamentally determined by the rotation speed unless the light source is very intense.

Two ellipsometer configurations without a retarder are the rotating polarizer configuration,

Source $\Rightarrow$ Continuously Rotating Polarizer $\Rightarrow$ Sample $\Rightarrow$ Analyzer $\Rightarrow$ Detector,

and the rotating analyzer configuration,

Source $\Rightarrow$ Polarizer $\Rightarrow$ Sample $\Rightarrow$ Continuously Rotating Analyzer $\Rightarrow$ Detector.

In the next section we discuss the relative strengths and weaknesses of these two rotating polarizer configurations.

### Rotating analyzer vs. rotating polarizer ellipsometers

The operating characteristics of these configurations are very similar. However, a rotating polarizer system requires the light source to be totally unpolarized. Any residual polarization in the source will be a source of measurement error unless corrected. Correspondingly, a rotating analyzer system is susceptible to polarization sensitivity in the detector. Polarization sensitivity is a notable problem with photomultiplier tube detectors. However, solid-state semiconductor detectors, like those used in J.A. Woollam Co., Inc. systems, have extremely small polarization sensitivities. The use of solid-state detectors has led J.A. Woollam Co., Inc. toward the use of rotating analyzer systems where residual polarization in the source is not an issue.

For rotating polarizer/analyzer systems there is still an issue of where to locate the device (either monochromator or ccd (or diode)-array) that selects measurement wavelengths. Wavelength selection can be incorporated into the detector or the source. If it is incorporated into the source, then ambient light is easily rejected. This occurs because the ambient light is split into its component wavelengths and there is not enough ambient intensity at any one wavelength to compete with the probe beam intensity at the detector. If wavelength selection is part of the source, the probe beam is monochromatic and there is no wavelength splitting element in the detector. This means the ambient intensity at all wavelengths together competes with the monochromatic probe beam.

From the point of view of ambient light rejection, placing wavelength selection with the detector has the advantage. However, there are two problems with such a design. First, the monochromator or ccd/diode array will almost certainly have a significant amount of polarization sensitivity. Second, collecting the probe beam to pass it through the monochromator reduces the beam intensity.

Different J.A. Woollam Co., Inc. ellipsometers will select the wavelength at either the source or detector. The VASE® and VUV-VASE® place a monochromator with the light source. Combined with a rotating analyzer arrangement, VASE® instruments are insensitive to residual source polarization and minimize detector polarization sensitivity. The problem of ambient light is addressed by using a chopped probe beam and synchronous detection techniques.
The M-44®, M-88®, and M-2000® ellipsometers use a broad band light source and place diode or CCD array in the detector unit. They have the advantage of simultaneous detection of all wavelengths, which make them faster than VASE® instruments. Also, because the MXX instruments have no moving parts and since the detectors correspond to fixed wavelengths, it is much easier to calibrate the detector polarization sensitivity than it is for scanning monochromator with a continuous wavelength range. (A scanning monochromator with a moving grating does not permit simultaneous measurements at multiple wavelengths).

Rotating analyzer ellipsometer with adjustable retarder

The primary drawback of the rotating analyzer ellipsometer is that it is most accurate when the beam entering the detector is nearly circularly polarized (\(\Delta \approx 90^\circ\)) and less accurate when the beam entering the detector is nearly linearly polarized (\(\Delta \approx 0^\circ\) or \(180^\circ\)). A less critical drawback is that \(\Delta\) actually ranges from \(0^\circ\) to \(360^\circ\), but with the rotating analyzer ellipsometer it is not possible to determine the handedness of the reflected beam polarization ellipse, hence \(\Delta\) is mapped into the \(0^\circ - 180^\circ\) range. Stated in another manner, a rotating analyzer ellipsometer cannot determine which quadrant \(\Delta\) lies in, and as a result (for example) a RAE system cannot distinguish between left- and right-circularly polarized light entering the analyzer / detector.

Both of these drawbacks may be alleviated by the addition of a variable compensating element under computer control to the rotating analyzer system. The variable retarder is placed after the input polarizer and before the sample, such that through the use of the polarizer / compensator combination, any input polarization may be generated prior to reflection from the sample. Thus, the input polarization may be adjusted to provide a reflected beam which is always close to circularly polarized, and the hybrid system will measure \(\Delta\) accurately over the entire range of \(0^\circ - 360^\circ\).

Rotating compensator ellipsometer

Another approach that introduces a compensator into the ellipsometer beam path is to implement the rotating compensator ellipsometer (RCE) configuration. There are many advantages to the RCE configuration, including: accurate measurement of the ellipsometric \(\Psi\) and \(\Delta\) parameters over the complete measurement range (\(\Psi=0-90^\circ\), \(\Delta=0-360^\circ\)), no residual input or output polarization sensitivity (due to a fixed polarizer on input and a fixed analyzer on output), and the capability to directly measure depolarization effects.

However, only recently have spectroscopic RCE systems been constructed. The prior lack of spectroscopic RCE systems, in spite of the well-known advantages to this configuration, was mainly due to the perceived difficulty of constructing a mechanically rotatable compensator element that behaves ideally (retardance about 90°) over a wide spectral range. Recently, this challenge has been successfully addressed in a number of ways, leading to both the IR-VASE® and the M-2000® instruments.
2.7 The rotating analyzer ellipsometer

In this section we discuss the rotating analyzer ellipsometer design, which is the basis of both the VASE®, M-44®, and M-88® instruments. The ellipsometer configuration is discussed, as is the use of the rotating analyzer / detector combination to measure beam polarization states. We use the Jones matrix formalism to derive expressions for $\Psi$ and $\Delta$ for the rotating analyzer ellipsometer, discuss the determination of the polarizer angles, and consider the sensitivity of the experiment as well as errors which may occur. Finally the benefits and drawbacks associated with the incorporation of a variable retarder into the rotating analyzer ellipsometer are discussed.

Configuration

The typical configuration of the rotating analyzer ellipsometer is as follows:

Source ⇒ Polarizer ⇒ Sample ⇒ Continuously Rotating Analyzer ⇒ Detector.

The input polarizer serves to linearly polarize the beam incident on the sample, and the combination of rotating analyzer and detector allow the measurement of the polarization state of the reflected beam.

Measurement of the reflected beam polarization state

The following examples show the detector signal for different polarization states after passing through a rotating analyzer.

![ Detector signal for a linearly polarized beam entering the rotating analyzer polarization detector.](image)

Figure 2.8. Detector signal for a linearly polarized beam entering the rotating analyzer polarization detector.
Circularly Polarized
Input Beam: (reflected off sample)
Detector (converts light to voltage)
Rotating Analyzer:
\[ A(t) = a(t) = 2\pi ft \]
- constant DC signal (the circularly polarized beam always has a component that passes through the rotating analyzer, regardless of its orientation)

Figure 2.9. The detector signal associated with a (right or left) circularly polarized beam entering the rotating analyzer polarization detector.

Elliptically Polarized
Input Beam: (reflected off sample)
Detector (converts light to voltage)
Rotating Analyzer:
\[ A(t) = a(t) = 2\pi ft \]

Figure 2.10. The detector signal associated with an arbitrarily elliptically polarized beam entering the rotating analyzer polarization detector.

For a general elliptical polarization the detected signal is a sinusoid with a DC offset of the form:

\[ V(t) = DC + a \cdot \cos(2\omega t) + b \cdot \sin(2\omega t) \]  
\[ (2.11) \]

The two important quantities measured by the ellipsometer are \( \alpha \) and \( \beta \), which are the normalized Fourier coefficients of the signal. They can be represented in terms of the \( \Psi \) and \( \Delta \) values for the sample and the (known) polarizer azimuthal angle as follows.

\[ \alpha = \frac{a}{DC} = \frac{\tan^2(\Psi) - \tan^2(P)}{\tan^2(\Psi) + \tan^2(P)} \]  
\[ (2.12) \]

\[ \beta = \frac{b}{DC} = \frac{2\tan(\Psi)\cos(\Delta)\tan(P)}{\tan^2(\Psi) + \tan^2(P)} \]  
\[ (2.13) \]

This result is obtained from a Jones matrix analysis of the RAE optical system, as described in the next section. \( \Psi \) and \( \Delta \) are the ellipsometric parameters that characterize the sample, and \( P \) is the input polarizer azimuth with respect to the plane of incidence. (\( P = 0^\circ \) is in the plane of incidence.) The above equations may be inverted to obtain \( \Psi \) and \( \Delta \) from the measured \( \alpha \) and \( \beta \) and the known \( P \).
Jones matrix analysis of the rotating analyzer ellipsometer

In this section we use the Jones matrix formalism described previously to develop a model for the rotating analyzer ellipsometer which can predict the measured quantities (\( \Psi \) and \( \Delta \)) in terms of the optical properties of the sample and the polarizer and analyzer azimuthal angles. For this purpose, we need to calculate the time dependent beam intensity at the detector, as this is the actual quantity measured by the ellipsometer.

The detector intensity is proportional to the magnitude of the electric field of the beam at the detector squared:

\[
I_D \propto |E_D|^2. \tag{2.14}
\]

Thus, our calculation will proceed by tracking the polarization state of the light beam through the ellipsometer, and then evaluating the square of the resulting electric field of the beam at the detector. We can express the electric field of the beam at the detector by multiplying, in order, the electric field of the input beam by the Jones matrices appropriate for each element in the optical system. Thus, the expression for the beam at the detector will appear as follows:

\[
E_D = \text{[Analyzer matrix]} \text{[Sample matrix]} \text{[Polarizer matrix]} \text{[Input beam]}. \tag{2.15}
\]

Now we simply need expressions for the Jones matrices of the analyzer, sample, and polarizer in order to evaluate the electric field of the beam at the detector.

Assume we have rotated our coordinate system such that the axis of the input polarizer is in the p-direction (in the rotated coordinate system). The beam leaving the input polarizer is then p-polarized. We must then rotate the coordinate system back to the p- and s-coordinates of the ellipsometer. If the azimuthal angle between the polarizer axis and the plane of incidence is denoted by \( P \), the beam leaving the input polarizer (and incident on the sample) will have a Jones vector given by the product of the rotation matrix which returns the coordinate system to the ellipsometer coordinates with the Jones vector of p-polarized light:

\[
\text{Input polarizer Jones matrix.}
\]

\[
\text{Beam incident on sample} = \begin{bmatrix} \cos P & -\sin P \\ \sin P & \cos P \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix}. \tag{2.15}\]

If the sample is isotropic and not too rough, there will be no off-diagonal elements in the sample Jones matrix, and we can use the following matrix to describe the sample:

\[
\text{Sample Jones matrix} = \begin{bmatrix} \tilde{R}_p & 0 \\ 0 & \tilde{R}_s \end{bmatrix}. \tag{2.16}\]

where \( \tilde{R}_p \) and \( \tilde{R}_s \) are the complex Fresnel reflection coefficients for the p- and s-directions, respectively. Further on we will show how to calculate these quantities for real samples.

The analyzer Jones matrix is evaluated by rotating the coordinate system such that the new p-direction lies along the analyzer axis and then multiplying with the p-oriented polarizer Jones matrix. We do not need to rotate back to the ellipsometer frame, as we are now at the detector and this final rotation matrix will drop out in the evaluation of the square of the electric field. The total Jones matrix for the analyzer is then given by (assuming the angle between the analyzer axis and the plane of incidence in the ellipsometer frame to be \( A \)): 
Analyzer Jones matrix = \[
\begin{bmatrix}
1 & 0 \\
0 & 0
\end{bmatrix}
\begin{bmatrix}
\cos A & \sin A \\
-\sin A & \cos A
\end{bmatrix}.
\] (2.17)

The total expression for the electric field at the detector is then:
\[
E_D = \begin{bmatrix}
1 & 0 \\
0 & 0
\end{bmatrix}
\begin{bmatrix}
\cos A & \sin A \\
-\sin A & \cos A
\end{bmatrix}
\begin{bmatrix}
\tilde{R}_p & 0 \\
0 & \tilde{R}_s
\end{bmatrix}
\begin{bmatrix}
\cos P & -\sin P \\
\sin P & \cos P
\end{bmatrix}
\begin{bmatrix}
1 \\
0
\end{bmatrix}.
\] (2.18)

This is easily evaluated, and yields the following results:
\[
E_D = \begin{bmatrix}
\tilde{R}_p \cos P \cos A + \tilde{R}_s \sin P \sin A \\
0
\end{bmatrix}.
\] (2.19)

We may then evaluate the intensity of the beam at the detector by multiplying the non-zero element in the above Jones vector by its complex conjugate. Performing this calculation and invoking a few trigonometric identities yields
\[
I_D \propto \tilde{R}_p^2 \cos^2 P + \tilde{R}_s^2 \sin^2 P \\
+ \left[ \tilde{R}_p^2 \cos^2 P - \tilde{R}_s^2 \sin^2 P \right] \cos(2A) \\
+ 2\Re(\tilde{R}_p \cdot \tilde{R}_s^*) \sin P \cos P \sin(2A)
\] (2.20)

Now, we can normalize the above expression so that the DC component is unity by dividing by the term which is independent of the analyzer azimuthal angle \( \Phi \). This yields
\[
I_D \propto 1 + \frac{\tilde{R}_p^2 - \tan^2 P}{\cos(2A) + \frac{2\Re(\tilde{R}_p \cdot \tilde{R}_s^*) \tan P}{\tan^2 P}}
\] (2.21)

Let us now define the complex ellipsometric parameter \( \rho \).
\[
\tilde{\rho} = \frac{\tilde{R}_p}{\tilde{R}_s}.
\] (2.22)

This is what the ellipsometer actually measures.

The ellipsometric parameter \( \rho \) is only a function of the Fresnel reflection coefficients of the sample, and represents the total information we can obtain from a single ellipsometric measurement. \( \rho \) is commonly expressed in terms of the two real-valued ellipsometric parameters \( \Psi \) and \( \Delta \) as follows:
\[
\tan \Psi \exp(i\Delta) \equiv \tilde{\rho}
\] (2.23)

such that \( \tan \Psi \) equals the magnitude of the ratio of the p- to s-direction complex reflection coefficients for the sample, and \( \Delta \) is the phase difference between the \( p \)- and \( s \)-reflection coefficients.

We can now substitute \( \rho \) for the ratio of Fresnel coefficients in our equation for the detector intensity and obtain the detector signal as a function of \( \Psi \), \( \Delta \), \( P \), and \( A \) only:
Now, this expression has the form of a Fourier series in twice the analyzer azimuthal angle:

\[ I_D \propto 1 + \frac{\tan^2 \Psi - \tan^2 P}{\tan^2 \Psi + \tan^2 P} \cos(2A) + \frac{2 \tan \Psi \cos \Delta \tan P}{\tan^2 \Psi + \tan^2 P} \sin(2A). \]  

(2.24)

The analyzer angle A is actually a harmonic function of time, since the analyzer is rotating continuously:

\[ A(t) = 2\pi f_0 t + \theta \]  

(2.26)

Thus, if we measure the detector signal as a function of time, we can perform a Fourier transform on the experimentally measured detector signal to obtain the Fourier coefficients \( \alpha \) and \( \beta \) of the signal, effectively eliminating the analyzer azimuthal angle \( A \) as an experimental parameter. We can then identify the expressions for \( \alpha \) and \( \beta \):

\[ \alpha = \frac{\tan^2 \Psi - \tan^2 P}{\tan^2 \Psi + \tan^2 P}, \]

(2.27)

\[ \beta = \frac{2 \tan \Psi \cos \Delta \tan P}{\tan^2 \Psi + \tan^2 P}, \]

and solve for \( \Psi \) and \( \Delta \) as functions of the Fourier coefficients \( \alpha \) and \( \beta \) and the polarizer azimuthal angle \( P \):

\[ \tan \Psi = \sqrt{\frac{1 + \alpha}{1 - \alpha}} |\tan P|, \]

(2.28)

\[ \cos \Delta = \frac{\beta}{\sqrt{1 - \alpha^2}} |\tan P|. \]

These equations are used to get \( \Psi \) and \( \Delta \) from the measured detector signal.

These equations form the basis of the ellipsometric measurement with the rotating analyzer ellipsometer. To summarize, the detector signal is measured as a function of time, the measured signal is Fourier analyzed to obtain the Fourier coefficients \( \alpha \) and \( \beta \), and finally \( \Psi \) and \( \Delta \) are calculated from \( \alpha \) and \( \beta \) and the known azimuthal angle of the input polarizer.

This constitutes half of our optical model for ellipsometric experiments. Now, given the complex reflection coefficients of the sample, we can predict the values of \( \Psi \) and \( \Delta \) which will be measured from the sample by our rotating analyzer ellipsometer (provided the off-diagonal reflection coefficients of the sample equal zero – see next section). The second half of the optical model consists of calculating the reflection coefficients of the sample from knowledge of the structure and optical properties of the sample, which will be treated later.
Anisotropic or depolarizing samples

Some types of anisotropy may cause the sample Jones matrix to exhibit off-diagonal elements, as may significant surface, interfacial, and/or grain boundary roughness in or on the sample. In this case, the sample Jones matrix may have no non-zero elements:

\[
\begin{bmatrix}
J_{pp} & J_{ps}
\end{bmatrix}
\]

(2.29)

When the sample Jones matrix is not diagonal we can still predict the \( \Psi \) and \( \Delta \) values that the rotating analyzer ellipsometer will measure using the same approach, but with considerably more algebra involved. The final result is that equations 2.28 are still valid, but \( \alpha \) and \( \beta \) as given in equations 2.27 are replaced by

\[
\alpha = \frac{\left( |\tilde{R}_{pp}|^2 - |\tilde{R}_{sp}|^2 \right) \cos^2 P + \left( |\tilde{R}_{ps}|^2 - |\tilde{R}_{ss}|^2 \right) \sin^2 P + 2 \Re(\tilde{R}_{pp}^* \tilde{R}_{ps}) - \Re(\tilde{R}_{ss}^* \tilde{R}_{sp}) \sin P \cos P}{\left( |\tilde{R}_{pp}|^2 + |\tilde{R}_{sp}|^2 \right) \cos^2 P + \left( |\tilde{R}_{ss}|^2 + |\tilde{R}_{ps}|^2 \right) \sin^2 P + 2 \Re(\tilde{R}_{pp} \tilde{R}_{ps}^*) + \Re(\tilde{R}_{ss} \tilde{R}_{sp}^*) \sin P \cos P},
\]

(2.30)

\[
\beta = \frac{2 \Re(\tilde{R}_{pp}^* \tilde{R}_{ps}) \cos^2 P + \Re(\tilde{R}_{ss} \tilde{R}_{ps}^*) \sin^2 P + \Re(\tilde{R}_{pp}^* \tilde{R}_{ss}^*) + \Re(\tilde{R}_{sp} \tilde{R}_{ps}^*) \sin P \cos P}{\left( |\tilde{R}_{pp}|^2 + |\tilde{R}_{sp}|^2 \right) \cos^2 P + \left( |\tilde{R}_{ss}|^2 + |\tilde{R}_{ps}|^2 \right) \sin^2 P + 2 \Re(\tilde{R}_{pp} \tilde{R}_{ps}^*) + \Re(\tilde{R}_{ss} \tilde{R}_{sp}^*) \sin P \cos P},
\]

These equations can be used to calculate expected ellipsometric data for any sample for which all four reflection coefficients are known. An interesting aspect of equations 2.30 is that they predict that when the off-diagonal reflection coefficients are non-zero, the measured \( \Psi \) and \( \Delta \) will depend on the polarizer azimuthal angle, which is not the case when the sample reflection matrix is diagonal.

Some non-idealities of the sample and/or ellipsometer may lead to a partially polarized beam at the detector. Examples of such cases are non-uniform films, back-surface reflections, non-zero monochromator bandwidth effects, and effects due to angular spread of the beam or curved sample surfaces. These effects may be treated by dividing the beam at the detector into many component beams, each of which has a well defined polarization state. The detector signal due to each of the component beams may then be calculated, and the total detector signal (from which the measured Fourier coefficients \( \alpha \) and \( \beta \) are obtained) may then be evaluated as the sum of the contributions to the detector signal from each of the component beams. It is important to sum the contributions to the detector signal rather than average the \( \Psi \) and \( \Delta \) values of the component beams, as this averaging procedure will at best yield approximately correct results.
Calibration of the polarizer angles

There are three experimental parameters which must be determined prior to acquisition of data with a rotating analyzer ellipsometer - the absolute position of the polarizer and analyzer axes and the relative attenuation of the a.c. signal with respect to the d.c. component of the detector signal due to the signal processing electronics. The procedure by which these parameters are determined is discussed in this section. Note that this information is excerpted from “Regression calibration method for rotating element ellipsometers,” by Blaine Johs, Thin Solid Films, 234, 395-398 (1993).

We define the three calibration parameters as follows. First, we let $P_s$ and $A_s$ denote the angular difference between the dial reading for the polarizer and analyzer and the true azimuthal angle between the polarizer and analyzer axes and the plane of incidence. In other words, if we take the dial reading for the polarizer (denoted by $P$) and subtract the calibration parameter $P_s$, we obtain the azimuthal angle between the polarizer axis and the plane of incidence. The measured Fourier coefficients $\alpha$ and $\beta$ are now given as follows, with $\eta$ representing a calibration parameter equal to the relative attenuation of the AC component of the detector signal with respect to the DC component.

$$\alpha = \frac{1}{\eta} [\alpha' \cos(2A_s) - \beta' \sin(2A_s)], \quad (2.31)$$

$$\beta = \frac{1}{\eta} [\alpha' \sin(2A_s) + \beta' \cos(2A_s)] \quad (2.32)$$

where

$$\alpha' = \frac{\tan^2 \Psi - \tan^2 (P - P_s)}{\tan^2 \Psi + \tan^2 (P - P_s)}, \quad (2.33)$$

$$\beta' = \frac{2 \tan \Psi \cos \Delta \tan(P - P_s)}{\tan^2 \Psi + \tan^2 (P - P_s)}. \quad (2.34)$$

To calibrate the ellipsometer, a sample must first be mounted and aligned. This sample must exhibit a reflected beam with a well-defined polarization state (i.e. no depolarizing effects such as anisotropy or extreme roughness) and it is helpful (but not required) that the reflected beam be nearly circularly polarized. A good choice for the sample is to use the standard sample (a 20 nm thermal oxide on silicon) and calibrate at 500 nm wavelength and 75° angle of incidence.

With the sample mounted and aligned, the Fourier coefficients of the detector signal $\alpha$ and $\beta$ are measured as a function of the position of the input polarizer $P$. Equations 2.31 - 2.34 are then fit to the measured Fourier coefficients and residual function to determine the values of the three calibration parameters.

There are a number of advantages of this procedure over previous calibration techniques, which relied on fitting the residual quantity near the region where the polarizer axis lies in the plane of incidence. The residual is defined as follows:

$$\zeta = 1 - \alpha^2 - \beta^2, \quad (2.35)$$

and is expected to exhibit a parabolic minimum at the position where the polarizer axis lies in the plane of incidence. The use of the full regression fit to the Fourier coefficients and the residual is advantageous in that it is fully automated and yields
rigorous error bars on the calibration parameters. Also this calibration technique may be performed on any arbitrary sample, if necessary.

As an example, here are the results of a calibration on the J. A. Woollam Co., Inc. VASE® instrument performed on the standard oxide on silicon wafer at 75° angle of incidence and 500 nm wavelength. The measured and calculated Fourier coefficients and residual are plotted as a function of polarizer angle in Figure 2.11.

![Calibration fit from a fine mode calibration.](image)

The calibration fit shown above yielded the following results:

MSE=0.955

\[
\psi = 16.778 \pm 0.00478
\]

\[
\Delta = 87.915 \pm 0.016
\]

\[
\alpha = 174.35 \pm 0.0137
\]

\[
\beta = 99.103 \pm 0.00429
\]

\[
\text{Attn} = 0.9602 \pm 0.00046
\]

Note that the best-fit calculated data are indistinguishable from the measured data, indicating the model is very good and the ellipsometer is functioning nearly ideally. The results of the calibration fit are listed to the right of the calibration plot. Note that \( \Delta \) was found to be 87.92°, very close to 90°, and that the calculated 90% confidence limits on the calibration parameters are very small.

**Error (sensitivity) analysis - polarizer tracking**

\( \psi \) and \( \Delta \) as a function of \( \alpha \), \( \beta \), and \( P \) are given by the following

\[
\tan(\psi) = \frac{1+\alpha}{1-\alpha} \tan(P) \tag{2.36}
\]

\[
\cos(\Delta) = \frac{\beta}{\sqrt{1-\alpha^2}} \tag{2.37}
\]

Noise in the measured \( \psi \) and \( \Delta \) values comes directly from noise in the measured \( \alpha \) and \( \beta \). The noise in \( \alpha \) and \( \beta \) is minimized by J.A. Woollam Co., Inc. ellipsometers by averaging multiple analyzer rotations, and the magnitude of the noise is estimated from the fluctuations of \( \alpha \) and \( \beta \) from revolution to revolution. This measurement noise is then converted to standard deviations on \( \psi \) and \( \Delta \) which are saved with the data set. These standard deviations are then used to weight the
contributions of each data point to the mean-squared error (MSE) during the fitting process, such that very noisy data points are effectively excluded from the fit.

It is expected that the noise levels on $\alpha$ and $\beta$ will depend only the probe beam intensity, not the particular polarization state of the beam. However, the corresponding noise on $\Psi$ and $\Delta$ values will depend on the polarization state being measured. The minimum amount of noise is expected when $\alpha = 0$ and $\beta = 0$. This corresponds to circularly polarized light entering the detector, and is the condition at which there is minimum sensitivity to calibration errors. This is due to the fact that a circularly polarized beam entering the detector yields a nearly constant detector signal, which is always much greater than the noise floor.

By adjusting the polarizer setting, $P$, it is possible to keep $\alpha = 0$, for a wide range of $\Psi$ values. This is done by setting $P = \Psi$ for each measurement. (For $\Psi < 10^\circ$ and $\Psi > 80^\circ$, it is not practical to track the polarizer to $\Psi$ because the intensity of the probe beam reflected from the sample is very low.) In practice it is sufficient to keep $P$ within several (10) degrees of $\Psi$.

Keeping $\Delta$ near $90^\circ$ is a slightly more complicated issue. For a given sample and at a single wavelength, only the angle of incidence can be varied to adjust $\Delta$. This is one reason why an automated variable angle system, like a VASE® system, can be so useful. Coincidentally, for a wide range of samples, sensitivity to layer thicknesses and optical constants is greatest when $\Delta = 90^\circ$. Therefore, measuring $\Delta$ near $90^\circ$ is important for more than just noise consideration.

As a final note, calibrating on a sample is the most accurate way to obtain $\Psi$ and $\Delta$ at the given wavelength and angle of incidence for that sample, with the tradeoff being considerably increased acquisition time. It is possible with the WVASE® software to acquire spectroscopic ellipsometric scans where the regression calibration is performed at each point to obtain $\Psi$ and $\Delta$. This scan may also be performed on depolarizing samples to determine not only $\Psi$ and $\Delta$ but the off-diagonal reflection Jones matrix coefficients as well.

### 2.8 Variable vs. fixed angle of incidence

In this section, we discuss the benefits of acquiring data at multiple angles of incidence. Typical spectroscopic ellipsometers can measure over a wide range of angles, however, acquiring data at many different angles is not always necessary nor is it usually the best approach. In most situations only 2 or 3 well-chosen angles are needed.

The primary reason for using a variable angle of incidence instrument is to acquire data at angles of incidence near the pseudo-Brewster angle for each sample. When the angle of incidence is near the pseudo-Brewster angle the measured $\Delta$ values are around $90^\circ$, and this range of $\Delta$ values provides the most sensitive measurement of the sample. For semiconductor samples the pseudo-Brewster angle is typically around $75^\circ$, while for lower index materials like glass the pseudo-Brewster angle is typically closer to $60^\circ$. Choosing optimal angles of incidence is thoroughly presented in the chapter - “VASE® Data Acquisition - Procedures and Strategies”.

For samples with a single transparent layer, spectroscopic ellipsometry is routinely used to measure both the layer thickness and the layer index of refraction. With variable angle measurements on certain samples, spectroscopic ellipsometry can measure the thickness and both the real and imaginary parts of the complex refractive index for an absorbing film. For certain samples, data from multiple angles can be used to fundamentally increase the available information about a
sample. This occurs when by changing the angle of incidence you are also changing the path length of the probe beam as it travels through a film. If you have such a sample, it may be worth measuring the sample at more than 3 angles of incidence.

For a simple substrate with no layers, changing angles cannot directly increase the available information about the sample. (Measurements at multiple angles can, of course, still be used to place \( \Delta \) in the proper ranges). Furthermore, if a sample does have coatings or overlayers, but the layers are very thin compared to the wavelength of the probe beam, then again multiple angles do not directly increase the available information. Finally, if semiconductor samples are being measured, they will often have a high refractive index (\( n>3 \)) and in this case the large amount of refraction means the path length inside the sample changes little even for large changes in the angle of incidence.

For a more detailed look at why measurements at multiple angles of incidence do not always produce the desired effect of enhancing information content, consider the task of determining optical constants at \( W \) wavelengths of a substrate that has a film of known optical properties but unknown thickness. The total number of real valued unknowns is \( 2W+1 \) (\( n \) and \( k \) at each wavelength, plus the layer thickness). For ellipsometric data acquired at one angle of incidence the total number of measured values is \( 2W \), hence the system is underdetermined (fewer measured values than parameters). By measuring the sample at a second angle of incidence the number of measured values increases to \( 4W \) and the system might appear to be over determined. However, in some cases of interest, the system still has no unique set of fit parameters because there is strong correlation in the information content between data at different angles. This is especially true when the overlayer is thin (i.e., native oxides, surface roughness). This information correlation is easily observed in the pseudodielectric spectra as shown in the comparison between \( \Delta \) spectra and \( \langle \varepsilon \rangle \) spectra, for an InP substrate with a thin oxide overlayer. The pseudodielectric function is defined simply as the dielectric function calculated directly from the ellipsometric data assuming the sample is a bulk structure with no overlayers.

![Figure 2.12. Ellipsometric \( \Delta \) data from measurements on an InP substrate with a native oxide. The data from two angles of incidence are shown.](image-url)
Even though the measured $\Delta$ spectra at the two angles are quite different, the $\langle \epsilon_1 \rangle$ and $\langle \epsilon_2 \rangle$ spectra at each angle are identical within the noise level. In this case, the second angle of incidence contributes no additional information, and therefore no additional parameters can be determined.

However, multiple angles are always valuable in several ways. First, measurements at the same wavelength are independent with respect to measurement noise, and therefore the extra information helps to reduce noise in the fitted parameters. Second, the additional measurements improve the statistical determination of confidence limits by further over determining the model. Third, the proper choice of multiple angles ensures that for each wavelength, at least one pair of $\psi$ and $\Delta$ values will be near the optimum measurement regime for the type of ellipsometer being used (e.g., a rotating-analyzer ellipsometer is most accurate for $\Delta \sim 90^\circ$). Finally, angles may be chosen at which $\psi$ and $\Delta$ are most sensitive to the model parameters. For an absorbing substrate with only a very thin overlayer, this also occurs when $\Delta \sim 90^\circ$.

### 2.9 J. A. Woollam Co., Inc. Spectroscopic Ellipsometers

The J.A. Woollam Co., Inc. manufactures a wide range of different spectroscopic ellipsometers that cover the spectrum from the vacuum ultraviolet to the infrared. The table below lists each type of Woollam spectroscopic ellipsometer with the corresponding range that it covers.

<table>
<thead>
<tr>
<th>Model</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>VASE®</td>
<td>190 nm – 3200 nm</td>
</tr>
<tr>
<td>VUV-VASE®</td>
<td>146 nm – 2500 nm</td>
</tr>
<tr>
<td>IR-VASE®</td>
<td>1.7 $\mu$m – 30 $\mu$m</td>
</tr>
<tr>
<td>M-44®</td>
<td>280 nm – 1100 nm*</td>
</tr>
<tr>
<td>M-88®</td>
<td>280 nm – 760 nm</td>
</tr>
<tr>
<td>M-2000®</td>
<td>193 nm – 1700 nm*</td>
</tr>
</tbody>
</table>

*the listed spectral range may not be available from a single instrument, but instead is covered by the different available ranges within that model.
The VASE® is a traditional rotating analyzer ellipsometer (RAE). This design is very accurate and well understood. The following is a list of some key features of the VASE®.

- Input polarizer is fixed, while the analyzer continuously rotates. Best measurement accuracy and sensitivity when $\Delta$ is near 90°.
- The rotating analyzer is a continuous motion stepper motor. Data acquisition is perfectly synchronized without use of position encoders.
- Monochromator is placed before the sample, which insures that monochromatic, low-intensity light is incident on the sample. This is important when studying photosensitive materials such as photoresists.
- A beam chopper is placed at the output of the monochromator.
- Synchronous detection techniques to reject ambient light and allow measurements to be acquired with room lights on.
- Solid state detectors are used. These are more reliable, more linear, less polarization sensitive, and less expensive than photomultiplier tubes.
- Stacked detector unit to allow measurement over a large spectral range. The silicon detector has a usable spectral range of 185nm to 1100nm. The InGaAs detector has a usable spectral range from 800nm to 1700nm. In typical use the stacked detector unit provides a continuously measurable spectral range from 193nm to 1700nm.
- Automated angle of incidence with vertical or horizontal sample mounts.
- The AutoRetarder® option introduces a computer-controlled retarder into the beam path after the fixed polarizer. The AutoRetarder® allows measurement of $\Delta$ from 0° to 360° without ambiguity or “trouble” regions of other designs. Also measures '% depolarization'.

A VASE® system schematic is shown in Figure 2.14. In addition to the basic instrument shown, optional upgrades include:

- AutoRetarder®.
- Focusing optics to decrease beam diameter to 200 microns.
- Automated and manual sample translation stages.
- Liquid cell for studying liquid/solid interfaces.
- Cryostat for variable sample temperature from 4.2 to 700 Kelvin.
VASE®

Figure 2.14. The Woollam Co. variable angle spectroscopic ellipsometer (VASE®). Components include: 1) monochromator, 2) fiber optic cable, 3) input unit with polarizer, 4) alignment detector, 5) sample stage, 6) goniometer base for automated angle control, 7) detector unit with rotating analyzer and solid state detectors, and 8) motor control box.

VUV-VASE®

The VUV-VASE® Gen-I and Gen-II systems are based on the same technology as the VASE® with a few added features to allow measurements into the vacuum ultraviolet (to 146nm).

- Rotating analyzer ellipsometer with AutoRetarder®.
- Nitrogen purged chamber to avoid ambient absorption from oxygen and water vapor in the vacuum ultraviolet region.
- Convenient sample load lock to provide fast sample exchange.
- Dual deuterium/xenon arc lamp light sources. The deuterium lamp provides light from 146nm to 300nm and the xenon arc lamp provides light from 190 to 1700nm.
- Dual photomultiplier tube/solid state detector system. A photomultiplier tube is used for measurements from 146nm to 300nm and the solid state detector is used from 300nm to 1700nm.
- Fully automated sample alignment and angle of incidence control.
- A single fully contained unit.

Photos of the VUV-VASE® Gen-I and Gen-II systems are shown in Figure 2.15.
Figure 2.15: The Woollam Co. variable angle spectroscopic ellipsometer for the vacuum ultraviolet (VUV-VASE® Gen-I and Gen-II systems).

IR-VASE®

The IR-VASE® is a rotating compensator ellipsometer (RCE) that covers a spectral range from 1.7 to 30 microns ($333\text{cm}^{-1}$ to $5900\text{cm}^{-1}$). Features include:

- Fourier Transform Infrared (FTIR) spectrometer as the light source.
- RCE design allows measurement of $\Delta$ from 0-360°, as well as advanced measurements of ’% depolarization’ and anisotropy.
- High precision, computer controlled angle of incidence

A photo of the IR-VASE® is shown in Figure 2.16.

Figure 2.16. A variable angle spectroscopic ellipsometer for the infrared (IR-VASE®) from the J.A. Woollam Co., Inc.
M-44® and M-88®

The M-44® and M-88® spectroscopic ellipsometers use a patented rotating analyzer diode array system for fast accurate measurements. Both instruments reflect polarized white light from a sample through the rotating analyzer. The light is then dispersed off of a grating onto either 44 or 88 silicon detectors simultaneously. In this manner, either 44 or 88 wavelengths are measured simultaneously. These instruments are primarily for in-situ process monitoring or ex-situ mapping, where rapid data acquisition is necessary. Features include:

- Various spectral ranges to choose from:
  - M-44UV 44 wavelengths from 280nm to 600nm.
  - M-44VIS 44 wavelengths from 410nm to 750nm.
  - M-44NIR 44 wavelengths from 600nm to 1100nm.
  - M-88 88 wavelengths from 280nm to 760nm.
- Typical measurement time is less than one second for all wavelengths.
- Fixed, manual, or automated angle of incidence available.
- Simultaneous calibration of all wavelengths.

A schematic of the M-44® ellipsometer is shown in Figure 2.17.

Figure 2.17. The J. A. Woollam Co., Inc. M-44® spectroscopic ellipsometer.

M-2000®

The M-2000® is a rotating compensator ellipsometer (RCE) with CCD array detection to provide fast, accurate ellipsometry over a large spectral range. The large number of wavelengths measured simultaneously provides maximum versatility. Like the M-44® and M-88® ellipsometers, the M-2000® reflects white light from a sample. The white light is dispersed onto a CCD detector array to allow spectroscopic measurements simultaneously. Features include:

- Large variety of spectral range options:
Reflection of polarized light from planar structures

In this section we develop a mathematical formalism to model the reflection of polarized light from planar structures, consisting of a substrate that may or may not have any number of films deposited on its surface. We first establish the measurement geometry and the meaning of the optical constants, and then proceed to calculate the reflection coefficients for bulk structures, from which the ellipsometric parameters $\Psi$ and $\Delta$ are evaluated. The summation of multiple reflections is discussed for single film samples, and formalisms for the treatment of multilayers are reviewed. Finally, brief descriptions of the treatment of superlattices, graded layers, and roughness are given.
Measurement geometry

Ellipsometry measures the sample parameters $\Psi$ and $\Delta$, by launching a probe beam with a known polarization state onto the sample and then measuring the polarization state of the reflected beam. In the following figure, a linearly polarized input beam is converted to an elliptically polarized reflected beam.

1. linearly polarized light ...

2. reflect off sample ...

3. elliptically polarized light !

Figure 2.19. Measurement geometry for ellipsometric experiments

The coordinate system used to describe the ellipse of polarization is the $p$-$s$ coordinate system. The $s$-direction is taken to be perpendicular to the direction of propagation and parallel to the sample surface. The $p$-direction is taken to be perpendicular to the direction of propagation and contained in the plane of incidence. The plane of incidence (shaded in Figure 2.19) is defined as that plane which contains the input beam, the output beam, and the direction normal to the sample surface.

The angle of incidence is defined as the angle between the input beam direction and the direction normal to the sample surface. For any angle of incidence greater than 0° and less than 90°, $p$-polarized light and $s$-polarized will be reflected differently. This means that $R_p \neq R_s$.

Optical constants and what they mean

Ellipsometry is the premier technique for measuring optical constants.

Ellipsometry is an optical technique that requires an accurate model of the measurement process to analyze the measured data. The key components of all ellipsometric models are the optical constants of the substrate and sample layers and the thicknesses of the layers. To obtain good model fits to the measured data, highly accurate optical constants are required. While this sensitivity to optical constants might at first seem to be a problem, it can be used to measure optical constants of materials. In the near-UV, visible, and near-IR wavelength ranges, ellipsometry is the premier technique for measuring optical constants.

Within WVASE® optical constants are expressed as a complex dielectric function, $\varepsilon = \varepsilon_1 - i\varepsilon_2$, or as a complex refractive index, $\tilde{n} = n - ik = \sqrt{\varepsilon}$. WVASE® considers any optical constants with a positive imaginary part to represent an absorbing material.

With regard to the available published optical constant sets, spectroscopic ellipsometry has had something of an iterative history. First, simple samples were measured and the data analyzed to obtain useful optical constants. Then those optical constants were used in modeling more complicated samples that in turn yielded optical constants for additional materials. In this way a large base of optical constants has already been accumulated.
Alternatively, some materials do not seem to have intrinsic optical constants, in that the optical constants depend on the deposition process. Materials such as TiN, TiO\(_2\), and polycrystalline silicon exhibit a range of optical constants depending on how they are deposited. Metal films are also notable because the grain structure and surface morphology greatly impact their apparent optical constants.

The optical constants of all materials have some sort of expected dispersion as a function of wavelength. The following graphs show some typical optical constant spectra for different materials.

**Figure 2.20.** Real and imaginary parts of the complex dielectric function for crystalline silicon, a semiconductor.

**Figure 2.21.** Real part of the dielectric function for silicon dioxide (fused silica), a dielectric.

**Figure 2.22.** Real and imaginary parts of the complex dielectric function for silver, a metal.
Most optical constants have been published as wavelength tabulated lists, and tabulated lists form the basic set of optical constants used by WVASE®. However, this means a great deal of information is required to describe each material. At 200 wavelengths, 400 different real valued parameters are needed to describe a material. Further if the optical constants need to be measured, 400 different values will have to be measured. Optical constants for real materials, however, are not random functions of wavelength. They are generally smooth functions of wavelength and there is a causality relationship (the Kramers-Kronig relationship) between the real and imaginary parts. Because of this, the optical constants for many materials can be very adequately modeled using functional forms. WVASE® supports a variety of function-based optical constant models and allows you to easily work with optical constants in different formats.

Bulk materials

A bulk material is a bare substrate, with no coatings or overlayers.

Given the measurement geometry shown in figure 2.15 and assuming the sample to be optically thick with no coatings or overlayers, we now wish to calculate the Fresnel reflection coefficients of the sample, such that the expected \( \Psi \) and \( \Delta \) values may be calculated via equations 2.22 or 2.23. The reflection of the beam from the sample is described by the following Jones matrix equation:

\[
\begin{bmatrix}
\tilde{E}_r^p \\
\tilde{E}_r^s
\end{bmatrix} =
\begin{bmatrix}
\tilde{r}_p^r & 0 \\
0 & \tilde{r}_s^r
\end{bmatrix}
\begin{bmatrix}
\tilde{E}_p^p \\
\tilde{E}_p^s
\end{bmatrix}
\]

(2.38)

The analogous equation for the transmitted beam is

\[
\begin{bmatrix}
\tilde{E}_t^p \\
\tilde{E}_t^s
\end{bmatrix} =
\begin{bmatrix}
\tilde{t}_p^r & 0 \\
0 & \tilde{t}_s^r
\end{bmatrix}
\begin{bmatrix}
\tilde{E}_p^p \\
\tilde{E}_p^s
\end{bmatrix}
\]

(2.39)

Thus, there are four equations that define the Fresnel reflection coefficients:

\[
\tilde{r}_p^r \equiv \frac{\tilde{E}_r^p}{\tilde{E}_p^p} \quad \tilde{r}_s^r \equiv \frac{\tilde{E}_r^s}{\tilde{E}_p^s}
\]

(2.40)

\[
\tilde{t}_p^r \equiv \frac{\tilde{E}_t^p}{\tilde{E}_p^p} \quad \tilde{t}_s^r \equiv \frac{\tilde{E}_t^s}{\tilde{E}_p^s}
\]

(2.41)
The p- and s- components of the incident, reflected, and transmitted electromagnetic waves may now be written as follows.

\[ \tilde{E}_{p,s}^{\text{incident}} (\vec{r}, t) = \tilde{E}_{0,p,s}^{\text{incident}} \exp \left( -\frac{i 2 \pi n_0}{\lambda} \vec{q}_{\text{incident}} \cdot \vec{r} \right) \exp (i \omega t), \]  
\[ \tilde{E}_{p,s}^{\text{reflected}} (\vec{r}, t) = \tilde{E}_{0,p,s}^{\text{reflected}} \exp \left( -\frac{i 2 \pi n_0}{\lambda} \vec{q}_{\text{reflected}} \cdot \vec{r} \right) \exp (i \omega t), \]  
\[ \tilde{E}_{p,s}^{\text{transmitted}} (\vec{r}, t) = \tilde{E}_{0,p,s}^{\text{transmitted}} \exp \left( -\frac{i 2 \pi n_1}{\lambda} \vec{q}_{\text{transmitted}} \cdot \vec{r} \right) \exp (i \omega t), \]

Note that the angle of propagation of each beam is contained in the unit vector q, which lies along the direction of propagation of the beam.

We may now insert the expressions for the incident, reflected, and transmitted fields into the definitions for the Fresnel reflection and transmission coefficients (equations 2.40 - 2.43). We then require the phase quantities to be identical at all points on the interface, and we require the tangential components of \( \tilde{E} \) and \( \tilde{H} \) and the normal components of \( \tilde{D} \) and \( \tilde{B} \) to be continuous across the interface. This calculation yields three useful results.

First, we find that the reflected angle must be equal to the angle of incidence. In other words, the reflection of the beam will be specular. Second, from the equality of phase at the interface we obtain the well known Snell’s law:

\[ \vec{n}_0 \sin \phi_0 = \vec{n}_1 \sin \phi_1, \]  
where \( \phi_0 \) is the angle of incidence of the incident beam measured between the incident beam and the sample normal, and \( \phi_1 \) is the angle of propagation of the transmitted beam in the sample, measured again between the propagating beam and the axis of the sample normal. Note that if the (bulk) sample is absorbing such that the sample index of refraction \( \vec{n}_1 \) is complex, the transmitted angle \( \phi_1 \) will be complex as well. Note also that this equation is valid for any interface, and in a multilayer it can be used repeatedly from top to bottom in the stack to track the angle of propagation of the beam all of the way through the sample.

Finally, we are able to obtain expressions for the Fresnel reflection and transmission coefficients for the surface of the bulk sample:

\[ r_p = \frac{\vec{n}_1 \cos \phi_0 - \vec{n}_0 \cos \phi_1}{\vec{n}_1 \cos \phi_0 + \vec{n}_0 \cos \phi_1}, \]  
\[ r_s = \frac{\vec{n}_0 \cos \phi_0 - \vec{n}_1 \cos \phi_1}{\vec{n}_0 \cos \phi_0 + \vec{n}_1 \cos \phi_1}, \]
Fresnel transmission coefficients.

\[
\tilde{t}_p = \frac{2\tilde{n}_0 \cos \phi_0}{\tilde{n}_1 \cos \phi_0 + \tilde{n}_0 \cos \phi_1}, \quad (2.50)
\]

\[
\tilde{t}_s = \frac{2\tilde{n}_0 \cos \phi_0}{\tilde{n}_0 \cos \phi_0 + \tilde{n}_1 \cos \phi_1}, \quad (2.51)
\]

It is now a simple matter to evaluate \( \Psi \) and \( \Delta \) for the bulk sample case, by inserting equations 2.48 and 2.49 into the ellipsometric equation 2.23. It is instructive to use these equations to examine the behavior of \( \Psi \) and \( \Delta \) as functions of angle of incidence for different choices of the sample index of refraction. In all cases we choose the ambient index to be one, with no absorption, corresponding to air or free space.

We first consider the case of a transparent substrate, for which the extinction coefficient \( k \) is zero. We will assume that the index of the substrate is 1.5 at the wavelength of interest (a reasonable assumption for many glasses), and calculate \( \Psi \) and \( \Delta \) as a function of angle of incidence from normal incidence \( (0^\circ) \) to grazing incidence \( (90^\circ) \).

\( \Psi \) vs. angle of incidence for bare glass.

![Figure 2.24. Ellipsometric \( \Psi \) calculated versus angle of incidence for a transparent material with index \( n = 1.5 \).](image)

\( \Delta \) vs. angle of incidence for bare glass.

![Figure 2.25. Ellipsometric \( \Delta \) calculated versus angle of incidence for a transparent material with index \( n = 1.5 \).](image)

Examine the behavior of \( \Psi \) and \( \Delta \) carefully. \( \Psi \) equals \( 45^\circ \) and \( \Delta \) equals \( 180^\circ \) at normal incidence, which corresponds to the reflected beam exhibiting the same polarization state as that of the incident beam. At normal incidence, this will
always be the case as the plane of incidence is not defined in this case and there is no distinction between the p- and s- direction reflection coefficients.

As the angle of incidence increases, \( \Psi \) decreases until it reaches 0° at about 56° angle of incidence. At this angle, \( \Delta \) changes abruptly from 180° to 0°, and remains at 0° for angles up to 90°. The angle at which these effects occur is known as the Brewster angle, and for bare substrates with no coatings or overlayers it may be calculated from:

\[
\phi_B = \tan^{-1}\left( \frac{n_1}{n_0} \right) \tag{2.52}
\]

where \( \phi_B \) denotes the (complex) Brewster angle. For our assumptions of the substrate index equal to 1.5 and the ambient index equal to 1.0, we obtain the Brewster angle from equation 2.52 as 56.322°, which is easily verified from the above figures. Note that the Brewster angle will be complex if the substrate is absorbing.

To further understand the dependence of \( \Psi \) on angle of incidence, recall that \( \tan(\Psi) \) equals the square root of the ratio of the p- to s- intensity reflectances. The p-reflectance is defined as the intensity reflectance (intensity of reflected beam divided by the intensity of the incident beam) measured with the incident beam linearly polarized in the p-plane, and an analogous definition holds for the s-reflectance. The p- and s- reflectances may be calculated from the Fresnel reflection coefficients of the sample as follows, with an asterisk superscript denoting complex conjugation.

\[
R_p = |\vec{r}_p|^2 = \overline{\vec{r}_p} \cdot \overline{\vec{r}_p}^*, \tag{2.53}
\]

\[
R_s = |\vec{r}_s|^2 = \overline{\vec{r}_s} \cdot \overline{\vec{r}_s}^*. \tag{2.54}
\]

\( R_p \) and \( R_s \) for bare glass.

\[
\begin{align*}
\text{Angle of Incidence in degrees} & \quad 0 & \quad 20 & \quad 40 & \quad 60 & \quad 80 & \quad 100 \\
\text{Reflection} & \quad 0.0 & \quad 0.2 & \quad 0.4 & \quad 0.6 & \quad 0.8 & \quad 1.0 \\
\hline
\text{s-polarized} & \quad \text{---} & \quad \text{---} & \quad \text{---} & \quad \text{---} & \quad \text{---} \\
\text{p-polarized} & \quad \text{---} & \quad \text{---} & \quad \text{---} & \quad \text{---} & \quad \text{---}
\end{align*}
\]

\textit{Figure 2.26. The p- and s- polarized intensity reflectance calculated versus angle of incidence for a transparent substrate with } \( n = 1.5 \).

Note the p- and s-reflectances are identical at normal incidence, due again to the indistinguishability of the p- and s- directions at normal incidence. The s-reflectance increases monotonically from normal to grazing incidence, where it approaches unity. The p-polarized reflectance, however, decreases to zero at the Brewster angle and then increases to unity at grazing incidence.
The addition of absorption in the substrate modifies the above behavior somewhat. Let us now look at silicon, at a wavelength of 633 nm. At this wavelength, the index of refraction of crystalline silicon is 3.875 and the extinction coefficient for crystalline silicon is 0.023. We first calculate the $p$- and $s$-polarized intensity reflectance for crystalline silicon at 633 nm.

$R_p$ and $R_s$ for crystalline silicon (c-Si).

![Reflection vs Angle of Incidence plot](image)

Figure 2.27. $p$- and $s$-polarized intensity reflectance for crystalline silicon at 633 nm, $n = 3.875$ and $k = 0.023$.

Note the qualitative similarity of the angular dependence of the reflectances calculated for crystalline silicon to those calculated for glass. There are several important differences, however. First, due to the much higher index of refraction of silicon, the normal incidence reflectance is considerably higher, around 0.35, as opposed to about 0.09 for glass. This is physically reasonable, as a higher mismatch between the ambient and substrate index should scatter more of the beam back into the ambient, leading to higher reflectance. A second difference is that the Brewster angle is now around 76°, as opposed to 56° for glass. The Brewster angle will as a general rule increase with increasing index of refraction.

Finally, even though it is not apparent from the above plot, the $p$-polarized reflectance does not go identically to zero at the Brewster angle due to the non-zero absorption of silicon at 633 nm. Rather, the minimum value of the $p$-polarized reflectance (occurring at the Brewster angle, 75.5°) is $8.3 \times 10^{-6}$, which is extremely small but not zero. The absorption in the substrate prevents the $p$-reflectance from going to zero, and the value of the $p$-polarized reflectance at the minimum (Brewster angle) will increase as the value of the extinction coefficient increases. We now calculate $\Psi$ and $\Delta$ for crystalline silicon.
ψ vs. angle of incidence for c-Si.

![Figure 2.28. Ellipsometric ψ calculated for bare crystalline silicon as a function of angle of incidence, n = 3.875, k = 0.023.](image)

Δ vs. angle of incidence for c-Si.

![Figure 2.29. Ellipsometric Δ calculated for bare crystalline silicon as a function of angle of incidence, n = 3.875, k = 0 (solid curve), and k = 0.023 (dashed curve).](image)

Here is an expanded view of the ψ and Δ data shown above from 60° to 85° only.

![Figure 2.30. Same as figure 2.28, plotted from 70° to 80° angle of incidence only.](image)
Figure 2.31. Same as figure 2.29, plotted from 70° to 80° angle of incidence only.

Note that although qualitatively the simulated data shown for crystalline silicon is very similar to those shown for glass with no absorption, there are some important differences. First, the Brewster angle is now around 75.5°, and the minimum in $\Psi$ now occurs at this angle. Second, $\Psi$ does not go to zero, rather its minimum value at the Brewster angle is ~ 0.19°. Third, $\Delta$ does not change abruptly from 180° to 0° at the Brewster angle, rather this transition occurs over a range of angles of incidence centered on the Brewster angle. As a general rule for bulk samples (bare substrates), increasing values of the extinction coefficient lead to larger values of $\Psi$ at the Brewster angle and a broader transition region for $\Delta$.

To illustrate this point, we now compare the dependence of $\Psi$ and $\Delta$ on angle of incidence for crystalline and amorphous silicon at 633 nm. The amorphous silicon (a-Si) optical constants at 633 nm are $n = 4.516$ and $k = 0.249$, such that a-Si exhibits a higher index and extinction coefficient.

c-Si vs. a-Si.

Figure 2.32. Ellipsometric $\Psi$ calculated as a function of angle of incidence for crystalline silicon ($n = 3.875, k = 0.023$) and amorphous silicon ($n = 4.516, k = 0.249$).
c-Si vs. a-Si.

Figure 2.33. Ellipsometric $\Delta$ calculated as a function of angle of incidence for crystalline silicon ($n = 3.875, k = 0.023$) and amorphous silicon ($n = 4.516, k = 0.249$).

Note the higher index of a-Si leads to a larger value of the Brewster angle, and that the larger extinction coefficient for a-Si causes a shallower minimum in $\Psi$ at the Brewster angle. Also, the larger extinction coefficient yields to a broader region of transition for $\Delta$ from $180^\circ$ to $0^\circ$.

As an extreme case, we now consider polycrystalline silver at 633 nm, for which $n = 0.135$ and $k = 3.990$.

$\Psi$ vs. angle of incidence for silver.

Figure 2.34. Ellipsometric $\Psi$ calculated versus angle of incidence for polycrystalline silver, $n = 0.135, k = 3.990$.  

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$\Delta$ vs. angle of incidence for silver.

Figure 2.35. Ellipsometric $\Delta$ calculated versus angle of incidence for polycrystalline silver, $n = 0.135$, $k = 3.990$.

The extinction coefficient is now very large, and we see that the minimum in $\Psi$ is correspondingly very shallow, with $\Psi$ only decreasing to about 44.1° at the Brewster angle. Also, the transition of $\Delta$ from 180° to 0° is very broad.

Bulk samples with no overcoats or overlayers are rarely encountered in the real world. Most materials will oxidize in atmosphere, and most samples of interest have one or more films deposited on the substrate. In the next section we extend our mathematical formalism to include the case of a single film on a thick substrate, and then in the following section review formalisms valid for multilayered structures.

**Single films on thick substrates**

*Advanced.*

The case of polarized light reflection from a single film on an optically thick substrate may be solved in a number of ways. The most instructive is an analytic solution based on the summation of all reflected beam components, which will be demonstrated here.

Figure 2.36. Multiple reflected and transmitted beams for a single film on an optically thick substrate.

The multiple reflections of the incident light beam that occur in the film for the case of a single film on an optically thick substrate are shown in Figure 2.36.
There are in principle an infinite number of reflected and transmitted beams, however the splitting of the beam into reflected and transmitted components at each reflection quickly reduces the amplitude of the subsequent reflections such that eventually the reflected and transmitted beams die out. Also, any absorption in the film will attenuate the beams as they propagate in the film.

We now take advantage of the fact that our previous derivation for the Fresnel reflection and transmission coefficients of a bulk system is locally valid for the reflection and transmission of a beam from any interface. Thus, we can calculate Fresnel reflection coefficients which are functions of the ambient and film indices of refraction and the angle of incidence which are valid for any beam incident on the air / film interface. The same holds for beams incident from either direction upon either interface in the system.

The terminology for this calculation will be as follows. First, the incident beam is denoted by $\vec{E}_{\text{incident}}$, which represents either a p- or s-polarized wave of unit amplitude. The reflected beams will be labeled $\vec{E}_n^r$, where the subscript ‘n’ denotes the n\textsuperscript{th} reflection and the superscript ‘r’ denotes reflected beams. Transmitted beams will be labeled $\vec{E}_n^t$, where the subscript ‘n’ indicates the n\textsuperscript{th} transmitted beam and the superscript ‘t’ denotes transmitted beams.

Quantities relating to the ambient medium will have the subscript ‘0’, quantities relating to the film will have the subscript ‘1’, and quantities relating to the substrate will have the subscript ‘2’. This notation is used because it is easily extended to any number of layers. Fresnel reflection and transmission coefficients for both interfaces will be given two numbers for a subscript, where the first number denotes the region from which the beam is incident on the interface, and the second number denotes the region on the other side of the interface.

Our calculation will be performed independently for p- and s-polarized incident beams, as any incident beam of arbitrary polarization can be described as a linear combination of the p- and s-polarization states. As a result, we do not need to label the Fresnel coefficients with ‘p’ or ‘s’. For example, $\tilde{r}_{01}$ denotes the complex Fresnel reflection coefficient for a beam incident upon the film (region ‘1’) from the ambient medium (region ‘0’), while $\tilde{t}_{21}$ denotes the Fresnel transmission coefficient for a beam incident on the film / substrate interface from the film side.

In order to complete the model we must also be able to connect the propagating waves between the top and bottom interfaces of the film. A propagating wave will have the form given in equation 2.5, and it is a simple matter to show that propagation of a wave across the film (in either direction) yields a resulting wave of the following form.

$$\vec{E}_{\text{after}} = \vec{E}_{\text{before}} \cdot \exp(-i 2 \beta), \quad (2.55)$$

where $\beta$ is the phase thickness (or optical thickness) of the film (for the given wavelength and angle of incidence), given by

$$\beta = 2 \tilde{n}_1 \frac{d}{\lambda} \cos \phi_1 = 2\pi \frac{d}{\lambda} \sqrt{n_2^2 - n_0^2 \sin^2 \phi_0}, \quad (2.56)$$

in which $d$ is the film thickness and $\lambda$ is the wavelength, in the same units as the film thickness. It is now a simple matter to write down the expressions for the successive reflected beams:

$$\vec{E}_{i}^r = \tilde{r}_{01} \vec{E}_{\text{incident}}, \quad (2.57)$$
\[ \tilde{E}_2 = \tilde{E}_0 \tilde{r}_1 e^{-i2\beta} \tilde{E}_{\text{incident}}, \quad (2.58) \]
\[ \tilde{E}_3 = \tilde{E}_0 \tilde{r}_1(\tilde{r}_1)^2 e^{-i4\beta} \tilde{E}_{\text{incident}}, \quad (2.59) \]
\[ \tilde{E}_4 = \tilde{E}_0 \tilde{r}_1(\tilde{r}_1)^3 e^{-i6\beta} \tilde{E}_{\text{incident}}, \quad (2.60) \]

and so on. We can now identify the following general form for the \( n \)th reflected beam:
\[ \tilde{E}_n = \tilde{E}_0 \tilde{r}_1(\tilde{r}_1)^{n-2} e^{-i(2n-2)\beta} \]
\[ (2.61) \]

Now we sum the reflected beams using this functional form, as shown below.
\[ \tilde{E}_{\text{total}} = \left[ \tilde{r}_0 + \tilde{r}_0 \tilde{r}_1 e^{-i2\beta} \sum_{n=2}^{\infty} \tilde{r}_0(\tilde{r}_1)^{n-2} e^{-i2n\beta} \right] \tilde{E}_{\text{incident}}, \quad (2.62) \]

We next take advantage of the following identities, which may be derived from equations 2.48-2.51:
\[ \tilde{r}_0 = -\tilde{r}_1, \quad (2.63) \]
\[ \tilde{r}_1 \tilde{r}_0 = 1 - \tilde{r}_0^2. \quad (2.64) \]

Inserting 2.63 and 2.64 into 2.62 and evaluating the resulting convergent series, we find the following expression for the total reflected beam.
\[ \tilde{E}_{\text{total}} = \left( \frac{\tilde{r}_0 + \tilde{r}_1 e^{-i2\beta}}{1 + \tilde{r}_0 \tilde{r}_1 e^{-i2\beta}} \right) \tilde{E}_{\text{incident}}, \quad (2.65) \]

This equation is valid for p- or s-polarized input beams, provided the corresponding p- or s-polarized Fresnel reflection coefficients for the interfaces are employed. We now define the pseudo-Fresnel reflection coefficients for any arbitrary sample in terms of the incident, reflected, and transmitted beams. If we use p-polarized Fresnel coefficients for the evaluation of 2.65, we can find the p-polarized pseudo-Fresnel reflection coefficient \( \tilde{R}_p \) as follows
\[ \tilde{R}_p \equiv \frac{\tilde{E}_{\text{total}}}{\tilde{E}_{\text{incident}}} = \frac{\tilde{r}_0 + \tilde{r}_1 e^{-i2\beta}}{1 + \tilde{r}_0 \tilde{r}_1 e^{-i2\beta}}, \quad (2.66) \]

with a similar equation holding for the s-polarized case. These coefficients are easily identified from 2.65. We may now calculate \( \Psi \) and \( \Delta \) from a broader definition of the ellipsometric parameters, valid for any sample exhibiting pseudo-Fresnel p- and s-polarized reflection coefficients \( \tilde{R}_p \) and \( \tilde{R}_s \), respectively:
\[ \tilde{\rho} = \tan \Psi e^{i\Delta} = \frac{\tilde{R}_p}{\tilde{R}_s}. \quad (2.67) \]

In summary, the expected \( \Psi \) and \( \Delta \) for a single film sample at a given wavelength and angle of incidence may be calculated with the following procedure:

1. Calculate the phase thickness of the film (\( \beta \)) from 2.56.
2. Calculate the p-plane reflection coefficient for a beam incident on the film from the ambient (from 2.48, with subscript ‘0’ denoting the ambient and ‘1’ denoting the film.

3. Calculate the p-plane reflection coefficient for a beam incident on the substrate from the film (from 2.48, with subscript ‘0’ denoting the film and ‘1’ denoting the substrate).

4. Calculate the p-polarized pseudo-reflection coefficient for the sample from 2.66, using the interfacial reflection coefficients calculated in steps 2 and 3.

5. Repeat steps 2 - 4 for the s-polarized case, using equation 2.49 instead of 2.48 in steps 2 and 3, and obtaining the s-polarized pseudo-reflection coefficient for the sample.

6. Evaluate $\psi$ and $\Delta$ from the p- and s-polarized pseudo-reflection coefficients via equation 2.67.

Note that the summation of multiple transmitted beams may also be performed in a similar manner to obtain the polarization state of the transmitted beam.

**Multilayer formalisms**

There are many mathematical formalisms which may be used to calculate the pseudo-reflection coefficients and/or $\Psi$ and $\Delta$ for multilayered structures. In this section we discuss two common types, but due to the involved nature of these calculations we do not go into great depth.

It is possible to evaluate the pseudo-reflection coefficients by summing the multiple reflections from multilayered samples, but the difficulty of this calculation increases dramatically with increasing number of layers.

Many formalisms are based on the use of “characteristic matrices” to describe the individual layers and the substrate. These matrices relate the field components (electric and/or magnetic) at the top of the film to those at the bottom. Results valid for a multilayered structure are then obtained by multiplying the appropriate matrices together in order through the stack. These formalisms are very powerful, are not computationally intensive, and lend themselves well to the evaluation of superlattices, graded films, and other structures with large numbers of layers. Formalisms based on 2 x 2 matrices exist for isotropic samples, while useful formalisms based on 4 x 4 matrices have been developed to encompass optical and magneto-optical effects in multilayer structures, as well as other anisotropic sample effects and depolarizing effects.

**Superlattices**

The characteristic matrix approach is particularly useful for superlattices, where the same group of layers is repeated many times in the structure. In this, the characteristic matrix of a single period of the superlattice is first evaluated. It is then only necessary to multiply this matrix by itself as many times as there are periods in the superlattice.
Grading

Grading of the optical properties of a film along the direction of the film normal (from top to bottom through the film) is usually described by breaking the film up into many much thinner layers, each of which is itself uniform, but with the properties of each layer slightly different from the layers above and below. The properties of the individual layers are calculated from the specified grading profile of the film.

Composite materials and roughness - EMA models

There are a number of models in the literature for the calculation of the effective optical constants of a mixture of two or three materials, known as effective medium approximations (EMA). The simplest EMA is to simply linearly interpolate between the constituent optical constants, as shown in equation 2.68.

\[ \tilde{\varepsilon} = f_A \tilde{\varepsilon}_A + f_B \tilde{\varepsilon}_B + f_C \tilde{\varepsilon}_C, \]  

(2.68)

where \( \tilde{\varepsilon} \) is the effective complex dielectric function of the mixture, \( f_A, f_B, \) and \( f_C \) are the volume fractions (ranging from zero to one) of each constituent material, and \( \tilde{\varepsilon}_A, \tilde{\varepsilon}_B, \) and \( \tilde{\varepsilon}_C \) are the complex dielectric functions of the constituent materials. The volume fractions must total unity, and equation 2.68 is valid for three constituent EMA models as shown, and for two constituent EMA models if \( f_C \) is fixed at zero. The linear interpolation EMA (2.68) is not highly accurate, but is often used for graded layers to reduce calculation time.

The Maxwell-Garnett and Bruggeman EMAs are the most common, and can be used to model a wide range of mixing effects such as surface and interfacial roughness, mixing of c-Si with a-Si, and index grading. The Maxwell-Garnett EMA is derived assuming spherical inclusions of one (or two) material(s) (denoted materials ‘B’ and ‘C’) exist in a host matrix of the second material (denoted material ‘A’):

\[ \frac{\tilde{\varepsilon} - \tilde{\varepsilon}_A}{\tilde{\varepsilon} + 2\tilde{\varepsilon}_A} = f_B \frac{\tilde{\varepsilon}_B - \tilde{\varepsilon}_A}{\tilde{\varepsilon}_B + 2\tilde{\varepsilon}_A} + f_C \frac{\tilde{\varepsilon}_C - \tilde{\varepsilon}_A}{\tilde{\varepsilon}_C + 2\tilde{\varepsilon}_A}. \]  

(2.69)

Equation 2.69 must be solved for the effective complex dielectric function \( \tilde{\varepsilon} \) given the volume fractions of two of the constituents \( f_B \) and \( f_C \) (\( f_A \) is assumed to equal \( 1 - f_B - f_C \)) and the dielectric functions of all three materials. Equation 2.69 is valid for a three constituent Maxwell-Garnett EMA, and the two constituent case may be obtained by fixing \( f_C \) at zero.

The Bruggeman EMA (sometimes referred to as the coherent potential approximation) makes the self-consistent choice of the host material complex dielectric function equaling the final effective complex dielectric function of the multi-constituent material. The Bruggeman EMA requires the numerical solution of the following equation, valid for three constituents, or for two constituents with \( f_C \) fixed at zero.

\[ f_A \frac{\tilde{\varepsilon}_A - \tilde{\varepsilon}}{\tilde{\varepsilon}_A + 2\tilde{\varepsilon}} + f_B \frac{\tilde{\varepsilon}_B - \tilde{\varepsilon}}{\tilde{\varepsilon}_B + 2\tilde{\varepsilon}} + f_C \frac{\tilde{\varepsilon}_C - \tilde{\varepsilon}}{\tilde{\varepsilon}_C + 2\tilde{\varepsilon}} = 0 \]  

(2.70)

This equation can be quite difficult to solve correctly, particularly for three constituent EMA models. It is a complex equation and will yield an infinite number of solutions, such that the software must correctly choose the appropriate solution branch.
2.11 Regression analysis of optical data

How do we get layer thicknesses and optical constants from \( \Psi \) and \( \Delta \)?

Ellipsometry is a model dependent technique in that the measured quantities are the physical quantities we wish to determine, and a numerical analysis of the experimental data based on some mathematical model is required to obtain useful physical information about the sample under study. In this section we discuss the regression analysis of optical data to obtain physical parameters for the sample and, in some cases, the ellipsometer.

Description of the problem

Assume that we are studying a sample from which we have measured ellipsometric data as a function of wavelength and angle of incidence. We also have an optical model for our sample, consisting of any number of layers on a substrate and parameterized by the optical constants of the various materials and the thicknesses of the films on the sample. We now wish to vary some parameters in this model such that ellipsometric data calculated from the model matches our experimental data as closely as possible. A flowchart of this general procedure is shown in Figure 2.37.

![Figure 2.37. Flowchart of the procedure for an ellipsometric experiment.](image)

First we must define some quantity (called a maximum likelihood estimator) which represents the quality of the match between the data calculated from the model and the experimental data. The maximum likelihood estimator must be positive and should go to zero (or at least an absolute minimum) when the calculated data matches the experimental data exactly. \( \text{WVASE}^{TM} \) uses the following maximum likelihood estimator, the mean-squared error (MSE):

\[
\text{MSE} = \sqrt{\frac{1}{2N-M} \sum_{i=1}^{N} \left( \frac{\Delta_{i}^{\text{mod}} - \Delta_{i}^{\text{exp}}}{\sigma_{\Delta_i}^{\text{exp}}} \right)^2 + \left( \frac{\Psi_{i}^{\text{mod}} - \Psi_{i}^{\text{exp}}}{\sigma_{\Psi_i}^{\text{exp}}} \right)^2} = \sqrt{\frac{1}{2N-M} \chi^2}, \quad (2.71)
\]

where \( N \) is the number of \( (\Psi, \Delta) \) pairs, \( M \) is the number of variable parameters in the model, and \( \sigma \) are the standard deviations on the experimental data points. Another common maximum likelihood estimator, the chi-square (\( \chi^2 \)) is defined in equation 2.71 for comparison.

The MSE as shown in equation 2.71 represents a sum of the squares of the differences between the measured and calculated data, with each difference weighted by the standard deviation of that measured data point. For a very noisy...
measurement, the corresponding standard deviation will be large and that measurement will not be strongly weighted in the fit.

We have now reduced the fitting problem to finding a set of values for the variable model parameters which yields a single unique absolute minimum of the MSE. This is a minimization problem in that we are trying to find the minimum value of the MSE. For the results to be meaningful, this minimum should occur at a small value of the MSE, and should be fairly sharp as a function of the variable parameters. Also, it must be the lowest MSE obtainable from the given model, and only one set of variable parameters should yield the minimum MSE. Parameter correlations and insensitive parameters may prevent such a minimum from existing, and these problems will be discussed in further sections.

The discussion of minimization methods in the following sections requires the definition of some terms before proceeding. First, we will henceforth denote all of the measured data points as \( y_i \), where each \( y_i \) is either a measured \( \Psi \) or \( \Delta \) value. The corresponding \( \Psi \) or \( \Delta \) value calculated from the model is denoted \( y(x_i; \bar{a}) \), with \( x_i \) representing all known model parameters (such as angle of incidence, wavelength, known thicknesses, known optical constants, etc.) and the vector \( \bar{a} \) consisting of all variable model parameters. Thus, each element of \( \bar{a} \) is a variable parameter such as a layer thickness or optical constant, and the individual elements will be denoted \( a_j \), where \( j \) ranges from 1 to \( M \), the total number of variable parameters. Finally, \( \sigma_i \) will denote the standard deviation of the \( i^{th} \) data point.

### The gradient method

**Advanced.**

The gradient method is a very simple means for minimizing the MSE. We simply calculate the gradient of the MSE function with respect to each model parameter. If we think of the MSE as a surface defined in an \( M \)-dimensional space (where \( M \) is the number of variable model parameters), we are evaluating gradient of the MSE surface in this space, at the point defined by the current values of the variable parameters.

The gradient of the MSE surface will be an \( M \)-component vector with one component for each variable parameter. The elements of the gradient vector are given by

\[
\frac{\partial \chi^2}{\partial a_k} = -2 \sum_{i=1}^{N} \left( y_i - y(x_i; \bar{a}) \right) \left( \frac{\partial y(x_i; \bar{a})}{\partial a_k} \right),
\]

from which the factor of -2 is conventionally removed by the definition:

\[
\beta_k \equiv -\frac{1}{2} \frac{\partial \chi^2}{\partial a_k}.
\]

To take a step along the direction of the gradient from our current position on the MSE surface, we adjust the current values of the variable parameters by adding a multiple of the gradient.

\[
\bar{a} = \bar{a} + (\text{constant}) \cdot \bar{\beta},
\]

such that each individual parameter is modified according to

\[
a_i = a_i + (\text{constant}) \cdot \beta_i,
\]
or, if we define the adjustment vector \( \Delta \alpha \) as an M-vector composed of the adjustments to the variable parameters, we can calculate the elements of the adjustment vector as follows:

\[
\Delta \alpha = (\text{constant}) \cdot \beta_j. \tag{2.76}
\]

The problem with this approach is that the constant in equation 2.76 must be chosen arbitrarily, as there is no rigorous means of estimating an appropriate value. Too small of a value for the constant will cause the MSE to be improved very slightly, and many iterations will be required for the fit to reach the MSE minimum. If the constant value is chosen too large, the algorithm will overshoot the minimum, and may leapfrog back and forth across the minimum for many iterations.

**The inverse Hessian method**

A second method for minimizing the MSE is the inverse Hessian method. Close to the minimum, we can reasonably expect the MSE to be a quadratic function of the variable parameters, as the MSE is a sum of squares. In this case, we may write

\[
\chi^2(\tilde{\alpha}) \approx \gamma - \tilde{\alpha} \cdot \tilde{\alpha} + \frac{1}{2} \tilde{\alpha} \cdot \tilde{D} \cdot \tilde{\alpha},
\]

where \( \tilde{\alpha} \) is an M-component vector and \( \tilde{D} \) is an M x M matrix. If this approximation is good, it can be shown from equation 2.77 that the MSE minimum will occur at values of the variable parameters specified as follows:

\[
\tilde{\alpha}_{\text{min}} = \tilde{\alpha}_{\text{current}} + \tilde{D}^{-1} \cdot [-\tilde{\nabla} \chi^2(\tilde{\alpha}_{\text{current}})].
\tag{2.78}
\]

If the approximation 2.77 is exact, equation 2.78 will yield the exact location of the minimum. If the approximation 2.77 is good, equation 2.78 will yield variable parameters that yield an MSE which is close to the minimum. If the approximation 2.77 is bad, equation 2.78 will yield new values of the variable parameters which may or may not improve the MSE or be any closer to the minimum.

To evaluate the matrix \( \tilde{D} \) in equation 2.78, we first take an additional partial derivative of equation 2.70 with respect to the variable parameters.

\[
\frac{\partial^2 \chi^2}{\partial \alpha_i \partial \alpha_i} = 2 \sum_{i=1}^{N} \left[ \frac{\partial y_i(\tilde{x}; \tilde{\alpha})}{\partial \alpha_k} \frac{\partial y_i(\tilde{x}; \tilde{\alpha})}{\partial \alpha_l} - \left[ y_i - y(\tilde{x}; \tilde{\alpha}) \right] \frac{\partial^2 y(\tilde{x}; \tilde{\alpha})}{\partial \alpha_k \partial \alpha_l} \right], \tag{2.79}
\]

where it is again conventional to remove the prefactor 2 by defining

\[
\alpha_{kl} = \frac{1}{2} \frac{\partial^2 \chi^2}{\partial \alpha_k \partial \alpha_l}. \tag{2.80}
\]

Note that the matrix \( \tilde{\alpha} \) (known as the curvature matrix) is equal to one half times the matrix \( \tilde{D} \) (the Hessian matrix) in equations 2.77 and 2.78.

The adjustment vector which must be added to the current variable parameter vector to move to the minimum may be calculated by solving the following system of linear equations:
This algorithm works very well when starting from a point close to the final minimum, but fails as the quadratic approximation 2.77 begins to fail with increasing distance from the minimum. The Levenberg-Marquardt algorithm integrates the gradient and inverse Hessian methods smoothly to yield a robust algorithm which works well both close to and far from the minimum, and is described in the next section.

The Levenberg-Marquardt algorithm

WVASE™ employs the Levenberg-Marquardt algorithm for all model minimizations and for analysis of the calibration data to obtain calibration parameters. This algorithm provides a means of smoothly interpolating between the gradient and inverse Hessian methods described previously.

Consider the constant in equation 2.76 for the gradient method. As mentioned in that section, there is no means for estimating the value of this constant, which is a major drawback of the gradient method. Marquardt deduced that while the gradient vector itself contains no information useful for estimating the value of this constant, the Hessian matrix should provide some information as to the size of the constant.

Now, the elements of the gradient vector $\beta_k$ have the inverse dimensions of the corresponding variable parameters. As a result the constant in equation 2.76 must have the dimensions of $a_k^{-2}$. The only quantity in the $\tilde{\alpha}$ matrix that will have these dimensions is the reciprocal of the diagonal element corresponding to the $k^{th}$ variable, i.e. $1/c_{kk}$. Thus, the constant in equation 2.76 may be represented as follows

$$\delta \alpha_i = \frac{1}{\lambda \alpha_{ii}} \beta_i,$$  

(2.82)

where we have retained a ‘fudge factor’ $\lambda$. We now define a new $\tilde{\alpha}$ matrix (denoted $[\alpha']$) from the old one as follows.

$$\alpha'_{jj} \equiv \alpha_{jj} (1 + \lambda), \quad \text{if } j \neq k,$$

(2.83)

$$\alpha'_{jk} \equiv \alpha_{jk} \quad \text{if } j \neq k.$$  

(2.84)

We then replace both 2.81 and 2.76 by

$$\sum_{l=1}^{M} \alpha'_{il} \delta \alpha_i = \beta_k.$$  

(2.85)

This is the Levenberg-Marquardt algorithm, with the ‘fudge factor’ $\lambda$ now acquiring identity as the Marquardt parameter. At a given point on the MSE surface, we calculate the adjustments to the variable parameters as the solutions of the linear set of equations 2.85. Note that equation 2.85 reduces to equation 2.76 (the gradient method) when the Marquardt parameter becomes very large, and that it reduces to equation 2.81 (the inverse Hessian method) when the Marquardt parameter $\lambda$ is zero. Thus, by varying the value of the Marquardt parameter we can smoothly shift between the gradient method, which is desirable when far from the minimum, to the inverse Hessian method, which is desirable close to the minimum.
A typical approach then, is to choose some value of the Marquardt parameter and calculate the adjustment to the variable parameters. Then calculate the new MSE at the adjusted values of the variables. If the MSE is improved, divide the Marquardt parameter by ten (shift toward the inverse Hessian algorithm) and repeat the process. If the MSE is not improved, revert back to the original values of the variable parameters and multiply the Marquardt parameter by ten (shift toward the gradient method).

Convergence is reached when successive iterations are unable to improve the MSE. Normally, some minimum bound is set such that when the MSE is improved by less than this bound iteration will cease, and a maximum number of iterations may also be enforced as well.

The primary drawback of this algorithm is that it can settle on local minima of the MSE surface, yielding an incorrect result. Thus it is a good idea to try fitting from widely separated initial guesses for the variable parameters to ensure that the best-fit minimum located by the fitting algorithm is the true minimum on the MSE surface.

**Evaluating the best-fit results**

_Never skip this step!

Once a fit is completed, the resulting best-fit parameter values must be evaluated for sensitivity and for possible correlations. The sensitivity is expressed in terms of a confidence limit and describes “how much” information is available about a given parameter. Fit parameter correlation is expressed in terms of a set of two-parameter correlation coefficients and describes “how independent” the fit parameters are.

Both of these pieces of information come from an important element of the fitting procedure, the curvature matrix \( \alpha \), whose elements are given as follows.

\[
\alpha_{ij} = \sum_{i=1}^{N} \left[ \frac{1}{\sigma_{i}^{2}} \frac{\partial \Phi}{\partial a_{i}} \frac{\partial \Phi}{\partial a_{j}} + \frac{1}{\sigma_{ij}^{2}} \frac{\partial \Phi}{\partial a_{i}} \frac{\partial \Phi}{\partial a_{j}} \right]
\]  (2.86)

The curvature matrix is related to the covariance matrix of the fit parameters by

\[
[C] = [\alpha]^{-1}.
\]

The standard 90% confidence limit (SCL) found in text books, and the figure of merit (FOM) we have adopted to describe confidence in the \( i \)th fit parameter are given by

\[
SCL_{i} = 1.65 \times \sqrt{C_{ii}} \quad \text{and} \quad FOM_{i} = SCL_{i} \times \sqrt{\text{MSE}}.
\]  (2.87)

\( C_{ii} \) is the \( i \)th diagonal element of the covariance matrix. When WVASE\textsuperscript{®} returns the “error bars” on a fit parameter the FOM is used. WVASE\textsuperscript{®} treats the terms “confidence limit”, “confidence FOM”, and "error bar" as the same quantity. The returned format is Fit Value±FOM. The assumptions required to accurately determine confidence limits and methods of interpreting confidence limits are briefly discussed next. A much more in depth discussion may be found in chapter 13 - ‘VASE\textsuperscript{®} Data Analysis’.

**Interpretation of confidence limits**

In the case of a good fit with no systematic errors, the MSE tends toward unity and \( FOM_{i} \) reduces to the standard 90% confidence limit. This FOM combines information about the sharpness of the fit minimum (\( C_{ii} \)) with information about the
overall quality of the fit. The FOM is primarily related to the combined measurement and fitting process. Using the FOM as direct quantitative information about the sample is only valid when \( \sigma_{\varphi}^{\exp} \) and \( \sigma_{\Delta}^{\exp} \) are known to be accurate in magnitude, and when random (not systematic) measurement errors dominate the fit.

Assigning an independent confidence limit to a fit parameter also requires that the parameter be uncorrelated. This is usually a simple matter of checking the two-parameter correlation coefficients given by

\[
S_{jk} = \frac{c_{jk}}{\sqrt{C_{jk}^{\varphi} C_{jk}^{\Delta}}}
\]

(2.88)

An absolute value of \( S_{jk} \) near 1 indicates correlation between the \( j \)th and \( k \)th fit parameters. The correlation coefficients, computed from the same covariance matrix as the confidence limits, are much less dependent on the absolute magnitude of the standard deviations. The correlation coefficient can be objectively evaluated even when the confidence limit can not. A very detailed discussion of the interpretation of the confidence limits from a fit is given in chapter 13 - ‘VASE® Data Analysis’.

## 2.12 Optical properties of materials and thin films

In this section we present a brief tutorial on the optical constants of materials. We begin with a discussion of the physical meaning of the optical constants, and proceed to discuss the dominant optical absorption processes encountered in materials. Classification of materials by optical properties is discussed, as are the primary classes of materials - dielectrics, semiconductors, and metals. Finally, anisotropic materials are briefly discussed, as are differences between bulk and thin film optical constants for the same material.

### Optical constants - what are they?

The optical constants are parameters which characterize how a material will respond to excitation by an electromagnetic field at a given frequency. For isotropic materials, two real parameters (or one complex parameter) are sufficient for this purpose. Consider a point inside of the material of interest at which some externally applied electric field \( \vec{E} \) exists. The polarization field \( \vec{P} \) is defined as the additional electric field induced at that point by the external field, and is (in the absence of non-linear effects) proportional to the external field:

\[
\vec{P} = \tilde{\chi}_e e_0 \vec{E},
\]

(2.89)

where \( \tilde{\chi}_e \) is called the electric susceptibility of the material, and \( e_0 \) is the free space dielectric constant. The displacement field \( \vec{D} \) may be shown from Maxwell’s equations to equal the external electric field plus the polarization field, yielding

\[
\vec{D} = (1 + \tilde{\chi}_e) e_0 \vec{E}.
\]

(2.90)

The complex dielectric function of the material is then defined as the constant of proportionality between the displacement and electric fields:

\[
\tilde{\varepsilon} \equiv (1 + \tilde{\chi}_e) e_0,
\]

\[
= \tilde{\varepsilon}_r e_0,
\]

(2.91)
where $\varepsilon$ is the complex dielectric constant of the material ($\varepsilon = \varepsilon_1 + i\varepsilon_2$), and $\varepsilon_r$ is the (complex) relative dielectric constant for the material. Thus, the displacement and (external) electric fields are related by

$$\tilde{D} = \varepsilon \tilde{E}. \quad (2.92)$$

We have assumed that the response of the material to the applied field is isotropic, i.e. equal in all directions. If this is not the case (as will occur for many crystals of non-cubic symmetry) then the complex scalar dielectric function in equation 2.92 must be replaced with a $3 \times 3$ tensor dielectric function.

Thus, we have shown that the dielectric function represents the degree to which the material may be polarized by an applied electric field. It is a complex quantity, and the imaginary part of the dielectric function has the useful property of being directly proportional to the amount of power absorbed per unit time and unit volume at a point in the material from the applied field. This is a natural quantity for calculation from physical absorption models. The real and imaginary parts of the relative dielectric function are very commonly tabulated in the literature as optical constants of materials.

A second representation of the optical properties of a material is also possible, based on the effect the material has on an electromagnetic wave propagating through the material. Recall equation 2.5 for a propagating electromagnetic wave, restated below:

$$\tilde{E}(\tilde{r}, t) = \tilde{E}_0 \exp \left( \frac{i2\pi}{\lambda} \tilde{q} \cdot \tilde{r} \right) \exp(-i\omega t) \quad (2.93)$$

The complex index of refraction $\tilde{n}$ ($= n + ik$), where $k$ is the extinction coefficient) appears in this equation, and governs the change in amplitude and phase of the wave as it propagates. The complex index of refraction and the complex dielectric function of a material are related by

$$\tilde{\varepsilon} = \tilde{n}^2. \quad (2.94)$$

The length of propagation of the wave in the material after which the phase of the propagating wave will have changed by $2\pi$ is determined by the real part of the index of refraction ($n$), and equals the wavelength of the propagating wave (in free space) divided by the real part of the material index of refraction. The amplitude of the propagating wave will decay to $1/e$ of its original amplitude after propagating a distance equal to the wavelength divided by $2\pi$ times the imaginary part of the complex index of refraction (the extinction coefficient).

Thus, the optical constants $n$ and $k$ (the real and imaginary parts of the complex index of refraction) represent the optical properties of a material in terms of how an electromagnetic wave will propagate in that material. Alternatively, the real and imaginary parts of the dielectric function contain the same information in terms of how the material responds to an applied electric field. Both types of optical constants are commonly encountered in the literature, and the choice of optical constant type is generally determined by the application.

**Kramers-Kronig relations**

The real and imaginary parts of the complex index of refraction are not independent quantities, nor are the real and imaginary parts of the complex dielectric function. The Kramers-Kronig relation, derived from the requirement that the material cannot respond to an applied electric field prior to the application of the
field, connects the real and imaginary parts of the complex index of refraction and complex dielectric function as follows:

\[ n(E) - 1 = \frac{2}{\pi} \int_0^\infty \frac{E' k(E')}{E'^2 - E^2} \, dE', \quad (2.95) \]

\[ \varepsilon_1(E) - 1 = \frac{2}{\pi} \int_0^\infty \frac{E' \varepsilon_2(E')}{E'^2 - E^2} \, dE', \quad (2.96) \]

In other words, if the spectrum of the absorptive part of the optical constants is known, the real part may be evaluated from equation 2.95 or 2.96. Also, examination of the denominator of equations 2.95 and 2.96 shows that the integrand should not contribute significantly unless \( E' \) is fairly close to \( E \), such that absorption processes far removed from the photon energy of interest do not contribute strongly to the dispersion of the index or real part of the dielectric constant at that energy.

This is easily seen in the optical constants of crystalline silicon. When the silicon absorption is significant, there is very strong dispersion of the silicon index of refraction and the real part of the silicon dielectric function. At energies below the bandgap energy, silicon is not absorbing and the silicon index and real part of the dielectric function exhibit weak dispersion, decreasing monotonically with decreasing photon energy.

**Crystalline silicon optical constants.**

![Figure 2.38](image.png)
Crystalline silicon optical constants.

Figure 2.39. Real and imaginary parts of the silicon complex dielectric function, plotted as a function of photon energy.

The optical properties of all materials are determined completely by the types and strengths of the optical absorption processes that occur in the material. In the next few sections we discuss the primary mechanisms by which energy is absorbed from a light beam by materials.

**Interband absorption**

The most important type of optical absorption is interband absorption. This occurs when an electron in a bound state in the material absorbs a single photon from the light beam and jumps to a higher energy level in the material. This process may occur as stated, with the electron’s crystal momentum remaining unchanged, or absorption and/or emission of a phonon may also occur such that the crystal momentum of the electron changes as well.

Semiconducting and dielectric materials exhibit an energy gap in their band structure, with the Fermi level of the material lying somewhere within the bandgap. Thus, interband absorption will not occur for such materials until the photon energy exceeds the energy difference between the highest occupied electron energy level and the lowest unoccupied electron energy level. If these two levels occur for the same value of the crystal momentum, the onset of absorption occurs with direct transitions, requiring no change in the electron crystal momentum. This is the case, for example, for GaAs. If the highest occupied and lowest unoccupied levels occur at different crystal momenta, the onset of absorption occurs through indirect transitions, requiring the emission and/or absorption of a phonon for conservation of both crystal momentum and energy. Absorption due to interband transitions dominates the optical spectra in the UV-VIS-NIR for nearly all semiconducting and dielectric materials. Metals exhibit interband absorption structure in the optical constants as well, but also show strong absorption effects due to the absorption of photons by free carriers.

**Intraband absorption**

A second important type of optical absorption is intraband absorption, in which an electron absorbs a photon from the light beam but jumps to a different energy state within the same band. This process requires the emission or absorption of a phonon unless the initial and final electron states occur at identical values of the energy.
crystal momentum. A special case of intraband absorption is absorption by free carriers, discussed in the next section.

**Free carrier absorption**

Metals and other conducting materials contain a ‘sea’ of conductors which are not bound to any specific atom or location within the material. These free carriers exhibit a distinctive optical absorption, which may be derived by solving for the trajectories of free carriers under the influence of a driving electromagnetic field. Examples of free carrier absorption spectra will be presented in the following sections. Note that the Drude model for free carrier optical absorption may be obtained as a special case of a single Lorentz oscillator with the center energy fixed at zero. This is due to the fact that metals exhibit no bandgap, as the Fermi energy for a metal lays within one of the electron energy bands.

**Dielectric materials and semiconductors**

The most commonly encountered classes of materials in ellipsometry are dielectric materials and semiconductors. These two types of materials are equivalent for purposes of discussing their optical properties. The optical constant spectra of a typical semiconductor or dielectric may be divided into two distinct spectral regions. The first region extends from the photon energy where the material begins to absorb to higher energies. The onset of absorption is due to the onset of interband transitions above the bandgap energy, and the material will usually be absorbing for all energies higher than the energy at which absorption begins to occur. Near the onset energy, the extinction coefficient (or imaginary part of the dielectric function) tends to increase smoothly with energy, but may show complicated dispersion as the energy increases due to contributions from many different interband transitions.

At photon energies less than the bandgap energy, the extinction coefficient (imaginary part of the dielectric function) will be zero, and the index of refraction decreases slowly and monotonically with decreasing photon energy. The index cannot show strong dispersion in this region, as previously discussed with respect to the Kramers-Kronig relations.

A good example of this type of material is crystalline silicon, whose optical constants are shown in Figures 2.38 and 2.39. Another example is silicon dioxide, for which only the second region may be observed in the UV-VIS-NIR region of the spectrum. The absorption edge for silicon dioxide is located deep in the UV, and is not normally observed in optical measurements.

Probably the most important point of this section is that the index of refraction (real part of the dielectric function) of a material should never increase with decreasing photon energy (or increasing wavelength) if the extinction coefficient (imaginary part of the dielectric function) of the material in the spectral range of interest is zero. This is very useful for identifying unphysical results of model fits when fitting for the index of transparent films.

**Metals**

The optical constants of metals are determined by contributions from both inter- and intraband absorption, as well as a contribution from free electron absorption. As a result the dispersion of the optical constants of metals tends to be rather complicated. For our purposes, metals are defined as any material that does not exhibit vanishing optical absorption anywhere in the UV-VIS-NIR regions of the
Bulk vs. thin film optical constants

As a final note, there can be very significant differences between the optical constants measured from a bulk specimen of a material and the optical constants of a thin film of the same material. This is primarily related to microstructural differences in the film, but can also be due to size effects for very thin films. It is dangerous, as a result, to employ bulk optical constants from the literature for the analysis of thin films of the same material, and this analysis technique should only be employed as a last resort.

Further Reading

The following list of references is provided to encourage further investigation to advance the ideas presented in this short course. They have been grouped according to the topics of this chapter.

Spectroscopic ellipsometry overviews

Special wavelength range SE


Polarized light and optical components

**Ellipsometry configurations and calibration**


**Optical constants**


**Data regression**


**Applications**

Chapter 3 Navigating WVASE®

3.1 Working in the Microsoft Windows® XP operating system

You can skip this chapter if you are an experienced Windows® 98 user.

This section contains information and examples intended to help the new user quickly become proficient with the Microsoft Windows® environments under which WVASE® will run (Windows® 95, Windows® 98, Windows® XP® and Windows® 7®, with some exceptions for Windows® NT). It is assumed from the outset that the user has no previous experience with Windows® XP. Keep in mind that the best way to learn is by doing. As you read these instructions, we recommend running WVASE® and trying the functions described below. The WVASE® program is written specifically for Windows® environments and uses the Windows® user interface. As a result, some knowledge of Windows® operation is required for efficient use of the program.

Starting Windows® XP or Windows® 7®

Windows® XP and Windows® 7® starts automatically when the computer is turned on. Windows® will start with a screen similar to the following.

The Windows® XP Desktop.

Figure 3-1. A possible Windows® XP Desktop display.
Windows® XP basics

In this section the major components of the Windows® operating system are described as well as the basic user interface. Figure 3.1 shows the basic component layout, consisting of the Windows Desktop, the Taskbar, and the Start menu button. First, a brief description is given on using the mouse in the Windows® environment.

Using the Mouse

The mouse is a very important part of the Windows® user interface. This section briefly describes the basics of using the mouse and the ‘mouse terminology’ that will be used throughout the rest of the manual.

The mouse is a graphical pointing device. It typically appears on the screen as an arrow. This is called the mouse cursor. The appearance of the cursor may change from time to time to indicate when different functions can be performed. For example, the mouse will take the form of an hourglass when the computer is busy performing a task and not able to take input from the user. The basic operation of the mouse involves moving the cursor over the item (icon, menu, etc.) you wish to activate and clicking the left mouse button. When ever this manual states ‘click the mouse’, it indicates the user should move the mouse onto the specified object and click the left mouse button. In some cases it is necessary to click the left mouse button twice in quick succession. This is called a ‘double-click’.

Sometimes it is necessary for the user to click the right mouse button to perform an operation. This manual will explicitly state ‘click the right mouse button’. For more information on using the mouse see the Windows® XP documentation or online help.

The Desktop

A typical Desktop is shown in Figure 3.1. It covers the entire area of the computer screen. When applications are running, they run on the Desktop. The Desktop also contains several icons. These icons represent applications (programs) and folders (directories) which are commonly used. In the above picture there are eleven icons, one of which represents the WVASE® program. To run the program associated with an icon or to open the folder associated with an icon, move the mouse over the icon and double-click.

The Taskbar

The Taskbar is the narrow bar that extends across the bottom or sides of the Desktop. This bar contains the Start menu button at the far left, and the time at the far right. Programs which are currently running will also appear on the task bar in the form of buttons. For example, Figure 3.2 below shows the Taskbar when Microsoft Word (used to write this manual) and the Calculator applications are running. The button which is pressed represents the application that is active, or on top of the others. Clicking the mouse on a different application’s button makes that application active and puts it on top of the others on the Desktop.

The Start menu

From the Start menu, all of Window’s functions and applications can be accessed. To activate the Start menu, move the mouse over the Start button and click. The Start menu will appear similar Figure 3.3. The icons at the top of the
menu, above the ‘Programs’ folder, will vary from computer to computer as these are configurable. The items from the bottom of the menu to the ‘Programs’ folder will appear on every computer running Windows® XP. Only two of these items will be discussed here: ‘Shut Down’ and ‘Programs’. Please see the Windows® XP documentation or online Help for information on the other items.

Figure 3-3. The Windows® XP Start menu and Programs menu. Different icons may appear at the top of the menu for various computers as they are configurable.

The ‘Shut Down’ item on the Start menu is used to shut down Windows® XP and the computer. Do not turn off the computer without using the ‘Shut Down’ item unless the computer has locked up (does not respond to the keyboard or mouse). Improperly shutting the computer down may result in loss of data on the computer’s hard drive.

The ‘Programs’ item is where icons for all of the windows applications can be found. Selecting this item with the mouse causes a second menu to appear (as indicated by the arrow after the word ‘Programs’). This second menu displays icons for programs as well as more program groups (the ones with arrows after them). Selecting a program item causes that program to be executed. Generally, WVASE® program can be found in the Start menu itself.

**Working with Applications**

As mentioned before, applications can be accessed in Windows® XP in a couple of ways. If the desired application appears on the Desktop, then the easiest way to run the application is to double-click the application’s icon. For example, to start WVASE®, place mouse over the WVASE® icon and double-click. Another way to access applications in Windows® XP is to use the Start menu on the Taskbar previously as described.

Some of the more common applications provided by Windows® XP are located in the Accessories Program group on the Start menu as seen in Figure 3.3. These applications include Notepad (a simple text editor) and other system tools. Any of these applications can be run by clicking on them.

Starting applications.

For example, if we were to point the mouse at the icon labeled ‘Notepad’ in the Accessories folder and click the mouse, the Notepad program begins running in a window.
Closing applications.

To close an application, place the mouse cursor over the small box in the upper right corner of the window (a gray box with a black X in the middle as shown in Figure 3.4) and click the mouse. This will close the window and exit the program. For example, let us say that the 'Notepad' program had been opened by clicking on the 'Notepad' icon as in the previous paragraph. If we then click on the box with an ‘X’ in the upper right corner of this window, the 'Notepad' program is closed, and we are back to the Windows® XP Desktop.

Windows® XP is best learned by practice!

Try experimenting with opening and closing folders and programs. To exit Windows® XP, choose Shut Down from the Start Menu. Always exit from Windows® XP by using the Shut Down command.

Menus

Individual applications will usually contain various menus of functions which the user can select. The headings of these menus are displayed on the bar (the menu bar) across the top of the window as shown in Figure 3.4.

![Figure 3-4. The menubar from the Notepad program window.](image)

Shortcut: when a word has an underlined letter, that menu can be accessed by holding <Alt> down and then pressing the same underlined letter.

Menus provide you with options.

In Figure 3.4, menus titled 'File', 'Edit', 'Search', and 'Help' are provided. To see the contents of one of these menus, use the mouse to place the cursor over the title of the menu you wish to select and click the left mouse button. Alternatively, you can hold down the <alt> key and press the underlined letter in the title of the menu you wish to access. A list of options contained in the menu will be displayed under the menu title that you clicked on.

![Figure 3-5. The File menu from the Notepad program’s menubar.](image)

To select one of the menu options, place the arrow over the option and click the left mouse button or press the key or combination of keys displayed in the menu next to the desired option. The program will then perform the requested function. For specific information on Windows® 98 menu options, consult the Windows® 98 documentation or online help. We will discuss the menu options provided by the WVASE® program in detail later.

Minimizing and maximizing windows

A window can be removed from the screen without actually closing it. The 'minimize' function allows us to remove an active window from view and yet leave the application running. The icons at the bottom of the screen next to the Start button on the Taskbar represent all applications currently running. To bring the window of an active program to the front, click on that programs icon in the Taskbar.
To minimize a window, click once on the box in the upper right corner of the window which contains the single horizontal line (see Figure 3.4). This will erase the application's window from the Desktop but will not remove it from the task bar. The program continues running even though it isn’t visible on the desktop. To open the application again, use the mouse to position the cursor over the icon for the application in the Taskbar and click the left mouse button. A window will open in exactly the same state as it was just prior to being minimized. This feature is very useful when you need to use another program but don't wish to close the program you are currently running. For example, we might wish to use the calculator supplied with Windows® XP while working on a document with the Microsoft Word™ word processor. To do this, we would minimize the Word™ window, click on the calculator icon in the 'Accessories' folder, do our calculations, close or minimize the calculator window, and click on the Microsoft Word™ icon in the Taskbar to bring the word processor back on the screen.

Along with the minimize function, Windows® XP has a maximize function which will increase the size of a window to fill the entire screen. To switch between maximum size and normal size windows, click on the box in the upper right corner which contains either a single square box or two overlapping square boxes. If the window is normal size, only the single box will be present as in Figure 3.4. Doing this will switch the window to its alternate condition, i.e. from normal to maximum or from maximum to normal.

In the normal size, windows can be scaled in size by pointing the arrow at the edge of the window, holding the left mouse button down, and dragging the edge of the window to whatever position you desire. This can be done to any of the four edges of the window, such that windows can be adjusted to any size desired. Move windows by holding the mouse button over the titlebar and ‘dragging’ the window to a new location. The WVASE® program is structured to take full advantage of this feature to allow the user to easily switch between the different sections of the program.

Note that multiple windows can be present on the screen at any time. In the screen shown below, there are three open windows: Microsoft® Word, WVASE®, and Notepad. Any of these windows can be brought to the foreground by pointing the arrow anywhere within the window and clicking the left mouse button or by selecting that application from the Taskbar.

Figure 3-6. A Desktop with multiple open and overlapping windows.
Dialog boxes

WVASE® makes extensive use of dialog boxes for communicating with the user. For example, selecting the ‘Angles’ menu option from the Experimental Data window will cause the dialog box shown in Figure 3.7 to appear.

![Figure 3-7. A dialog box used by WVASE®.](image)

There are several important features of the above dialog box which are common to all dialog boxes used by WVASE®. First, there are a number of 'text' boxes which contain information used by the WVASE® program. The above dialog box contains eleven such information cells, three of which contain numbers. In this example, the user is telling WVASE® that the angle of incidence is 65°. Only one information cell is active at a given time, and the active cell will contain the cursor or will be highlighted. To move between cells, either use the mouse to point and click on the cell you wish to move to, or use the <Tab> key to move from cell to cell. Information can be typed directly into the active cell.

The smaller boxes on the right side of the above dialog box can be checked or unchecked. These check boxes are accessed in the same way as the information cells - by pointing and clicking or using the <Tab> key. To toggle the check box on/off, press the space bar when the box you want is active. In WVASE®, check boxes are often used to define fit parameters. Finally, note that some characters in the dialog box are underlined (the numbers 1-5 in the above example). Pressing <Alt> and the underlined letter will directly access that particular option from the dialog box. For example, pressing <Alt> and '3' within the above dialog box will allow the user to specify the third angle of incidence. Keystrokes which provide rapid access to menus or menu items (denoted by an underlined letter in the menu title or menu item name) are often referred to as ‘hot’ keys.

Selecting the ‘Open File’ menu option from the Experimental Data window will cause the dialog box of Figure 3.8 to appear. A very similar dialog box is used when saving files to disk.
You will use this dialog box often, so learn it well!

Figure 3-8. Standard dialog box used for selecting a file name to open.

This dialog box contains several different items to help you find the file name you want.

‘Look in:’ List

This drop-down list box is used to choose what drive (or computer if hooked up to a network) the file will be loaded from.

Directories and Files List

This large selection box is used to choose the directory and file. To view a specific directory, double click on the directory in this list. To select a file from the current directory, click on the file in the list or type the file name into the ‘File name’ text box.

File name

In addition to displaying the filename you might have chosen using the selection boxes, this is an editable text box. In this edit box you can type an explicit filename which includes the drive and directory specification. If you do not specify a drive and directory then the path displayed in the ‘Look in’ list will be used.

‘Files of Type’ list

This selection box contains “masks” for what kind of files the program wants (what file extensions are acceptable). Only files of the selected type are displayed in the directory and file list.

Open button

This button is used when the appropriate name has been selected and you want the ‘Open’ command to be completed.

Cancel button

This button is used to cancel the ‘Open’ command.

Summary of Windows® XP functions

As a final note, all of the above functions can be performed from the keyboard, without using the mouse. Expert Windows® users often find that it is much easier to get around in Windows®98 (and WVASE®) quickly by using keystrokes rather than the mouse. The following table summarizes the functions described above, and how to perform them with the mouse or with the keyboard.
### Windows® XP Functions

<table>
<thead>
<tr>
<th>Function</th>
<th>Mouse</th>
<th>Keyboard</th>
</tr>
</thead>
<tbody>
<tr>
<td>Open a Program.</td>
<td>Place the arrow over the icon for the program on the Desktop and double click the left button, or select the program from the Start menu.</td>
<td>Press the Start menu keyboard button and use the arrow keys to navigate the Start menu, selecting the program you wish to run.</td>
</tr>
<tr>
<td>Close a program.</td>
<td>Use the mouse to click on the box with an ‘X’ in the upper right corner of the window.</td>
<td>Use &lt;Alt&gt;-f to select the 'File' menu, and select the appropriate menu option to close the application.</td>
</tr>
<tr>
<td>Minimize a window.</td>
<td>Click on the box in the upper right corner of the window containing a single horizontal line.</td>
<td>Press &lt;Alt&gt;-&lt;Space&gt; to activate the control menu. Select 'minimize' from this menu. Use the arrow keys to move the highlighted bar among menu options.</td>
</tr>
<tr>
<td>Toggle between maximum and normal size windows.</td>
<td>Click on the box in the upper right corner of the window containing two square boxes. If window is normal size, this box will contain only a single square box.</td>
<td>Press &lt;Alt&gt;-&lt;Space&gt; to activate the control menu. Select the appropriate option from this menu.</td>
</tr>
<tr>
<td>Switch between running applications.</td>
<td>Click on the window you wish to switch to or click on the desired application in the Taskbar.</td>
<td>Use &lt;Alt&gt;-&lt;Tab&gt; to switch between active windows.</td>
</tr>
<tr>
<td>Change window size and/or position.</td>
<td>Position the arrow on the boundary of the window. Hold the left mouse button down and drag the boundary to the desired position.</td>
<td>Press &lt;Alt&gt;-&lt;Space&gt; to open the control menu. Select the 'size' option. The arrow will change to a four-headed arrow. The arrow keys can be used to adjust the window boundaries. When done, press &lt;Enter&gt;.</td>
</tr>
<tr>
<td>Select Menu items.</td>
<td>Click on the menu title to open the menu, then click on the option you wish to select.</td>
<td>Each menu option has one letter underscored. Press &lt;Alt&gt; and the underlined letter to open that menu, and the underscored letter to select particular menu options.</td>
</tr>
</tbody>
</table>

These are the basic functions required to use Windows® XP. There are many other useful keystrokes available to the Windows® XP user, and the above list is by no means a complete summary of all Windows® XP functions. For a more thorough and detailed discussion of the Windows® XP environment, we refer the user to the Windows® XP documentation.

### 3.2 Starting WVASE®

To start WVASE® from Windows® XP, position the arrow tip of the mouse on the WVASE® icon and double-click the left mouse button, or select the WVASE® icon from the Start menu. The WVASE® icon looks like this:
3.3 Auto-launching WVASE® from .env, .mod, & .dat files

Select .env, .mod and .dat files from Windows™ Explorer to automatically launch WVASE®, then load the selected file. After the file is loaded, WVASE® will set the datadir (data directory) to that file’s location.

Set-up WVASE Auto-launch feature

Before using this feature, Windows® Explorer must recognize the extensions. In Windows® Explorer:

1. Right-click on a .env file
2. Choose ‘Open With >’
3. Select ‘Choose Program …’
4. Check ‘Always use the selected program to open this kind of file’
5. Select ‘Browse…’
6. In the ‘Open With’ dialog box, choose WVASE.exe as the program to open (You might need to choose ‘Browse’ to find WVASE.exe in the WVASE directory).

This procedure will allow Windows® Explorer to launch WVASE® when these extensions are selected.

3.4 WVASE® windows

The “V.A.S.E. for Windows” frame

WVASE® has six windows - one for data acquisition and five for data analysis and display.

Within the “V.A.S.E. for Windows” frame, there is one menubar and up to six main windows. The six windows are named as follows.

1. Experimental Data
2. Model
3. Generated Data
4. Graph
5. Fit
6. Hardware

The first five WVASE® windows are used for data analysis, while the sixth (the Hardware window) is used for data acquisition. These six windows are explained in full detail in separate chapters of this manual. These six main windows may all be displayed simultaneously. They may overlap each other, but they will always be contained within the “V.A.S.E. for Windows” frame. The frame and the windows within the frame are resizeable and may be dragged and dropped in the usual Windows®98 manner. Of the six windows, only one will be active (highlighted). The active window can be selected by clicking anywhere inside the desired window. This will highlight the selected window and bring it to the front.

A useful window arrangement is shown in Figure 3.10. This arrangement allows all five windows used for data analysis to be viewed simultaneously. This arrangement is easily organized at any time by choosing the Window menu and selecting ‘Reset Window Layout’. Alternatively, a window can be selected from the Window menu which is always present at the top of the ‘VASE for Windows’ menubar.
This arrangement is only one of the infinite possible arrangements of the main windows. You will undoubtedly find your own preferred window configuration. If WVASE® When you exit WVASE® your configuration will be saved and used the next time you start the program.

### Summary of main window functions

In this section we summarize the main functions of each of the six WVASE® windows. Note that throughout this manual the first letter of the name of the six WVASE® windows will be capitalized (i.e. Experimental Data window, Model window, etc.) when referring to that window.

**Experimental Data window**

The Experimental Data window contains the experimental data being used by WVASE® at any given time. Data acquired within the Hardware window is automatically placed in the Experimental Data window during acquisition. Options are provided in the Experimental Data window which allows the user to load and save experimental data files and select the range of wavelengths and angles of incidence which will be used by the WVASE® program for analysis.

**Model window**

The Model window is used to build an optical model for a given sample. When the Model window is active, the menubar contains options which allow the user to add and subtract layers of various types from the model, load and save models to disk, and set parameters in the model to be varied or held fixed during the analysis of experimental data.

**Generated Data window**

The Generated Data window contains any data (ellipsometric, reflectance, transmittance, etc.) which has been calculated by the WVASE® program based on the model specified in the Model window. Options provided by this window allow the user to load and save generated data files, set the ranges of wavelengths and angles
of incidence for which data is to be calculated, perform sensitivity calculations, and copy calculated data to the Experimental Data window.

**Graph window**

The Graph window is used to provide plots of the various sets of data used by the program. Options provided in this window allow the user to select which set of data (experimental, generated, optical constants) and what type of data (\(\Psi\) and \(\Delta\), reflectance, transmittance, pseudo-optical constants) will be plotted. Both experimental and calculated data can be viewed simultaneously such that you can monitor the quality of a fit during data analysis. Also, the entire contents of the Graph window can be copied directly to the Windows\(^{®}\) XP clipboard for use in other Windows\(^{®}\) XP applications.

**Fit window**

The Fit window contains no visible data, but provides many of the most important features in the WVASE\(^{®}\) program. Options provided by the Fit window pertain to the analysis of experimental optical data, and allow you to analyze the experimental data by varying parameters in the optical model defined in the Model window to best fit the experimental data. Statistics pertaining to the quality of the fit can be displayed, and the experimental data may be fit at all wavelengths simultaneously or one wavelength at a time.

**Hardware window**

The Hardware window is primarily used to acquire ellipsometric data. This window contains options which allow the user to initialize the ellipsometer hardware, align samples, calibrate the ellipsometer, and acquire experimental data for a given sample. Options are also implemented which allow the user to directly control the settings of the monochromator, filter wheel, and angle of incidence.

### 3.5 WVASE\(^{®}\) Navigation

**Menubars**

On the menubar, three menus, |Window, |Global, and |File are always present. The other menu items depend on which of the six main windows is currently active (highlighted). Only the |Window and |Global menus are constant. The items on the |File menu will change based on the active window. However, the Exit_WVASE item is always on the |File menu of every window.

---

*Figure 3-11. A WVASE\(^{™}\) menubar (from the Experimental Data window).*

---

The options available on the menubar will depend on which window is active.
Naming convention for this manual

Important

To facilitate use of this guide, a naming convention for menus and menu items is defined by example. For instance, the “File” menu with the Model window active is denoted Model|File, and the “Type” menu with the graph window active is Graph|Type. Note that the |Window and |Global menus require no window specification because they are always present. (Be advised that many menus, such as Model|AddLayer or Fit|Normal_Fit, directly cause an action without displaying a list of menu items.) The selectable items under the menus are similarly identified. The Open_Model item in the Model|File menu is denoted Model|File|Open_Model. The Experimental_Data item in the |Window menu is denoted |Window|Experimental_Data.

Universal Hot Keys in WVASE®

The following keyboard shortcuts are now available, independent of the active WVASE window:

- **Ctrl-A** Add Layer
- **Ctrl-D** WVASE Defaults
- **Ctrl-F** Normal Fit
- **Ctrl-G** Generate Data
- **Ctrl-I** Experimental Data Information
- **Ctrl-O** Open Experimental Data
- **Ctrl-R** Experimental Range Select
- **Ctrl-S** Fit Stats
- **Ctrl-T** Toggles between $\psi$, $\Delta$, $\varepsilon_1$, $\varepsilon_2$, $n$, $k$, Transmission*, Reflection*, %Depolarization*, & Current-Layer Optical Constants).

*If data are loaded selected in Experimental Data window.

Context Specific Pop Menus

Each WVASE window has been enhanced with context-specific “Pop Menus” that the user can access with a Right-click of the Mouse button.

For example:

Clicking right mouse button while the pointer is located within the Graph window will bring up a context-sensitive menu that includes all the features available in the pull-down menus at the top of the window.

However, if the pointer is inside the graph area, the pop menu includes the Edit 2D Graph Options & The Edit 3D Graph Options (Compare the left and right side of the following Figure).
The context sensitive pop-up menus are particularly useful in the WVASE Model window, where they facilitate the adding of simple-graded, functional-graded and anisotropic layers, and building Genosc layers from another layer.

The Context-specific pop-up menus for each window are discussed in greater detail within the chapter that describes that window.

**Recently used lists**

Up to twenty of the most recently used files are available at the bottom of the ‘File’ pull-down menus for the Environment, Data, Model, and Material files, as shown in Figure 3.13.

![Recently used lists](image)

**Mouse Scroll Wheel to Vary Model Parameters**

WVASE® incorporates the Mouse Scroll Wheel (Figure 3.14) to adjust fit parameters and re-generate the data automatically. In this manner, model parameters can be quickly adjusted to match experimental data before beginning a “Fit”. Two common uses of this feature:

1. Adjusting starting thickness (and other fit parameters) to values that will insure convergence of a “Fit”.

![Mouse Scroll Wheel](image)
2. Adjusting fit parameters to gain insight into how model variation adjusts the generated response.

![Mouse scroll wheel](image)

*Figure 3-14. Location of Mouse scroll wheel.*

**Adjusting Thickness**

To adjust thickness, position the mouse cursor overtop the Model Layer thickness (in this case 50nm) for SiO2_jaw. Then, begin rolling the mouse scroll wheel forward or backward to increase or decrease the thickness, respectively. Each time the thickness changes, the new curve for Generated Data is calculated and displayed.

![Model Window](image)

*Figure 3-15. To adjust thickness from model window, position the mouse arrow overtop the desired layer thickness in the model window as shown and rotate mouse scroll wheel.*

The thickness increases/decreases by a value $\delta_t$, based on the current thickness, as listed in the following table:

<table>
<thead>
<tr>
<th>Change in thickness ($\delta_t$)</th>
<th>STARTING THICKNESS 0 – 99.9 NM</th>
<th>STARTING THICKNESS &gt; 100 NM</th>
</tr>
</thead>
<tbody>
<tr>
<td>wheel only</td>
<td>0.1 nm</td>
<td>0.001 x current_value</td>
</tr>
<tr>
<td>with shift</td>
<td>1.0 nm</td>
<td>0.01 x current_value</td>
</tr>
<tr>
<td>with ctrl</td>
<td>1.0 nm</td>
<td>0.01 x current_value</td>
</tr>
<tr>
<td>with ctrl+shift</td>
<td>10.0 nm</td>
<td>0.1 x current_value</td>
</tr>
</tbody>
</table>

**Scroll-wheel adjustment of other fit parameters**

All fit parameters can be adjusted in a similar manner. However, this requires an additional step as additional fit parameters are not visible directly in the Model Window. For example, if the Cauchy A, B, and C terms are fit parameters, their values are not visible directly from the model (only upon opening the Cauchy layer).
To accommodate “scrolling” of additional fit parameters, access has been placed in the “Edit Fit Parameters” dialog box. First, set all parameters of interest as “fit” parameters in your model. Second, select ‘Edit Parms’ menu from the Fit window (Fit_window|Edit_Parms). You should see a dialog box such as shown in Figure 3.16.

![Figure 3.16. Edit Fit Parameters dialog box.](image)

Select the parameter you wish to vary in the list on the left (blue arrow, Figure 3.16). Then, place your mouse over the parameter value (red arrow). Scroll the mouse wheel up and down to adjust this parameter. The Generated data is automatically updated, so you will need to move this window out of the way of the Graph window before beginning. To increase the increment size of any parameter by a value of $\delta_{\text{parm}}$, use the SHIFT or CTRL+SHIFT buttons, and the (non-thickness) parameter will increases/decreases by a value as listed in the following table. Thickness parameters will always change according to the “Change in Thickness” table above.

<table>
<thead>
<tr>
<th>Change in (non-thickness) parameter ($\delta_{\text{parm}}$)</th>
<th>$\delta_{\text{PARAM}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>wheel only</td>
<td>0.001 x current_value</td>
</tr>
<tr>
<td>with shift</td>
<td>0.01 x current_value</td>
</tr>
<tr>
<td>with ctrl</td>
<td>0.01 x current_value</td>
</tr>
<tr>
<td>with ctrl+shift</td>
<td>0.1 x current_value</td>
</tr>
</tbody>
</table>

Each time the parameter changes, the new curve for Generated Data is calculated and displayed. If a parameter is beyond the region of interest and you want to reset it, enter the desired value in the box (red arrow, Figure 3.16) and press the ‘Change Value’ button.
3.6 Window menu

The Window menu is always available.

![Window menu](image)

Figure 3-17. The WVASE™ Window menu (available from all windows).

The Window menu is used to select which window is currently active. This menu is especially important if the window you want to activate has been closed or it is buried under other windows. There are seven items on this menu, six of which correspond to the six main windows.

1. Window\Model
2. Window\Graph
3. Window\Generated_Data
4. Window\Experimental_Data
5. Window\Fit
6. Window\Hardware

This menu, like the other menus, also supports short cut keys. The appropriate keystroke combination can be found by looking for the underlined letter in the menu name or menu item. For instance, Figure 3.17 shows what part of the WVASE™ screen might look like after typing <alt>-w. This same effect could have been achieved by clicking (left mouse button) on the word Window in the menu bar. From the figure, any of the six windows could be selected by pressing one of the letters underlined in the menu item, or by clicking on one of those items. Once selected, the menu could also be dismissed without making a selection by pressing the <esc> key. As an example, the Model window can be selected by clicking on the Window menu and then clicking on the Window\Model menu item. It could also be selected from the keyboard by typing <alt>-w to select the Window menu and then pressing 'm' to select the Window\Model option. Selecting Window\Reset_Window_Layout repositions the windows to match the arrangement shown in Figure 3.10.

3.7 Global menu

The Global menu is always available.

![Global menu](image)

Figure 3-18. The WVASE™ Global Menu (available from all windows).

The Global menu, as the name implies, deals with the larger configuration issues which are not specific to any particular window. The most commonly used item on this menu is the Global\Defaults item which allows you to specify working
units for thickness and wavelength, and to configure the memory allocation for WVASE®.

|Global|Help item

This item starts the on-line help feature. The on-line help and this printed user’s manual are essentially the same document.

|Global|Defaults item

This option brings up a dialog box like that shown in Figure 3.19.

![Image](image.png)

**Figure 3.19.** The dialog box opened by the |Global|Defaults menu item.

By setting the appropriate option buttons you can control the units used for layer thickness and for light wavelength. In this box, you can also determine whether optical constants will be expressed as a complex dielectric function (‘e1’ and ‘e2’) or as a complex refractive index (‘n’ and ‘k’).

The ‘Memory Allocation’ button allows the user to reconfigure the memory storage requirements. This button displays the four adjustable memory settings in a dialog box as shown in Figure 3.20. These can be very important options and an appropriate configuration will depend on the type of analysis being performed.

Recent versions of WVASE® will try to dynamically allocate memory based on the currently-loaded data set and other criteria. A typical configuration for a VASE® system is shown. In later chapters, suggestions will be made for different types of analysis as to how to adjust these settings.

![Image](image.png)

**Figure 3.20.** The dialog box is activated from the Memory Allocation button which is accessed from the |Global|Defaults menu item.

**Important**

WVASE® attempts to dynamically allocate based whenever a data file is opened. In most circumstances, changing the memory allocation will not remove the existing data, models, and graphs, but there are some circumstances where this is the case. If you set the allocation parameter values too large, the procedure will fail and WVASE® will terminate automatically.
WVASE® can take a large amount of memory from the computer, but more memory is fairly inexpensive and may well be worth it. This is especially true if you are trying to run WVASE® in conjunction with other applications, like Word for Windows®, which also use a large amount of memory. We suggest you use WVASE® in a Windows® XP environment that is not cluttered with a lot of different running applications. In addition to freeing up more memory, reducing the number of active applications can reduce the likelihood of the operating system crashing.

The ‘Material File Directories’ button allows the user to add directories to the Material files search path. This is useful when the user saves optical constant files (which are commonly) used to a directory other than the default WVASE® directories. When the user adds a file to a model, all directories in the search path are searched for the file. This is a time saving feature which, when used properly, eliminates the need to navigate to the specific directories to find a given material file.

|Global|Save_Current_Environment item

|Global|Save_Current_Environment menu option (see figure below) brings up a standard save dialog box that allows you to specify the file name and location. Environment files use the .env extension.

Environment files provide a convenient way to save the entire working environment of the WVASE® program. An “environment” includes everything in every window, including data, models, fit parameters, optical constants, etc. You can use this option can to quickly save your work and then return to the same point in your analysis, without having to manually rebuild the WVASE® environment.

Environments are a quick way to save your work part of the way through an analysis.

Compatibility of Environment files

Important: An Environment saved with one version of WVASE® is not necessarily compatible with every other version.

WVASE® environment files are usually forward and backward compatible with most of the recent WVASE® versions. However, the Woollam Company does not guarantee that an environment created using one version of WVASE® will be compatible with other versions. New features and other improvements are continuously being added to WVASE®, and some of the changes will not be compatible with older versions of the software.

Environments saved by versions before 2.989 are not compatible with later versions. Environments are intended to a convenient, but only intermediate, method of saving your work. Environments are never intended for long term archiving of information.

For complete forward compatibility use models (.mod files) and materials (.mat files) to save the data. If the user backups older versions of WVASE® whenever new versions are installed, old environments can then be opened using the appropriate backed-up version.
The user can also manually copy the correct WVASE® executable file into the same directory as the Environment file. This can be done whenever an environment file is saved. The WVASE® executable file, WVASE.exe, will be located in the \WVASE\ directory.

If you are unable to load an environment, you may contact the Woollam Company and we will try to help you.

**Global|Load_New_Environment menu item**

|Global|Load_New_Environment (see figure above) is the counterpart to the save option (green arrow in figure). When loading a new environment, the current environment is overwritten. Note that several of the most recently saved environments can be conveniently selected from a list located at the bottom of the Global menubar (see figure above).

When an environment is loaded or saved, the filename is displayed in the titlebar, which is located above the menubar in the WVASE® program window. When loading an environment file that was saved in a different WVASE® version, a Version Mismatch message box will appear (see next section).

When loading an environment file that was saved in a different WVASE® version, a Version Mismatch message box will appear (see figure below). It will ask, “Do you wish to proceed with the environment load anyway?”

![Version Mismatch](image.png)

*Figure 3-22. Environment Version Mismatch message box.*

Generally the user can simply select “Yes” and the environment file will load normally. This is because WVASE® environment files are usually forward and backward compatible with most of the recent WVASE® versions (see above).

**|Global|Run_WVASE_Tools item**

Selecting this option will allow the user to run any installed WVASE® tools. These are secondary programs which work in cooperation with WVASE® to perform a specific function.

**|Global|About item**

This item brings up a message box which displays the version number for WVASE® and for Windows® XP.

---

### 3.8 |File|Exit_WVASE item

Selecting this item is the standard way to terminate the program. The |File|Exit_WVASE command will always be present regardless of which window is currently active. A dialog box is used to confirm your intent. It is important that you have saved the models, graphs, and data files you care about before you respond “Yes”. Once you answer “Yes”, the current working environment is lost. However, the settings specified using the |Global|Defaults option, the window positions and sizes, and the important hardware settings are saved.
Chapter 4 Hardware Window: VASE®

4.1 Hardware window overview for VASE® systems

The Hardware window is used to acquire data.

J.A. Woollam Co., Inc. VASE® systems can be classified as either vertical systems (v-VASE®) or horizontal systems (h-VASE®), based on the sample orientation relative to the table top surface. For some of the measurement options, available from the Hardware window, the vertical and horizontal systems will operate slightly differently. These differences are noted where appropriate. The Hardware window for an M-XX system is significantly different and is covered in the next chapter.

The Hardware window is used to control the following elements of the VASE® system.

- Monochromator - used to set the probe beam wavelength.
- Goniometers - used to set the angle of incidence.
- Input polarizer - positions the input polarizer transmitting axis relative to the plane of incidence.
- Sample translator - (Optional) - allows automated acquisition of data at many points on a sample.

The exact configuration of your system is defined in a configuration file (hardware.cnf) which is stored in the c:\wvase directory. The syntax for this configuration file is described in detail in Appendix C.

Data acquired from the Hardware window is stored in the Experimental Data window. You are given the option of saving data immediately following data acquisition, or you may save the data at a later time by selecting the Exp_Data|File|Save_Exp_Data item with the Experimental Data window active.

Features displayed in the Hardware window

Figure 4.1 displays a typical Hardware window. The instrument status and current values of a number of instrument parameters are displayed.
The Hardware window displays a number of different features, which are listed below.

**Title bar**

The title bar identifies the Hardware window and displays status information when an instrument function is being performed.

**Motor position**

The primary moving elements of a VASE® system are stepper motor controlled. This section displays information as to where the WVASE® software "thinks" the motors are.

**Translator position**

For systems equipped with a sample translator, the current X-Y position of the sample stage is shown at the bottom of the Hardware window.

**Hardware window menubar**

As shown below, there are five items on the main menubar plus the |Window and |Global menus.

The general functions available from these menus are given in the following table. The specific actions which may be selected from the menus will be described in succeeding sections.
### Menu and Operation

<table>
<thead>
<tr>
<th>Menu</th>
<th>Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hardware</td>
<td>File</td>
</tr>
<tr>
<td>Hardware</td>
<td>Initialize</td>
</tr>
<tr>
<td>Hardware</td>
<td>Acquire Data</td>
</tr>
<tr>
<td>Hardware</td>
<td>Move</td>
</tr>
<tr>
<td>Hardware</td>
<td>Setup</td>
</tr>
</tbody>
</table>

### Summary of VASE® system options

The following list summarizes what effects some of the options listed above will have on the VASE® instrument and the Hardware window itself.

**Translator equipped systems**

For VASE® systems equipped with sample translators there will be an additional item on the Acquire_Data and Move menus. The configuration for a translator system is contained in the `hardware.cnf` configuration file. If the absence (or presence) of translator commands does not match your system, you may need to alter the `hardware.cnf` file. See Appendix C for information on how to do this.

**Infrared extended system**

VASE® systems may be optionally equipped with the IR extended option (InGaAs detector). For such systems, there are two detectors which must be calibrated. If WVASE® believes a second detector is present, there will be additional options available in the Hardware|Setup dialog box and for the Hardware|Acquire_Data|Calibrate item. If the absence (or presence) of second detector options does not match your system, you may need to alter the `hardware.cnf` file. See Appendix C for information on how to do this.

**PTI monochromator**

PTI monochromators require you to periodically keep WVASE® informed of the correct wavelength from the monochromator dial. Furthermore, the setting of the entrance slit on the PTI monochromator is manually controlled. If your system uses a PTI dual grating monochromator, then you should also be aware of the need for manual grating changes. You will need to maintain the proper grating identification and wavelength in the Hardware|Setup dialog box.

**CVI monochromator**

A CVI monochromator provides automated maintenance of the wavelength setting, grating setting, and slit settings. If your system uses a CVI monochromator, there will be additional Hardware|Setup items for controlling the slit width.
Common Hardware window message boxes

When working in the Hardware window, there are several dialog boxes which will appear with some regularity.

![Image of Replace existing Experimental Data? message box]

**Figure 4-3. Replace existing Experimental Data? message box.**

The "Replace existing Experimental Data?" message is encountered anytime you are starting acquisition of static spectroscopic data and data already exists in the Experimental Data window. If you do not want to overwrite data in the Experimental Data window you should use the ‘Cancel’ button. If you want to add new data to the existing data, then you should save the existing data (Exp_Data|File|Save_Exp_Data), acquire the new data (OK to replace), and merge the files in the Experimental Data window (Exp_Data|File|Merge_Exp_Data).

![Image of Save experimental data? message box]

**Figure 4-4. Save experimental data? message box.**

The "Save experimental Data?" message is encountered at the end of data acquisition scans. If you do not save newly acquired experimental data when the scan is completed, you can save it later using the Exp_Data|File|Save_Exp_Data menu item from the Experimental Data window.

4.2 Hardware|File menu

![Image of Hardware|File menu]

**Figure 4-5. The File menu from the Hardware window.**

The only option on the [File menu which is specific to the Hardware window is the Hardware|File|View_Log_File option. To save data acquired from the Hardware window use the Exp_Data|File|Save_Exp_Data option from the Experimental Data window.

**Hardware|File|View_Log_File item**

WVASE® maintains a log of many of the Hardware window functions. Initializations, calibrations, and some data acquisition are recorded in the log file. An example of the last few lines of the log file are shown below.
This log can be useful when comparing calibration constants from previous measurements. Under usual circumstances the ‘Attn’ calibration parameter should always stay the same, and the values of the ‘Ps’ calibration parameter should be very close to previous values. The ‘As’ calibration parameter values should change randomly after each hardware initialization.

Only the last 32000 characters are saved in the log file. Earlier information is discarded as newer log entries are added. The log file is saved in the \wvase directory as wvase.log. If you want to keep all information saved in the log file, you will need to periodically rename the log file. If wvase.log does not exist it will be created when the first entry needs to be logged.

### 4.3 Hardware|Initialize command

Before any data acquisition can occur the hardware must be initialized using the Hardware|Initialize command. When WVASE® is first started the Hardware window indicates the status of the instrument to be ‘Not Initialized & Not Calibrated’.

After starting the initialization process, the title bar changes to the following

During the initialization, the hardware.cnf configuration file is read, the analyzer motor is brought up to speed, the data acquisition is synchronized, and the monochromator is reset (CVI monochromators only).

When the initialization process is completed, WVASE® will ask for a user name to enter into the log file. The user name is only used for display in the log file.
4.4 Hardware|Acquire_Data menu

Always align the sample to obtain precise results!

Figure 4-10. The Acquire Data menu from the Hardware window.

These menu items represent all the main data acquisition options. The focusing probe items will only be visible if focusing probes were included with the ellipsometer system.

<table>
<thead>
<tr>
<th>Menu Item</th>
<th>Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Align_Sample</td>
<td>Used to align sample perpendicular to the probe beam.</td>
</tr>
<tr>
<td>Sample Z-Translation Alignment</td>
<td>Used to translate sample along z-axis (horizontally) so that its front surface is centered on sample stage axis of rotation.</td>
</tr>
<tr>
<td>Focusing Probe Alignment (also … Set#2) (if option is available with system)</td>
<td>Used to align focusing probes (visible only if option was included with system).</td>
</tr>
<tr>
<td>Calibrate_System</td>
<td>Used to calibrate polarizer offset, analyzer offset, and the detector attenuation.</td>
</tr>
<tr>
<td>Spectroscopic_Scan</td>
<td>Used to acquire ellipsometric data as a function of wavelength and/or angle.</td>
</tr>
<tr>
<td>Dynamic_Scan</td>
<td>Used to acquire time-dependent data at a few wavelengths and one angle of incidence.</td>
</tr>
<tr>
<td>R&amp;T_Data</td>
<td>Used to acquire intensity reflection or intensity transmission data.</td>
</tr>
<tr>
<td>Translation_Scan</td>
<td>(Optional) Used to acquire ellipsometric, reflection, and/or transmission data at multiple locations on one sample.</td>
</tr>
</tbody>
</table>

The use of these options is described in the following sections. For more insight into which data types, spectral ranges, and angles of incidence you should use for a particular sample, see chapter 12 - “VASE® Data Acquisition - Procedures and Strategies.”

4.5 Hardware|Acquire_Data|Align item

This menu item is used when mounting a sample for measurement. The alignment procedure ensures that the sample surface is placed perpendicular to the probe beam. Assuming the system is properly aligned, the angle of incidence will be correct to within the accuracy of the goniometers (±0.005°). The sample can be aligned to within 0.001° with respect to the probe beam.

The exact alignment procedure is slightly different for vertical and horizontal VASE® systems. However, the following general alignment procedure is common to both types of systems.
When the ‘Align’ menu item is selected, WVASE™ will prompt you to mount the sample and insert the alignment detector. Mount the sample and insert the alignment detector.

The sample surface must be oriented normal to the incident light beam. The computer controlled sample stage will move to 0° for alignment.

WVASE™ will move the monochromator to the ‘white light’ position, and dynamically display the alignment detector targeting crosshair.

The user must tilt the sample stage to center the alignment crosshair on the computer screen.

When the user cancels the alignment screen (by pressing <escape> or selecting Cancel from the menu) the computer returns the sample to the angle of incidence where it was prior to the alignment.

The user must translate the sample along its normal to center the reflected light beam on the detector iris.

After selecting the ‘Align’ item, you will be presented with a message box indicating that WVASE™ will expect a sample to be mounted and the alignment detector inserted. If this has not been done when this dialog box is closed, then the Hardware window will not display meaningful alignment data.

![Sample Alignment Message Box](image)

*Figure 4-11. Message box displayed at the start of the sample alignment procedure.*

If you do not cancel the alignment, WVASE™ will move the monochromator to the white light position. This will produce a visible probe beam for alignment.

For sample alignment, a special alignment detector is mounted in a socket just after the polarizer. (On most systems this is a removable unit.) The alignment detector is a four quadrant Si detector. A hole in its center allows the probe beam to pass through and strike the sample at normal incidence. The reflected beam (which is not perfectly collimated) returns and strikes the four elements of the detector. If an equal amount of light strikes all four detectors, the sample is aligned perpendicular to the probe beam. This assumes that the probe beam is uniform through its cross-section, any coatings on the sample are uniform, and there are no back-surface reflected beams reaching the alignment detector (which will not effect the alignment unless the top and bottom surfaces of the sample are not parallel).

The alignment screen shows the signal from each of the four detector quadrants. The signal is modulated by the beam chopper mounted on the monochromator. A crosshair indicates whether the reflected beam is too high or low, or too far left or right. The X-Y coordinates give a numerical representation of the beam location. By adjusting the tilt of the sample stage you should be able to position the crosshair at X=0±1, and Y=0±1. The Hardware window display of a properly aligned sample is shown below.
Figure 4-12. Typical Hardware alignment screen when aligning the SiO$_2$/Si calibration sample. The sample is very well aligned normal to the beam.

In the following figure, the alignment screen is shown with the sample stage deliberately rotated 0.01° away from normal incidence. Note that rotating the sample stage changes the X value approximately 7 units for each 0.01° of tilt. The exact amount of change depends upon the dimensions of the ellipsometer and alignment detector. Nevertheless, this demonstrates the extreme precision provided by this alignment technique.

Figure 4-13. Alignment crosshair with sample intentionally tilted 0.01° off normal.

The X-Y coordinates of the crosshair will exhibit a certain amount of random noise, typically ±0.3 along each axis. If the crosshair is jumping around more than that, you should check the ‘Gain’ value displayed on the top line of the window. If the gain value is 10 or greater then you probably are not detecting the probe beam at all. There are several things to check if this is the case.

- Is the alignment detector mounted securely in its socket?
- Is the sample oriented with a reflective surface facing the probe beam?
- Is the probe beam visible if you hold a piece of paper in front of it? The white light option is selected, and you should be able to see the beam. If the probe beam is not visible try homing the filter wheel ([Hardware]Setup[Home_Filter option]).
- Is the sample grossly misaligned such that you can visibly see the probe beam missing the alignment detector? If so, adjust the sample tilt as required to get the reflected probe beam to strike the alignment detector.
- Is the alignment detector cable plugged in?
• Is the electronics box (VB-200) turned on?

4.6 Hardware|Acquire_Data| Sample Z-Translation Alignment item

The Z-Translation alignment procedure is usually initiated automatically after exiting the tilt/alignment in the previous section. However, this menu item allows the user to initiate a z-axis alignment independently from the tip/tilt alignment.

The alignment procedure ensures that the sample surface is placed on the center of rotation of the sample stage, and that the probe beam will enter the center of the detector unit at all angles.

- When the ‘Sample Z-Translation Alignment’ menu item is selected, WVASE® will ask you to enter a Monochromator wavelength position, then a new angle of incidence. Under most circumstances, the default values of 500nm and 70° are acceptable.
- When the Z-Axis Alignment screen appears (see figure below), adjust the z-axis micrometer until the signal is maximized (red curve in figure).

![Figure 4-14. Z-Axis translation alignment screen.](image)

4.7 Hardware|Acquire_Data|Calibrate item

*Calibration is required prior to acquisition of ellipsometric data.*

Reflection and transmission may be measured without calibrating first.

The calibration procedure is used to align the transmitting axes of the polarizer and the analyzer relative to the sample plane of incidence. The calibration procedure also determines the relative gain of the DC and AC components of the rotating analyzer signal. The regression calibration procedure that WVASE® uses can be performed on any isotropic sample that does not depolarize the reflected beam. However, you may find it more convenient to use the calibration sample shipped with your VASE® system.

If the same calibration procedure is always performed on the same sample, it may be easier to detect system problems. In addition, always using the standard sample for calibration should maintain the confidence limits on the calibration parameters at relatively constant (and rather small) values. Previous calibration results can be examined in the log file (Hardware|File|View_Log_File) to evaluate long-term stability of the ellipsometer.
The analyzer and polarizer are stepper motor controlled and have defined "zero step" positions. Calibrating the system is necessary in order to find how the polarizer transmitting axis in the "zero" position relates to the plane of incidence of the sample. These polarizer offsets are internal to W\textsuperscript{VASE\textsuperscript{®}}, and are denoted ‘Ps’ (for the input polarizer) and ‘As’ (for the analyzer).

If the system has an IR extended detector then that detector will have its own As and Attn values, denoted ‘Ir-As’ and ‘Ir-Attn’. The calibration parameter ‘As’ also includes phase shifts induced by passage of the detector signal through the electronics, which may be different for the two detectors. The dominant component of the ‘As’ values is the physical location of the rotating analyzer, such that the values of ‘Ir-As’ and ‘Vis-As’ are generally close but not identical.

When and why to calibrate

When in doubt, calibrate. It does not require much time, and may save you a lot of time in the long run!

Each time you re-initialize the hardware you must calibrate the ellipsometer before acquiring ellipsometric data. The analyzer offset, ‘As’, is essentially a random number each time the system is initialized. Bringing the rotating-analyzer up to operating speed requires several motor steps and tracking every stepper motor pulse during the initial ramping of the motor is impossible. However, once the analyzer is rotating at operating speed, every step of the rotating analyzer motor is accounted for. This allows for a rotating analyzer system that operates with extreme speed precision, without the need for encoders to track the analyzer position. The calibrated ‘As’ values are essentially random after each hardware initialization, but should remain very stable (< ±0.02°) between initializations once the ellipsometer system has thermally stabilized (which usually requires 30-60 minutes from a cold start).

Between hardware initializations, the polarizer offset, ‘Ps’, should remain essentially the same. However, when the power is turned on or off it is possible for the stepper motors to pick up a few transient pulses. These transient pulses are undetectable by W\textsuperscript{VASE\textsuperscript{®}}, and as a result the ‘Ps’ value may change slightly between initializations, although it should not change significantly from calibration to calibration. You can examine the results of the most recent previous calibrations by viewing the log file (Hardware|File|View_Log_File).

The attenuation calibration constant ‘Attn’ is strictly a function of the electronic characteristics of the detector, and as such it should change very little from calibration to calibration. The attenuation may be slightly sensitive to the temperature of the system.

If you change the fiber or remount any of the input or detector elements you will need to recalibrate the system. (You may also need to perform a coarse calibration to relocate the polarizer.) Immediately after the power is turned on, there will be a slow drift as the system temperature reaches equilibrium. For the first few hours of operation, you may want to recalibrate every hour. Later you will need to recalibrate less frequently, perhaps once every four hours or so.

The calibration constants pertain to the ellipsometer, and you are not required to calibrate on each sample to be measured. See the discussion later in this section about the benefits of calibrating on the standard SiO\textsubscript{2}/Si sample provided with the W\textsuperscript{VASE\textsuperscript{®}} system, as opposed to calibrating on an unknown sample from which data are to be acquired.

Overview of calibration procedure

The following steps are required to calibrate the W\textsuperscript{VASE\textsuperscript{®}} instrument.
If the system is not aligned, you will need to perform the system alignment procedure. See chapter 12 - “VASE® Data Acquisition Procedures and Strategies” for means by which you can determine whether or not the system is fundamentally aligned.

If the hardware is not initialized you will need to initialize the system (Hardware|Acquire_Data|Initialize).

If the sample is not already aligned, you will need to align the sample to the probe beam (Hardware|Acquire_Data|Align) as described previously.

Acquire the calibration data using the Hardware|Acquire_Data|Calibrate menu item. See the next section for a description of the screen displays during acquisition.

Evaluate the quality of the calibration. See chapter 12 - “VASE® Data Acquisition Procedures and Strategies” for more information.

What happens during the calibration

During the calibration, the input polarizer is scanned over a range of positions with the polarizer optical axis on either side of the plane of incidence. The initial estimate for ‘Ps’ is taken from the most recent previous calibration. At each of the polarizer settings, the Fourier coefficients of the rotating analyzer signal are measured. The measured Fourier coefficient data are then fit to determine the calibration constants Ps, As, and Attn as well as the $\varphi$ and $\Delta$ for the sample.

If the system has an extended IR detector, then calibration data may also be acquired at a second wavelength within the range of the IR detector. On the dual detector system, the detectors that will be calibrated are selected using the Hardware|Setup|Current_Motor_Settings menu item.

The calibration dialog box

The parameters for controlling calibration data acquisition are entered in a dialog box like the following.

![Calibration Dialog Box](image)

Figure 4-15. Calibration dialog box for dual detector system.

During acquisition the Hardware window will display the percentage of points acquired until this percentage reaches 100%, at which point WVASE® will fit the calibration data, display the fit in the Graph window, and take appropriate action.
(described later) depending on the quality of the calibration fit. The following parameters may be set within the calibration dialog box.

**Calibration mode**

Selecting one of these two modes will set the other edit boxes in the dialog box to default values appropriate for that mode. A fine calibration is the typical calibration, but it requires that the previous calibrated Ps value is within about 20° of the new Ps value to be determined. If a large change in the correct Ps value is anticipated, you might use the coarse calibration mode which will span a wider range of polarizer settings to find Ps. If you perform a coarse calibration, make sure the sample has \( \psi < 45^\circ \) for the calibration wavelength. A coarse calibration should always be followed by a fine calibration.

**Revs per measurement**

This parameter determines how many analyzer revolutions will be averaged for measurement of the Fourier coefficients at each polarizer setting. The default values are 30 revs for a fine calibration and 10 revs for a coarse calibration. For a fine calibration, 30 revs is sufficient under most circumstances when using the calibration sample that comes with the VASE\(^\circledR\) system. However, if you find the resulting calibration to be noisy you may increase the number of revs. Increasing the revs to 50 would be typical. For a coarse calibration, there is no benefit to increasing the revs per measurement, since a coarse calibration should always be followed by a fine calibration.

**# of points**

The number of different polarizer settings at which the Fourier coefficients will be measured is displayed in this box. The default values for the different calibration modes are usually good. You can change this number if you want, but do not exceed 100 points.

**Degree span**

This is the range of polarizer settings over which data will be acquired. The minimum polarizer position will be \( \text{Ps} - (\text{Degree Span})/2 \) and the maximum will be \( \text{Ps} + (\text{Degree Span})/2 \). The last calibrated Ps value is assumed when setting the polarizer for the next calibration.

After the data is acquired, the Fourier coefficients are analyzed to determine Ps, As, and Attn for the system, and \( \psi \) and \( \Delta \) for the sample. For complete details on the regression calibration procedure see the section on calibration of the polarizer angles in chapter 2 - “A Short Course on Ellipsometry.” If necessary, a second As and Attn are found for the IR detector. The fit parameter results of the regression procedure are displayed in the WVASE\(^\circledR\) Log file (the Hardware_window|File|View_Log_File menu item is described in a previous section). A graph of the measured values and the model are displayed in the Graph window. (Like any data displayed in the Graph window, you can export the data to another application or a text file using items on the Graph|File menu. In the following figure, calibration results from the Graph window are displayed.)
Figure 4-16. Calibration fit for fine mode calibration, 10 revolutions per measurement. The true $Ps$ value was very near to the $Ps$ value from the previous calibration.

Figure 4-17. Calibration results for a coarse mode calibration when the $Ps$ value was very far from the previous measurement. The old $Ps$ value was approximately $Ps=189°$, and the new correct $Ps$ value is $Ps=99.098°$.

**Check the log file**

After a calibration you may want to check the log file to see how the results of the current calibration compare with those of previous calibrations. This is not essential to the operation of the VASE®, but can be helpful for troubleshooting.

Examine the log file and look for changes in $Ps$ from calibration to calibration. $Ps$ may change slightly ($< 1°$) from initialization to initialization, but larger changes often indicate that $Ps$ is very far from its true value. If $Ps$ is seen to change more than ~ $1°$ between initializations or calibrations, try performing a coarse calibration to absolutely determine $Ps$, then perform the fine calibration. Significant changes in $Ps$ from calibration to calibration may also be caused by misalignment of the sample on which the calibration is performed. It is always a good idea to align the sample on which you intend to calibrate very carefully.

Now examine the log file and look for changes in the value of the Attn calibration parameter from calibration to calibration which are larger than the error bar on Attn (displayed in the log file). This should only occur if calibrations were performed during the first hour (or so) after turning the system on, such that the system was drifting significantly between calibrations.

Finally, look for changes in $As$ from calibration to calibration (for the same initialization of the hardware) of more than about $0.01°$, as large changes in $As$ between calibrations may indicate hardware or sample alignment problems.
Evaluating the calibration results

After the calibration has been performed, you need to inspect the results. In this section, we discuss some of the things that can go wrong with a VASE® calibration.

Bad calibration

Some calibrations are simply incorrect. A sample which is very rough (depolarizes the probe beam) or an anisotropic sample are the two most common causes of a bad calibration. The calibration sample which comes with your VASE® system will not exhibit these problems.

The above bad calibration acquired from an anisotropic sample yielded the following results (located in Hardware log file).

- Final MSE: 48.18
- Psi: 17.227±0.26
- Delta: 64.367±1.19
- As: 174.21±0.962
- Ps: 99.297±0.36
- Attn: 0.9614±0.0236

A calibration which is this bad will bring up a calibration error dialog box similar to the following.

Figure 4-18. A bad calibration resulting from an anisotropic sample.

This dialog indicates that the error bars on the calibration parameters are above the acceptable limit and instructs the user to mount the standard SiO2/Si wafer supplied with every instrument and then perform a coarse and fine calibration.

Calibration error, but calibration OK

To determine if a calibration is in error, WVASE® gauges the final MSE from the regression fit to the calibration data. If the MSE is greater than 3, the calibration error dialog box is displayed. However, this dialog box does not always indicate that the calibration is in error. The reason this can occur is that even small systematic errors can make MSE large if the truly random errors on the measured...
Fourier coefficient data are driven toward zero. Furthermore, you can always reduce the random error by increasing the number of revolutions.

To demonstrate, we calibrated on the standard silicon sample at 500 nm wavelength and 75° angle of incidence. We repeated the calibration three times, averaging 30, 100, and 300 revolutions per measurement. All three calibrations yielded perfect fits (in the Graph window), identical calibration parameters, and nearly identical error bars on the calibration parameters. However, the final MSE increased from 1.427 for the calibration performed with 30 revs. per measurement to 2.848 for the calibration performed with 100 revs. per measurement, and reached 4.828 for the calibration performed with 300 revs. per measurement, a final MSE large enough to cause the calibration error dialog box to be displayed. In this case the calibration should be accepted in spite of the large MSE, as it is accurate.

**Check for polarizer off by 90°**

The regression calibration procedure can also produce an erroneous result if Ps has changed substantially since the last calibration. It is possible to find a Ps value which is off by 90° from the true value. If this occurs, the calibration data graph and fit parameters may look acceptable. However, if you try and fit ellipsometric data acquired with Ps off by 90°, you will see that generally Δ looks reasonable but ψ is reflected about 45°.

If you calibrate on the VASE® calibration sample at 500 nm and 75° angle of incidence, you can be assured that ψ < 45°. This means that if you see ψ > 45° in the calibration results displayed in the Fit window, you can be sure the calibration is incorrect. On other samples, it is harder to check for this problem because ψ may be > 45°. (i.e. a 100nm oxide on Si will have ψ>45° at wavelength=500nm).

The following example shows calibration results when Ps is off by 90°. Note that Psi=73.239° which is greater than 45°. Since these data were acquired on a VASE® calibration sample we know that Ps must be offset by 90°.

![Figure 4-20. Calibration example where Ps is in error by 90°.](image-url)

The results of the calibration fit shown above are listed below.
- Final MSE: 0.5594
- Psi: 73.239±0.0769
- Delta: 88.165±0.0491
- As: 55.638±0.0051
- Ps: 103.7±0.0825
- Attn: 0.96034±0.000231
If you suspect a calibration has yielded a Ps value which is offset by 90° from the true Ps value, perform a coarse calibration on a sample where \( \psi < 45° \) for the calibration wavelength and angle of incidence.

If the true Ps value has not changed more than about 20° since the last calibration, you should be able to calibrate on a sample exhibiting any \( \psi \) value (other than identically 0° or 90°). A movement of more than 20° by the polarizer axis since the last calibration indicates either a major change in the ellipsometer hardware or loss of a configuration file from the \( \text{wvase} \) directory.

Choice of calibration sample

*Calibrating on the ‘standard’ sample will always yield good results.*

The ‘standard’ calibration sample is a 3 inch diameter silicon wafer with a thermally grown SiO\(_2\) layer approximately 25 nm thick. This oxide is not sufficiently uniform to function as a thickness standard, however, it is a very good sample for performing precise system calibrations. We recommend always calibrating the \( \text{VASE}^\circledR \) system using the standard sample (or a similar thermally oxidized silicon wafer), as there are number of benefits to this practice.

First, you will always know the best wavelengths and angle of incidence to use for acquisition of the calibration data (500 nm and 75° for the UV-VIS detector, 1300 nm and 75° for the NIR detector), and you will know approximately what the calibration fit should yield for the \( \psi \) and \( \Delta \) values of the wafer if you always calibrate under the same conditions. The \( \psi \) and \( \Delta \) results may differ slightly due to the non-uniformity of the oxide film on the standard wafer.

A second important benefit to always performing calibrations on the standard sample under the same conditions is that this calibration will always yield very precise values for the calibration parameters (i.e. the error bars on the calibration parameters will be very small). The standard wafer is fairly reflective at 500 nm, and the signal-to-noise ratio for this measurement is very good.

The third benefit is that you will maintain roughly constant error bars on the calibration parameters, which will be the case provided you always calibrate on the same sample.

You may want to calibrate on the experimental sample if you will be performing long data acquisition on a sample and you can not tolerate remounting the sample (i.e. the sample is non-uniform). Because some drift of the calibration constants is possible, you may want to break the measurement into sections and recalibrate in between. Long acquisitions may occur if many revolutions, many angles, and/or many wavelengths are being used.

### 4.8 Hardware|Acquire_Data|Spectroscopic_Scan item

This menu item allows the user to acquire ellipsometric data at one location on a sample. For each of the chosen angles of incidence, the specified wavelength scan is performed. Spectroscopic scans can only be performed when the system has been calibrated. You will receive a warning message if data already exists in the Experimental Data window. The data from a spectroscopic scan will overwrite any data present in the Experimental Data window.

**The spectroscopic scan dialog box**

The scan options are entered in the dialog box shown below.
Figure 4-21. Dialog box used to control spectroscopic, variable-angle ellipsometric data scans. The wavelength units pull-down menu list is shown on the right.

The following items are present in the ‘Spectroscopic Scan’ dialog box.

**Wavelength range boxes**

The wavelength range boxes work in the current WVASE™ units shown on the right. (See |Global|Defaults.) The starting wavelength, ending wavelength, and wavelength step size are specified in these boxes. The units for the wavelength and step can also be selected via the pull-down list on the right (see Figure 4-23). A complete wavelength scan is performed for each of the specified angles of incidence.

**Angle range boxes**

The starting and ending angles of incidence and the angle of incidence step size are specified, in degrees, in these boxes. A complete wavelength scan is performed at each specified angle of incidence.

**Revs per measurement**

The value in this box specifies the number of analyzer revolutions to be averaged for each measurement point. Typically this is set to 10 to 50 revolutions. However, for certain low intensity spectral ranges and for some low reflectivity samples more than 100 analyzer revolutions may be averaged.

**Dynamic Averaging check box**

When checked, this activates the dynamic averaging feature. See Ellipsometric data acquisition options section below for a discuss of Dynamic Averaging.

**Settings Summary**

The current acquisition parameter settings are listed in the box in the lower left part of the spectroscopic scan dialog box.
More settings button

Selecting the ‘More Settings’ button will cause the Ellipsometric Data Acquisition Options dialog box to open. This dialog box is described in detail in the next section.

Save settings button

Selecting the ‘Save Settings’ button allows the user to save the current Ellipsometric Data acquisition settings in a .wmm file, for future use.

Open settings button

Selecting the ‘Open Settings’ button allows the user to load previously-saved data acquisition settings from a .wmm file.

Save File During Scan Interval

Selecting this option results in the experimental data being saved to file in time increments during the scan. The data is saved at the time increment specified in the text box next to the ‘Save File During Scan’ check box. This is very useful when the user is acquiring data for a long period of time (lots of wavelengths and/or lots of revs). If for some reason the scan is interrupted, the data taken up to the last save interval can be retrieved, so the entire scan does not have to be repeated.

Skip Wavelength Range: 1340-1450 nm

This option is useful when using an ellipsometer that has an IR extended detector in conjunction with a fiber designed for good throughput in the UV. The UV fiber has an absorption that occurs in the wavelength range 1340 nm to 1450 nm. Any data acquired in this wavelength region using the UV fiber will not be useful. Selecting this option results in the 1340-1450nm wavelength region being skipped. An IR optimized fiber (shipped with instruments with IR extended detectors) can be used to acquire good data over this region.

Cancel button

Cancels the spectroscopic scan and returns you to the Hardware window.

Ok button

Once a spectroscopic scan is started using the OK button, the wavelength and angle of incidence are set to the starting values and the scan begins. During a scan the Hardware window will look something like the following. The ψ and Δ values are displayed in the Graph window as they are measured.

Figure 4-22. Typical Hardware window display during a spectroscopic scan.

The top line of text in the Hardware window during the acquisition (as shown in the previous figure) shows the results and settings for the last measured point. Shown from left to right are: the angle of incidence (in degrees), the probe beam wavelength (current units), ψ ± σψ (degrees), Δ ± σΔ (degrees). The second line displays the polarizer setting, the slit width (not all systems), and the number of
Ellipsometric data acquisition options

Selecting the ‘More Settings’ button from either the spectroscopic scan or dynamic scan dialog box will cause the following dialog box to open.

![Ellipsometric Data Acquisition Options dialog box](image)

Figure 4-23. Ellipsometric Data Acquisition Options dialog box. The Sample Type pull-down list is shown on the right.

This dialog box is used to control the method by which the ellipsometer acquires ellipsometric data. The following items are available in the Ellipsometric Data Acquisition Options dialog box.

**Optical components box**

Options in this box allow the user to specify how the input polarizer is positioned for data acquisition. Options are present which control how the polarizer...
is positioned for data acquisition and how the variable retarder is used, if it is installed.

**Track polarizer option**

Selecting the ‘Track Polarizer’ option will cause the polarizer azimuth to be tracked to the psi value being measured, which minimizes errors in the measured data. Unless you have a good reason not to, always leave the polarizer tracking enabled for ellipsometric data acquisition.

**Fixed polarizer setting option**

Selecting the ‘Fixed Polarizer Setting’ option will cause the polarizer angle to be held fixed at the value specified by the user in the adjacent box during the acquisition of data.

**Zone average polarizer checkbox**

The third polarizer option, ‘Zone Average Polarizer’, will cause the measured data to be averaged over data acquired with the input polarizer positioned in each of the four quadrants. This can help to eliminate systematic errors due to errors in the knowledge of the polarizer calibration offset.

**Auto Retarder box**

This box is only available on systems with an installed auto-retarder option. The drop-down list box contains options for using the auto-retarder during a scan. The options are ‘Off’ and ‘High Accuracy’. If ‘Off’ is selected, the auto-retarder is not used for the measurement. If ‘High Accuracy’ is selected then data is acquired at five different positions of the retarder. This represents the most accurate data. One thing to note is that the Revs/Measurement value is divided between the different positions. For example, if ‘High Accuracy’ is selected and Revs/Measurement is set to 100, then each data point will consist of five 20 rev measurements.

**Revs/Measurement**

This is the number of analyzer cycles which will be averaged over for each measurement.

**Sample type box**

The various measurement types are described in some detail in the Ellipsometric data types section on page 6-6 of this manual.

This box is used to specify the type of measurement which will be performed. The most common measurement type is ‘Isotropic Sample’. This measurement assumes that an isotropic sample is being measured. There are several other types which are primarily for anisotropic samples. If an Auto-Retarder is installed depolarization measurement types will also be included in the list. The different options are described below.

**Isotropic Sample option**

When this option is selected, the standard ellipsometric parameters psi and delta are measured, based on the assumption that the sample Jones matrix is diagonal. This should be the case unless the sample is very rough or anisotropic.

**Isotropic + Depolarization**

This sample type is available if the ellipsometer has an auto-retarder installed. During acquisition both ellipsometric and depolarization data types will be stored in the Experimental data window. The depolarization can be used in the
modeling of layer thickness non-uniformity, patterned substrates, finite spectral bandwidth, finite angular bandwidth, and backside effects for transparent substrates.

**Slightly Anisotropic**

The Slightly Anisotropic mode works best if the Jones matrix representing the sample is dominated by the diagonal values $R_{pp} > R_{ps}$ and $R_{ss} > R_{sp}$. The mode assumes that the anisotropic effect is small enough that placing the Polarizer near the $\psi$ value is still a useful technique. Therefore tracking the polarizer is allowed for the anisotropic measurement mode

**Highly Anisotropic mode**

The Highly Anisotropic mode #1 is a regressed data type like the slightly anisotropic mode, but a fixed pattern of polarizer positions is used (-60°, -30°, 0, +30°, +60°, and +90°). This acquisition type can use the Auto-Retarder.

**Anisotropic (no regression)**

The Unregressed Anisotropic measurement mode was implemented early in the development of generalized ellipsometry. *Although this type can be used if light reaching the detector from the anisotropic sample is an incoherent mixture of light beams*, it is recommended that you use one of the Mueller-Matrix measurement modes instead.

The Unregressed Anisotropic mode is a robust anisotropic measurement mode, but it does not allow the Auto-Retarder to be used and the measured $\psi$ and $\Delta$ values do not have a direct Jones matrix representation. This anisotropic measurement mode acquires data with the polarizer set at +45°, -45°, 0° and 90° and then stores data of types E+45, E-45, E0, and E90. These stored-data are simply direct conversions of the measured $\alpha$ and $\beta$ values to $\psi$ and $\Delta$ with the polarizer set to the 4 values listed above. (For an explanation of $\alpha$ and $\beta$ and their relationship to $\Psi$ and $\Delta$, see Eqs. (2-27) and (2-28) in the “Jones matrix analysis of the rotating analyzer ellipsometer” section of Chapter 2.) These E+45, E-45, E0, and E90 data types can be modeled, but they do not have a direct physical significance.

**Mueller matrix mode**

For VASE® with AutoRetarder® instruments, the Mueller Matrix Mode measures the first 3 rows of the sample’s Mueller Matrix. The Mueller matrix data types are all real-valued quantities that describe how the sample transforms the Stokes vector of the incident light-beam. From the Mueller Matrix elements, WVASE® also automatically calculates and records the generalized ellipsometric parameters $AnE$, $Aps$ and $Asp$, as well as the Jones Quality factor $qJ$ data type.

**Dynamic averaging box**

This box contains options which allow the user to use dynamic averaging of the data rather than averaging over the same number of analyzer cycles at each measurement. Dynamic averaging lets WVASE™ determine the number of analyzer cycles to average by averaging the data until the standard deviation of the noise on the averaged data falls below some cutoff level. This should yield experimental data sets with roughly constant standard deviations, although it may not be possible to obtain the specified minimum standard deviation at each data point.

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2. The detected light beam can be a mixture of incoherent “sources” when, for example: (a) light is reflected from both the back and front sample surfaces, (b) thickness non-uniformity exists on one or more layers on the sample (especially for “thick” films $>$1μm), (c) the instrument spectrometer bandwidth is sufficiently wide that there are significant range of $\Psi$-$\Delta$ values across the band at each wavelength “step”, (d) beam focusing cause sufficient wide angle-of-incidence variation as to produce significant variations in $\Psi$-$\Delta$, and (e) the sample has patterning.
Dynamic averaging enabled check box

When this check box is enabled, the data acquisition will be performed with dynamic averaging of the measured data.

Maximum # of revs

This is the maximum number of analyzer cycles which will be averaged for any data point. If the maximum number of analyzer cycles is reached, the measured data are calculated from the averaged data, and the appropriate standard deviation (larger than the cutoff value for convergence of the dynamic averaging) will be stored with the data values in the Experimental Data window.

Threshold intensity

This is the minimum detector signal intensity for which dynamic averaging will be performed. If the detector signal intensity is less than this value, the maximum # of revs will be averaged for the given data point.

Min. Usable Intensity

This is the minimum intensity that must exist in order for a data point to be considered valid. If the intensity for a data point is below the minimum, the data point is skipped. The idea is to skip data points that would produce unusable data even if the full averaging was performed. This is primarily intended for DUV work and to skip over the IR absorption band near 0.87eV when using a UV enhanced fiber.

Monochromator slit width box

This box contains options which are only available for users with CVI monochromators, and allow the user to control the monochromator slit width used for data acquisition.

Max. slit width box

This is the maximum slit width which will be allowed at any data point during the scan. The maximum allowed value is 2000 mm.

Auto slit adjustment check box

If auto slit adjustment is not enabled, all data points will be acquired with the monochromator slit set at the value specified in the max. slit width box. If auto slit adjustment is enabled, the max slit width will be used at each data point unless the detector is overloaded. If a detector overload occurs, the slit width is decreased to half of its current value, and the measurement is repeated. This process is repeated until the slit width is small enough to prevent overloading of the detector, after which the measurement is performed. The slit width is then automatically increased at the next data point to provide the maximum possible signal without overloading the detector.

Principal Angle Scan

VASE systems can acquire (and graph) ellipsometric data in which the angle of incidence is automatically varied to maintain $\Delta \approx 90^\circ$ (or within any specified range) during the spectroscopic scan. This option is enabled checking the 'Enabled' box. The ‘Min.’ and ‘Max.’ boxes specify the tracking range for the measured Delta value, i.e., the angle of incidence will be adjusted until the measured Delta is within this range.
When the principle angle scan mode is enabled, the angle range values specified on the VASE Scan dialog box have different meanings: these values are used to guide the angle search algorithm. The starting and ending angles of incidence are used to bound the angle search range, the current angle of incidence is used to start the search, and the angle increment specifies the step size when searching for a $\Delta=90^\circ$ crossing (a bisection algorithm is used to narrow in on the correct angle after a $\Delta=90^\circ$ crossing is located).

**Transmission Measurement**

Selecting this option causes the ellipsometry measurement to be in transmission-mode. During measurement, the detector will remain fixed a $180^\circ$, and the resulting data will be marked as ellipsometric transmission data.

**Split Grating Changes Across Angles**

This option is used to speed data acquisition when using a CVI monochromator by acquiring data for all of the angles before switching gratings. (CVI monochromators take about three minutes to switch gratings.)

**Reset to defaults button**

Selecting this button will reset all options in the ellipsometric data acquisition dialog box back to their default values.

**Cancel button**

Selecting the cancel button will close the ellipsometric data acquisition dialog box, ignoring any changes made since it was opened.

**Ok button**

Selecting the Ok button will close the ellipsometric data acquisition dialog box and return the user to the spectroscopic (or dynamic) scan dialog box. The data acquisition settings box in the spectroscopic (or dynamic) scan dialog box will be updated to reflect any changes in the acquisition options.

### 4.9 Hardware|Acquire_Data|Dynamic_Scan item

*Dynamic scans are measurement of data as a function of time.*

You can also acquire time dependent ellipsometric data with a VASE© system. The acquisition speed will be limited by the scanning speed of the monochromator. You will only be able to use one angle of incidence. The wavelength range can be specified as a continuous range or as up to 9 discrete wavelengths. Running a VASE© in the dynamic mode is useful for slowly changing processes, but for high-speed and/or production line oriented measurements an M-XX system may be more suitable.

You will receive a warning message if data already exists in the Experimental Data window. The data from a dynamic scan will overwrite any data present in the Experimental Data window.

![Figure 4-24. Warning message when starting dynamic scan with data already present in the Exp_Data window.](image)
Selecting the ‘Yes’ button will cause the newly acquired data to be appended to the data already present in the Experimental Data window. Selecting the ‘No’ button will cause the newly acquired data to overwrite the data currently present in the Experimental Data window. Selecting the ‘Cancel’ button will cancel the dynamic scan and return to the Hardware window.

The dynamic scan dialog box

The options located on the left side of the Dynamic VASE Scan dialog box (highlighted by red rectangle in Figure 4-25) are the same as the standard VASE® data acquisition dialog box, which is described in detail in the previous section.

Figure 4-25. Dynamic VASE scan dialog box. The options on the left side of the box (highlight by red rectangle) are identical to the standard VASE® spectroscopic data acquisition options.

The following items are visible in the ‘Dynamic Scan’ dialog box.

**Grid vs. Discrete wavelengths**

The ‘Use Grid of Wavelengths’ button in the upper right corner of the Dynamic Scan Dialog box (figure above) activates the standard wavelength selection mode – the grid of wavelengths are set by the “Wavelength ___ to ___ by ___” entries in the upper left corner of the dialog box (figure above).

When the ‘Use Discrete Wavelength List’ button is selected, the ellipsometer acquires data at the wavelengths listed in the discrete wavelength list, located immediately below the button. Up to nine discrete wavelengths can be specified.

**Normal VASE Scan**

When the ‘Normal VASE Scan’ button is selected, the ellipsometer acquires only one data set using a single data acquisition scan – in other words, the data acquisition is identical to a static data acquisition described in the previous section. The data points do NOT contain a time stamp.

**Translator & Theta + Dynamic Scans**

The ‘Translator Scan’ and ‘Theta + Dynamic’ buttons are not used with the liquid cell attachment.
Dynamic Scan

When the ‘Dynamic Scan’ button is selected, the ellipsometer repeats the data acquisition scans (either Grid or Discrete List mode) over and over until Esc or Cancel are selected. A time stamp is added to each data point.

Minimum Cycle Period

‘Minimum Cycle Period (sec)’ value defines the minimum amount of time (in seconds) between data acquisition scans (either Grid or Discrete List mode). When the minimum cycle period is greater than the time required for a single data acquisition scan, then the program will wait the minimum time period before starting a new scan. When minimum cycle period is less than the time required for a single data acquisition scan (for example, Minimum Cycle Period (sec) = 0), the program will start a new scan immediately after the previous scan.

The effect of the minimum cycle period can be seen in Figure 4-26. On the left, only 3 scans were acquired in 4.5 minutes with a minimum cycle period equaled 120 seconds (2 minutes). On the right, 12 scans were acquired in 4.5 minutes when the minimum cycle period equaled 0 seconds. In this example, a single scan (@50 revs/meas with AutoRetarder) required 23 seconds (0.38 minutes).

Dynamic Fit

When the ‘Dynamic Fit’ button is selected, the program automatically fits the data after each scan is completed, using the current model. The user can view the dynamic parameter vs. time plot by right clicking in the Graph window and selecting Data|Point_by_Point_Fit_Parms. See Figure 4-27.
This option is selected if the user wishes to specify a wavelength range for the measurement, which will be repeated as a function of time. The wavelength range and increment need to be specified in the text boxes next to the ‘VASE Data’ button.

Note that the <Esc> key is used to stop a scan (as noted in the upper left corner of the Hardware window during a dynamic scan). If you stop a scan with the <Esc> key you will be given the option of saving the data acquired up to that point.

4.10 Hardware|Acquire_Data|R&T_Data item

This menu item is used to acquire intensity reflection and transmission data from a single point on a sample. You will receive a “Replace existing Experimental Data?” warning message after selecting this option if data already exist in the Experimental Data window. The data from a reflection or transmission scan will overwrite any data present in the Experimental Data window.

A VASE® system is capable of acquiring intensity reflection and transmission measurements; however this is a secondary function of the instrument and requires some care on the part of the user in order to obtain accurate data. Before making intensity reflection or transmission measurements a regular part of your sample analysis strategy, consult chapter 12 - “VASE® Data Acquisition Procedures and Strategies” in the Guide to Using WVASE® software manual for some insight as to when and why to use reflectance and transmission data.

When applicable, the most useful intensity measurement is normal incidence transmission. This data type provides information which is most complimentary to ellipsometric data, provided the sample is not completely opaque. Coincidentally, transmission is also the intensity measurement which is least susceptible to systematic errors.

At present, VASE® systems use the single beam technique, which requires a baseline scan and main data scan for the measurement of the reflection or transmission. The single beam technique is susceptible to errors due to fluctuations and/or drift of the light source intensity, so the baseline scan and main scans should be acquired in close succession.

Regardless of the measurement system or technique, relative intensity measurements are generally more susceptible to systematic errors than ellipsometric measurements. In ellipsometry, the baseline and data beams effectively propagate together. For ellipsometric measurements, there are almost no systematic errors due to fluctuations or drift of the light source intensity, to the throughput of the system optics, or to the detector collection efficiency.

With a VASE® system, normal incidence transmission measurements are the easiest intensity measurements to perform accurately. For this data type, the sample is simply inserted into the beam path after the baseline measurement, and, unless the sample is wedge shaped, the probe beam will not be deviated away from the detector. For transmission measurements at other than normal angles of incidence, the probe beam may be offset in passing through the sample, leading to a systematic error in the resulting transmission measurement.

Intensity reflection measurements require that the detector move between the acquisition of the baseline and main data scans. To obtain accurate reflection measurements, the probe beam must be collected in exactly the same way for both scans. See chapter 12 - “VASE® Data Acquisition - Procedures and Strategies” for tips on making accurate intensity measurements.
If your VASE® system has an IR extended dual detector unit, there is one more point to be aware of. The InGaAs detector used in the IR is physically much smaller than the silicon detector used in the UV and visible spectral regions. Because the probe beam and IR detectors are roughly the same size, intensity measurements on the IR detector are especially susceptible to systematic offsets.

The R&T scan dialog box

The reflection and transmission scan options are entered in the following dialog box.

![R&T scan dialog box](image)

*Figure 4-28. ‘R&T’ scan dialog box.*

The following items are visible in the R&T scan dialog box.

**Data acquisition mode**

All relative intensity measurements require both baseline and main data scans. However, you can use one baseline scan more than once. If you select the "baseline only" mode, the acquired data will be saved in the Experimental Data window. If you graph this data, you will see the intensity (in arbitrary units) for the spectral range specified. The "data only" mode will only be enabled when baseline data exists.

**Data type**

This is the data type that will be stored in the Experimental Data window. If you select either a p-polarized or an s-polarized data type, the polarizer will automatically be moved to 0° or 90° respectively. For general polarizer data types such as "uT" or "uRb", you can define the polarizer angle by entering a value in the ‘Polarizer Angle’ box, described below. Selecting the cross-polarized data types – for example, “ATps” (“ARps”) allows you to measure conversion of p-polarized incident light s-polarized light upon transmission (reflection). See Table below.
<table>
<thead>
<tr>
<th>Data Types</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>pT sT uT xT pR sR uR xR</td>
<td>Incident beam has one polarization state (p, s, u(^a) or x(^b)). All polarization states transmitted (or reflected) by the sample are measured.</td>
</tr>
<tr>
<td>ATpp ATps ATss ATsp ATuu ATux ATxu ARpp ARps ARss ARsp ARuu ARux ARxu</td>
<td>Incident beam has one polarization state (p, s, u(^a) or x(^b)). Only one polarization state (p, s, u(^a) or x(^b)) transmitted (or reflected) by the sample is measured.</td>
</tr>
</tbody>
</table>

\(^a\) User-defined polarizer azimuth taken from the ‘Polarizer Angle’ box described below.

\(^b\) \(x = u + 90^\circ, u = \) user-defined polarizer angle

User-defined polarizer azimuth taken from the ‘Polarizer Angle’ box described below.

If you are in the "data only" acquisition mode, the data type and polarizer setting for the baseline scan will be used. Both the baseline and main data scans must be taken at the same polarizer setting.

**Polarizer angle**

This is the polarizer angle used when acquiring one of the general data types such as "uT", "uR", “ATuu” and “ATux”, etc.

**Wavelength range & units boxes**

The wavelength range boxes work in the current wavelength units shown in the box on the right. The user can also choose different wavelength units from the pull-down menu in the units box. The starting wavelength, ending wavelength, and wavelength step size are specified in these boxes.

**Angle range boxes**

The starting and ending angles of incidence and the angle of incidence step size are specified, in degrees, in these boxes. The same spectroscopic baseline scan is used, regardless which incident angles are specified.

**Revs per measurement**

The value in this box specifies the number of analyzer revolutions to be averaged for each measurement. Typical values are from 20 to 60 revolutions. However, you might choose 100 revolutions or more for certain low intensity spectral ranges. You will probably want to average more revolutions for relative intensity measurements than you would for ellipsometric data on the same sample.
**Scatterometry**

The option should be set if the user wishes to scatterometry measurements. When this option is selected, the sample stage is set to the angle specified in the Angle section above, and the detector arm is scanned through the relative angle range. The relative angle range is (as the name implies) relative to the sample stage angle. For instance, if the sample stage is set to 75° for a reflection scatterometer measurement, then a relative angle range of –10° to 10° will result in the detector arm scanning from 140° to 160° (75° ± 10°).

**Translator Scan (deactivated for most systems)**

For VASE and VUV-VASE systems with sample translators. Contact J.A. Woollam for more information.

**Save Settings & Open Settings**

Once a desirable group of settings has been determined, the whole settings group can be saved to a file and then reloaded later using the Open Settings button and the Save Settings button.

**Change Settings button**

Selecting this button will open the “R&T Data Acquisition Options” dialog box (see Figure 4-29 below).

![R&T Data Acquisition Options dialog box](image)

**Figure 4-29.** ‘R&T Data Acquisition Options’ dialog box.

**Acquire baseline from reference sample**

Selecting this option will allow the user to acquire the baseline from a reference sample, such that the measured reflectance or transmittance will be with respect to the reflectance or transmittance of the reference sample, rather than absolute reflectance or transmittance.

**Baseline at special X-Y coordinate**

For VASE and VUV-VASE systems with sample translators. Contact J.A. Woollam for more information.
Go to white light for alignment

If this option is selected (i.e. the box is checked), the monochromator will move to the white light position for alignment of the probe beam to the detector prior to acquisition of the main data scan. If the sample is fully prealigned (see below), you do not need to use this option.

Use auxiliary detector

This option is only enabled for VASE® systems with an auxiliary intensity detector. If you are using an auxiliary detector, check this box and make sure the cables are properly connected.

Dynamic averaging box

This box contains options which allow the user to use dynamic averaging of the data rather than averaging over the same number of analyzer cycles at each measurement. Dynamic averaging lets WVASE® determine the number of analyzer cycles to average by averaging the data until the standard deviation of the noise on the averaged data falls below some cutoff level. This should yield experimental data sets with roughly constant standard deviations, although it may not be possible to obtain the specified minimum standard deviation at each data point.

Dynamic averaging enabled check box

When this check box is enabled, the data acquisition will be performed with dynamic averaging of the measured data.

Maximum # of revs

This is the maximum number of analyzer cycles which will be averaged for any data point. If the maximum number of analyzer cycles is reached, the measured data are calculated from the averaged data, and the appropriate standard deviation (larger than the cutoff value for convergence of the dynamic averaging) will be stored with the data values in the Experimental Data window.

Threshold intensity

This is the minimum detector signal intensity for which dynamic averaging will be performed. If the detector signal intensity is less than this value, the maximum # of revs will be averaged for the given data point.

Min. Usable Intensity

This is the minimum intensity that must exist in order for a data point to be considered valid. If the intensity for a data point is below the minimum, the data point is skipped. The idea is to skip data points that would produce unusable data even if the full averaging was performed. This is primarily intended for DUV work and to skip over the IR absorption band near 0.87eV when using a UV enhanced fiber.

Monochromator slit width box

This box contains options that allow the user to control the monochromator slit width used for data acquisition.
Permit Auto Slit Adjustment

When this option is checked, the monochromator slit will be adjusted to keep the intensity in the optimum range for the detector. This is useful when acquiring data where one or more of the lamps xenon lines are included in the wavelength range. At each wavelength, the program applies the same slit width for both the baseline and data acquisition.

The slit width is repeatable to within few \( \mu \text{m} \). This means that the slit width may not return to exactly the same width between the baseline and data scans. This is not a problem for single-wavelength measurements; where the slit remains fixed during acquisition of both the baseline and data. However, for multiple wavelength scans, auto slit adjustments can cause offset errors in Transmission and Reflection results. This is particularly true at wavelengths of high beam intensities, where the program might set the width to less than \( \sim 300 \mu \text{m} \). Baseline/Data Interleaving using a Grouping Time = 0 seconds will alleviate this problem by fixing the slit width for every wavelength (see ‘Interleave Baseline and Data check box’ section).

Max. slit width box

This is the maximum slit width which will be allowed at any data point during the scan.

Interleave Baseline and Data check box

The Interleave option enables the program to interleave the baseline and data acquisition scans, on a cycle set by the Grouping Time. Each “interleave group” consists of a background scan, followed by a data scan, then followed by another background scan. In order to determine the Transmittance or Reflectance values, the “true” background value is determined by interpolating between the two background scans. That “true” background value is then divided into the raw intensity values of the data scan.

During background data scans, the sample and detector stages are rotated to their “straight-through” positions (90° and 180°, respectively). VUV-VASE\textsuperscript{®} systems will also automatically translate the sample back at the same time. See “IMPORTANT NOTE for users of vertical VASE\textsuperscript{®} systems” below.

Important NOTE for users of vertical VASE\textsuperscript{®} systems

Users of vertical VASE\textsuperscript{®} systems must manually translate the sample back so that it is out of the beam path during the background scans. If normal-incidence Transmittance data are being acquired, then the Vertical VASE\textsuperscript{®} user can translate the sample back prior to the start of data acquisition. For other non-normal incident angles and data types (such as Reflectance), this will create errors in incident angles. This is not an issue for VUV-VASE\textsuperscript{®} system users (see above).

Grouping Time (sec)

This box enters the length of time allowed for the each of the two background scans as well as the data scan that makes up an Interleave Group. The larger the Grouping Time, the more wavelengths that will be included in each Interleave Group. A Grouping Time close to or equal to zero causes a baseline/data interleave at every wavelength. This takes longer but generally produces the most accurate results.

Scatterometry

The option should be set if the user wishes to scatterometry measurements. When this option is selected, The sample stage is set to the angle specified in the
Angle section above, and the detector arm is scanned through the relative angle range. The relative angle range is (as the name implies) relative to the sample stage angle. For instance, if the sample stage is set to 75°, then a relative angle range of –10° to 10° will result in the detector arm scanning from 85° to 65°.

### 4.11 Hardware | Acquire_Data | Translation_Scan item

These scans are only possible if you have an automated sample translator.

This option is only available on VASE® or M-44® systems equipped with a sample translator. This menu item is used to perform spectroscopic and/or variable angle measurements at different positions on the sample. Both ellipsometric and intensity reflection measurements can be performed at multiple sample locations.

**The translation scan dialog box**

A translation scan is configured using the following dialog box.

![Translation scan dialog box](image)

Figure 4-30. Translation scan dialog box. The VASE® Data acquisition mode with an X-Y mapping pattern is selected.

The following items are present in the ‘Translation Scan’ dialog box.

**Discrete wavelengths**

If this acquisition mode is selected, ellipsometric data will be acquired at the specified wavelengths. The number of wavelengths used is specified in the associated pull down selection box. Up to 9 wavelengths can be selected.

**VASE® data**

If this acquisition mode is selected, ellipsometric data will be acquired on a regular grid of wavelengths specified in the WvlBoxes. These boxes define the starting wavelength, the ending wavelength, and the wavelength step.
**Reflection/Transmission data**

If this acquisition mode is selected, relative intensity data will be acquired. This option is only enabled if a previously acquired baseline scan is available. Use the Hardware|Acquire_Data|R&T_Data to acquire the baseline. When the baseline data are acquired you will also be defining the wavelength set, the data type (reflection or transmission), and the polarizer setting for the acquisition of data. Performing a relative intensity translation scan can be thought of as performing a series of "data only" scans with using Hardware|Acquire_Data|R&T_Data, with the scans performed at different sample locations.

**Angles**

These boxes define what angles of incidence will be used at each translator location. These boxes define the starting and ending angles of incidence and the angle of incidence step size.

**Translator scan parameters**

This block is used to define the translator mapping pattern. In this section, you select the grid type (X-Y, or R-Theta) and the grid points. When the X-Y pattern is selected, the sample will be mapped on a rectangular X-Y grid. The starting X and Y positions, the ending X and Y position, and the X and Y direction step sizes are specified in the associated edit boxes. All values are given in cm.

When the R-Theta pattern is selected, the sample will be mapped on a polar R-Theta grid. For this pattern, you define starting and ending values and step sizes for R and Theta. R is defined in centimeters and Theta is defined in degrees. (If R=0 is included in the pattern, then the R=0 spot will be measured for each Theta value.) Note that an R-Theta scan is implemented using X-Y motion; the sample is not physically rotated.

**Data Acquisition Settings**

The currently selected options for the dynamic acquisition of ellipsometric data are displayed in this box.

**Change Settings**

Selecting this button causes the ellipsometric data acquisition options dialog box to open, allowing the user to change the data acquisition options. The ellipsometric data acquisition options dialog box is identical for dynamic or spectroscopic scans, and was described in the section titled Hardware|Acquire_Data|Spectorscopic_Scan.

**Revs/Meas**

This parameter specifies the number of analyzer revolutions to be averaged for each measurement.
4.12 Hardware|Move menu

Figure 4-31. Move menu from the Hardware window.

The items on this menu are used to directly reposition the VASE® system components.

**Hardware|Move|Monochromator item**

The dialog box shown below is displayed when this menu item is selected.

![Move Monochromator dialog box](image)

*Figure 4-32. Move Monochromator dialog box.*

**Enter new position**

In this editable text box, you enter the new desired wavelength. The current WVASE® wavelength units, displayed to the right, are set using the |Global|Defaults menu item. If you want to go to the white light position, use the White Light button; do not enter 0 for the wavelength.

**White light button**

Using this button moves the monochromator to the white light position.

*important*

If your system has a PTI monochromator, it is important that the internally stored WVASE® wavelength setting matches the actual dial reading on the monochromator. WVASE® will not intentionally move the monochromator past the mechanical limits of the monochromator, however, if WVASE® is misinformed as to the current dial reading, a mechanical limit could be exceeded. Exceeding the mechanical limit will most probably invalidate the wavelength calibration, but it may also destroy the internal mechanism of the monochromator.

**Hardware|Move|Angle_of_Incidence item**

The dialog box shown below is displayed when this menu item is selected.

![Change Angle of Incidence dialog box](image)

*Figure 4-33. Change Angle of Incidence dialog box.*
Enter new angle

In this editable text box, you enter the desired angle of incidence. Both the sample goniometer and the detector goniometer will move to the correct positions. Note this will only set the angle of incidence correctly if the goniometers are currently at the position \( \text{WVASE}^{\circledR} \) believes them to be. The internally stored \( \text{WVASE}^{\circledR} \) goniometer positions may be checked or reset using the Hardware|Setup|Current_Motor_Settings dialog.

Hardware|Move|Polarizer item

The dialog box shown below is displayed when this menu option is selected.

![Move Polarizer dialog box](image)

**Figure 4-34. Move Polarizer dialog box.**

Enter new position

In this editable text box, you may enter the desired polarizer angle. This angle is specified relative to the plane of incidence. The current calibration constant, \( P_s \), is used to determine the stepper motor offset. The polarizer will move to the specified position when ‘Ok’ is selected.

Hardware|Move|Translator item

This menu item is only available on \( \text{VASE}^{\circledR} \) systems equipped with a sample translator. The dialog box shown below will open when this option is selected.

![Move Translator dialog box](image)

**Figure 4-35. Move Translator dialog box.**

\( X \text{ in cm} \)

The desired \( X \) position (in cm.) is entered in this editable text box. This will be the radius if ‘R-T Coordinates’ is selected.

\( Y \text{ in cm} \)

The desired \( Y \) position (in cm.) is entered in this editable text box. This will be the angle theta if ‘R-T Coordinates’ is selected.
**X-Y & R-T Coordinates**

If ‘X-Y Coordinates’ are selected then the translation stage position is specified in Cartesian coordinates (x and y). If ‘R-T Coordinates’ is selected then the translation stage position is specified in polar coordinates (radius $r$ and angle $\theta$).

**Home stages button**

This button moves the translator in the negative X and Y directions until the limit switches are encountered.

The sample translator will move to the specified position when ‘Ok’ is selected. If this is not the case, check the translator settings in the configuration file `hardware.cnf` to ensure that they are correct.

---

### 4.13 Hardware|Setup menu

**Very important diagnostic options!**

The Setup menu from the Hardware window allows the user to check and/or modify the configuration of the VASE® instrument and hardware. Menu items are provided which allow the motor settings to be inspected and altered, the detector signal to be directly viewed, and the filter wheel position reset. The following list of options are available when the Setup menu is selected from the Hardware window.

![Figure 4-36. The Setup menu from the Hardware window.](image)

### Hardware|Setup|Current_Motor_Settings item

**Always check these settings before acquiring data. Incorrect settings will lead to bad data.**

The following items are present in the Current Motor Settings dialog box.

![Figure 4-37. Current Motor Settings dialog box.](image)
**Monochromator**

This box is only enabled when a PTI monochromator is part of the system. This box should contain the dial reading, not necessarily the actual probe beam wavelength. The actual wavelength is determined by the dial setting and the grating position. If the dial reading and the Monochromator setting do not match, **WVASE**® may try to move the grating past its mechanical limit. It is important to keep this setting current in **WVASE**®. With a PTI monochromator, you should check this setting each time you start **WVASE**® for data acquisition.

**Sample Stage or Source Stage**

This box contains the sample stage position (or Source stage position on an ellipsometer in the Horizontal configuration). All goniometer movements are relative, based on what **WVASE**® believes the current position to be. If this value does not match the actual dial reading for the stage, you may get an improper angle of incidence. There are limit switches on the sample stage designed to prevent mechanical damage. If the coarse degree reading matches, but the fine resolution dial on the stage is not exactly zero, see ‘Jog Buttons’ below.

**Detector stage**

This box contains the detector stage position. All goniometer movements are relative, based on what **WVASE**® believes the current position to be. If this **WVASE**® value does not match the actual dial reading for the stage, you may get the detector located in the wrong position for a measurement. There are limit switches on the sample stage designed to prevent mechanical damage. If the coarse degree reading matches, but the fine resolution dial on the stage is not exactly zero, see ‘Jog Buttons’ below.

**Auto home goniometers button**

This button is only enabled for horizontal **VASE**® systems. Selecting this button causes both the input and detector arms to find their home position by moving until they encounter the limit switches on the goniometers. This effectively calibrates the position of both arms.

**Jog buttons**

These buttons are used to move the sample stage or the detector stage one step at their finest resolution, 0.005°. When you turn the electronics box (VB-200) on or off, it is possible for a few spurious motor steps to be generated. The Jog Buttons may be used to zero the fine scale dials on the goniometers each time you turn the system on, however it is not critical that this be done. The detector arm only needs to be positioned within a few hundredths of a degree, so it is not strongly affected by a small offset on the dial. The sample stage motion is relative to the current position and the sample is aligned relative to the probe beam. Therefore, the angle of incidence is not affected if there is a slight offset on the sample stage dial.

If you have aligned a sample, using the sample stage Jog Button will invalidate that alignment.

**Grating position**

If you have a dual grating PTI system, this box is used to inform **WVASE**® as to which grating is currently selected. Any time you switch the grating you will need to change this setting. **WVASE**® uses the Grating Position in conjunction with
the Monochromator dial setting (at the top) to determine what the actual probe beam wavelength currently is.

**Slit width**

This option is only enabled when the monochromator has computer controlled slits (CVI Monochromator). This is the maximum width to which WVASE® will open the slits when attempting to increase probe beam intensity. If the automatic slit width adjustment is not enabled, this is the slit width used.

**Enable auto slit adjustment**

This option is only enabled when the monochromator has computer controlled slits (CVI Monochromator). When automatic slit width adjustment is enabled, WVASE® has some ability to adjust the probe beam intensity. By adjusting the intensity, some detector overload and low intensity conditions can be automatically eliminated.

**Detector system**

This option is only enabled for VASE® systems that have a dual detector unit. When both detectors are present you can control which detector(s) are calibrated with this setting. For instance, if you will not need to use the IR detector for a given data acquisition, you might select the UV-VIS option. Then when you calibrate the system, only the UV-VIS detector will be calibrated. If you have the UV-VIS & IR option selected, then both detectors will be calibrated when you use the Hardware|Acquire_Data|Calibrate_System command.

**Hardware|Setup|Display_Signal item**

This menu option allows you to examine the raw signal that WVASE® is acquiring. Immediately after selecting this item you will be presented with a dialog box where you enter the number of analyzer revolutions you want to average over. The signal is displayed, along with derived signal information, in a dialog box like that shown below. The signal display is updated whenever the specified number of analyzer revolutions have been averaged.

*Figure 4-38. Display Signal dialog box, after the system has been calibrated.*

The measured data values are shown as symbols. The corresponding ideally modeled signal is displayed as the continuous line. The acquired signal is double modulated. The high frequency modulation is due to the chopper. The desired rotating analyzer signal forms the envelope around the higher frequency.
The display includes data for the full 360° rotation of the analyzer. VASE® systems do not use a full featured lock-in amplifier. However, the combination of stepper motor driven chopper, a stepper motor driven analyzer, bandpass filtering, and digital signal analysis produce the same ability to remove noise sources at other frequencies.

**<Esc> exits**

This message in the upper left corner indicates that <Esc> key is used dismiss this dialog box and return to the main windows.

**Gain**

This is the current variable gain setting for the amplifier chain.

**Slit**

This is the monochromator slit width, for a system (CVI monochromator) with computer controlled slits.

**Chopper**

This is the magnitude of the Fourier coefficients at the chopper frequency. This is the DC rotating analyzer signal level value.

**Chop +2A**

This is the magnitude of the Fourier coefficients at the chopper frequency plus twice the analyzer frequency. This is the AC rotating analyzer signal value.

**alpha and beta**

These are the normalized Fourier coefficients, $\alpha$ and $\beta$, of the rotating analyzer signal. If the system has been calibrated since the last initialization, these $\alpha$ and $\beta$ values will have been corrected for calibration constants. If the system has not been calibrated, these will be uncorrected values. (Uncorrected values would be the same as corrected values if $Ps=0$, $As=0$ and $Attn=1$.)

**Psi and Delta**

The measured $\psi$ and $\Delta$ values for the displayed signal are shown if the system has already been calibrated.

**Hardware|Setup|Home_Filter item**

This menu option is usually only used when a problem has occurred with the order sorting filter wheel. On a VASE® system's monochromator there is a wheel containing several optical filters. These filters are used to prevent higher order wavelengths from appearing in the probe beam due to diffraction in the monochromator. For example, a filter is needed to prevent 1000 nm light from appearing in a 500 nm probe beam. WVASE® automatically tracks the position of this filter wheel to the currently selected wavelength.

Occasionally the filter wheel may lose tracking, or the configuration file may lose the appropriate home filter constant. When that occurs you will need to enter the appropriate value in the Home Filter dialog box, which appears when the ‘Home Filter’ option is selected.
Enter home filter constant

The value appropriate for your monochromator should be entered here. Usually the correct value will appear in the dialog box by default, and all you will need to do is use the OK button. If a zero appears in this box, it is almost certain that the configuration file containing this value has been lost. If you can not find your original system documentation with your correct filter constant, you can find it written inside the filter/chopper unit.
Chapter 5 Hardware Window: 
*M-Series*

5.1 Hardware window overview, *M-XX* systems

In this section we discuss the general functions associated with the Hardware window within WVASE® for *M-XX* systems. At the current time there are three basic *M-XX* system designs: the M-44, M-88, and M-2000. The M-44 and M-88 instruments are rotating analyzer ellipsometers with 44 and 88 wavelengths respectively. The M-2000 is a rotating compensator ellipsometer with anywhere from 150 to 1000 wavelengths depending on the version. The primary difference between rotating analyzer and rotating compensator ellipsometers is that a rotating analyzer instrument measures delta between 0° and 180° and a rotating compensator instrument measures delta between 0° and 360°. There are minor differences in the data acquisition and calibration dialogs for the two types of instruments. The menu structure is also different depending on whether the ellipsometer is used primarily for in situ or ex situ measurements. The basic differences will be addressed here but the best information for a specific system will be in that systems hardware manual.

5.2 Features displayed in the Hardware window

Figure 5.1 shows the appearance of the Hardware window after initialization of the hardware for a typical *M-XX* system.

![Figure 5-1. Typical Hardware window after initialization.](image)

The following features may be observed in figure 5.1.
**Title bar**

The title bar identifies the Hardware window and gives status information.

**Motor position**

The primary moving elements of a VASE® system are stepper motor controlled. This section presents information as to where the WVASE® software “thinks” the motors are.

**Calibration constants**

The calibration constants for the polarizer offset, analyzer offset, and detector attenuation are displayed.

**Hardware window menubar**

As shown in figure 5.2, there are five items on the Hardware window menubar, plus the |Window and |Global menus.

![Hardware window menubar](image)

*Figure 5-2. Menubar when Hardware window is active.*

The general functions available through these menus are listed in the following table. The specific actions will be described in succeeding sections.

<table>
<thead>
<tr>
<th>Menu</th>
<th>Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hardware</td>
<td>File</td>
</tr>
<tr>
<td>Hardware</td>
<td>Initialize</td>
</tr>
<tr>
<td>Hardware</td>
<td>Acquire Data</td>
</tr>
<tr>
<td>Hardware</td>
<td>Move</td>
</tr>
<tr>
<td>Hardware</td>
<td>Setup</td>
</tr>
</tbody>
</table>

**Common Hardware window message boxes**

When working in the Hardware window, there are several dialog boxes which will appear with some regularity.

![Common Hardware window message box](image)

*Figure 5-3. The Replace existing experimental data message box.*
The "Replace existing Experimental Data?" message shown in figure 5.3 is encountered any time you are starting acquisition of static spectroscopic data and data already exists in the Experimental Data window. If you do not want to overwrite the data in the Experimental Data window you should use the Cancel button. If you want to add new data to the existing data, then you should save the existing data (Exp_Data|File|Save_Exp_Data), acquire the new data (OK to replace), and merge the files in the Experimental Data window (Exp_Data|File|Merge_Exp_Data).

![Save experimental data message box](image1)

Figure 5-4.  The save experimental data message box.

The "Save experimental Data?" message shown in figure 5.4 is encountered at the end of data acquisition scans. If you do not save newly acquired experimental data when the scan is completed, you can save it later using the Exp_Data|File|Save_Exp_Data menu item from the Experimental Data window.

5.3 Hardware|File menu

![File menu](image2)

Figure 5-5.  The File menu from the Hardware window.

The only option in the File menu which is specific to the Hardware window is the Hardware|File|View_Log_File option. To save data acquired from the Hardware window use the Exp_Data|File|Save_Exp_Data option.

**Hardware|File|View_Log_File item**

**WVASE** maintains a log of some of the recently performed Hardware window functions. Initializations, calibrations, and some data acquisition are registered. An example of the last few lines of the log file are shown in figure 5.6.

![Log file](image3)

Figure 5-6.  Typical entries at the end of the log file.

This log can be useful when comparing calibration constants from previous measurements. Under usual circumstances the Attn and Ps calibration parameters should not change much from calibration to calibration. The As calibration parameter is a randomized number after each hardware initialization.
Only the last 32000 characters are saved in the log. Earlier information is discarded as newer log entries are added. The log file is saved in the `wvase` directory as `wvase.log`. If you want to keep all information saved in the log file, you will need to periodically rename the log file. If `wvase.log`, does not exist it will be created when the first entry needs to be logged.

### 5.4 Hardware|Initialize command

#### Figure 5-7. The Initialize option from the Hardware window.

You must initialize before calibrating or acquiring data.

Before any data acquisition can occur the hardware must be initialized using the Hardware|Initialize command. When WVASE® is first started the Hardware window title bar looks like the figure shown below.

#### Figure 5-8. The Hardware window title bar with the hardware un-initialized.

After starting the initialization process, the title bar changes to the following

#### Figure 5-9. The Hardware window title bar during hardware initialization.

During the initialization, the configuration file `hardware.cnf` is read, the analyzer motor is brought up to speed, the data acquisition is synchronized, and the monochromator is reset (if needed). When the initialization process is completed, WVASE® will ask for a user name to enter into the log file. The user name is only used for display in the log file.

#### Figure 5-10. The message box for user name entry.

### 5.5 Hardware|Align command

The Align menu does not contain any commands or dialog boxes. When this menu is selected the Hardware window is divided into four quadrants, and a crosshair will appear on the screen, as shown in figure 5.11. The system or sample can then be accurately aligned by centering the crosshair. The screen also displays the signals from the four quadrants of the alignment detector. When finished aligning, press the <Esc> key to close this screen.
The alignment screen.

![Alignment Screen](image)

**Figure 5-11.** The alignment screen with a positionally sensitive crosshair which allows the user to align the ellipsometer system or sample accurately.

## 5.6 Hardware|Calibrate command

*You must calibrate before acquiring ellipsometric data.*

The Calibrate menu will open a dialog box as shown in figure 5.12. The calibration procedure is divided into two parts: Normal & Coarse calibration and Straight-through calibration. The reason for this division is that some of the calibration parameters are sample/plane of incidence independent, while some are sample/plane of incidence dependent.

### The calibration dialog box

![Calibration Dialog Box](image)

**Figure 5-12.** The Calibration dialog box.

Parameters such as the signal phase shifts and signal intensity attenuations due to the electronic system, and the detector channel polarization sensitivities are plane-of-incidence independent. Therefore, these parameters are determined from the “Straight-through” calibration. The azimuths of the polarizer and analyzer, and the relative attenuation of the detector system, on the other hand, are plane-of-incidence dependent, and are calculated from the Normal/Coarse calibration.
In theory, the “Straight-through” calibration must be performed only once, when the instrument is first set up, and does not need to be performed every time the instrument is turned on. The calculated “Straight-through” calibration parameters are stored in the file motor_1.cnf and are used every time when the system is initialized. However, if this file is accidentally lost, or the “Straight-through” calibration is accidentally performed when the system is at a data-taking configuration with a sample in place, the “Straight-through” calibration must be performed in order to acquire data. Under normal operation conditions we still recommend that the user perform the “Straight-through” calibration occasionally (say every three months).

The “Normal/Coarse” calibration must be performed every time the system is turned on and data acquisition is to be carried out. The “Normal/Coarse” calibration can be performed with any sample, however, some samples, such as 900Å SiO₂ on silicon, tend to yield poor calibrations. In order to avoid problems, calibrate using the “Coarse” calibration mode on a “good” sample, such as 200-300Å of thermal SiO₂ on silicon. Then calibrate again using the “Normal” calibration mode with any sample (the sample under study, most likely).

Because the M-44® is primarily used in-situ, e.g., mounted on a vacuum chamber, it is usually not possible to conveniently change samples. In this case, the user should calibrate the system with a “good” sample on the multiple angle base which is a part of the M-44® system using the “Coarse” mode, and then mount the system back on the chamber to perform the “Normal” calibration on the sample in the chamber. Only the “Normal” calibration is needed later on if the WVASE® program has not been abnormally terminated while running the hardware due to a computer malfunction.

The following options and parameter settings are available within the Calibration dialog box.

**Normal**

Perform normal calibration when the instrument is in the data acquisition configuration. The “Degrees of Span” should be limited to less than 90°.

**Coarse**

Perform a coarse calibration when the instrument is in the data acquisition configuration. The “Degrees of Span” should be wide (more than 180°).

**Straight-through**

Perform the “Straight-through” calibration with the system input arm and output arm lining up such that the light beam leaves the input arm and proceeds straight into the detector unit. The “Straight-through” calibration is not needed every time the system is turned on.

**Revs per measurement**

One data point (ψ & Δ) can be determined every time the analyzer completes one revolution, however, the random noise on the measured data can be greatly reduced by averaging the measurements for many cycles of the analyzer. The more revolutions per measurement, the less noisy the data, but the longer the calibration process requires. The current analyzer speed is 25 revolutions per second, therefore, the M-44® can acquire data at 40ms per data array (one data array means the ψ and Δ of 44 different wavelengths in the spectrum the instrument covers, i.e., 44 ψ’s and 44 Δ’s).
# of points

The number of steps that the polarizer will take during the acquisition of the calibration data. The increment of steps will depend on the “Degrees of Span” discussed below. If the “Degree Span” is 90°, and the “# of Points” is 90°, then polarizer will move 90° steps with 1° increment during the calibration.

Degree span (of polarizer)

Defines the range (in degrees) over which the polarizer will be scanned. For the “Straight-through” calibration, 360° is recommended, while 180° is recommended for “Coarse” calibrations. A 90° span is usually sufficient for “Normal” calibrations.

Short wavelength / Long wavelength

Since the calibration process is carried out for all channels (wavelengths), the user may select either the shortest wavelength or the longest wavelength for the calibration to start at. In most cases, this choice will not affect the results of the calibration. Sometimes, depending on the random noise level, starting at one end of the spectrum may be better than starting with at the other.

Effect on other windows

The calibration process will affect the displays in the Experimental Data window and the Graph window. The calibration data will show up in the Experimental Data window, and the calibration data are plotted in the Graph window after the calibration process is finished. For the “Straight-through” calibration, the data plotted in the Graph window are shown in figure 5.13. Note that the X-axis represents the azimuthal angle of polarizer.

![Graph](image)

Figure 5.13. The “Straight-through” calibration data (of the starting channel) are shown in the Graph window.

The parameters calculated through the “Straight-through” calibration are the electronic phase shift (Eph), electronic attenuation (Attn), phase of polarization sensitivity (fd), and amplitude of the polarization sensitivity (Xp). These parameters are automatically stored in the file called motor_i.cnf.

The user may also view these data through the Graph window. To do this, activate the Graph window, and select ‘Point-by-Point Fit Parms’ from the ‘Data’ menu. A dialog box as shown in figure 5.14 will appear. A parameter may be selected from this list to be displayed as a function of the channel number (wavelength). The data may look like those shown in figures 5.15 - 5.18.
Figure 5-14. This dialog box allows the user to display the most currently calculated calibration parameters one at a time in the Graph window.

Figure 5-15. The electronic phase of each channel, from straight-through calibration.

Figure 5-16. The relative AC/DC attenuation of the signal from each detector channel, from straight-through calibration.

Figure 5-17. The magnitude of the polarization sensitivity of each channel of the detector array, from straight-through calibration.
The phase of the polarization sensitivity of each channel of the detector array, from straight-through calibration.

The “Normal” and “Coarse” calibrations have similar effects on the Experimental Data window and the Graph window. Figure 5.19 is typical for these types of calibrations. Because the calibration is carried out for all 44 wavelengths (the VASE® system calibration is done using only one or two wavelengths), the \( \psi \) and \( \Delta \) obtained through the calibration process are spectroscopic and can be plotted in the Graph window using the ‘Psi’ or ‘Delta’ options from the ‘Type’ menu in the Graph window. Figure 5.20 shows the spectroscopic \( \psi \) and \( \Delta \) obtained from a calibration procedure on a sample consisting of 25 nm of thermal SiO\(_2\) on a silicon wafer.
5.7 Hardware Ellipsometric Data command

Selecting this option will cause the dialog box shown in figure 5.21 to be displayed. This dialog box allows the user to acquire ellipsometric data in several different ways. The user can acquire a “single” scan data, meaning that spectroscopic data are acquired over the designated wavelength range. The user can also acquire dynamic real-time data with or without fitting the data in real-time. If the user wants to fit the data in real-time, an appropriate model must be built prior to the acquisition of data.

The ellipsometric data dialog box

![Ellipsometric Data dialog box](image)

Figure 5.21. The Ellipsometric Data dialog box.

The following items are present in the Ellipsometric Data dialog box.

Revs/meas

This text box specifies how many analyzer cycles will be averaged for each measurement. For the rotating analyzer ellipsometer, one data point (ψ & Δ) can be measured for each revolution of the analyzer. The current M-44° design rotates the analyzer 25 revolutions per second. Therefore, the fastest data acquisition rate is 40ms per data array (one data array means ψ and Δ of the 44 wavelengths in the designed spectral range). The faster the data acquisition rate, the more noise in the data. For in-situ applications, depending on the film deposition/removal rate, the user should average as many revolutions per measurement as possible to increase the signal-to-noise ratio.

Polarizer setting

For the M-44° system, the polarizer remains fixed during the acquisition of ellipsometric scans. Therefore, it is necessary to set the polarizer to a proper position to minimize systematic errors in the acquired data. The polarizer value should be set roughly equal to the average of the ψ values acquired over the entire spectrum. It is, of course, impossible to know the average of ψ before the data acquisition. The default value of 30° will usually provide good results.

Current angle of incidence

This parameter has no effect on the data to be acquired. However, the value shown in this text box will be recorded in the data file as the angle of incidence for each data point. When the data are analyzed, WVASe® will use this value to
calculate data from the optical model to compare with the experimental data. If the angle of incidence is not correct, \textit{WVASE}® will not be able to fit the experimental data well, or worse, will fit the data well and produce inaccurate results.

In order to accurately determine the angle of incidence, the user can fit the calibration data (if they are saved) first to find the angle of incidence, and then use this value for the real-time data analysis process. Alternatively, the user can define the angle of incidence as a variable parameter during a fit. To define the angle of incidence as a fit parameter, see chapter 6 - “The Experimental Data Window”. Keep in mind that the addition of more fit parameters usually leads to stronger correlations among the fit parameters, therefore, an independent means of determining the angle of incidence is preferred.

\textbf{Fit data to model in real-time}

The user can build a model and select this checkbox to fit the most current data that \textit{WVASE}® acquired. In this way, the user can directly view the changes of meaningful physical parameters such as layer thickness in real-time, rather than viewing the raw $\psi$ and $\Delta$ data which do not tell the user directly how the physical parameters are changing. Selecting this option may slow down the data acquisition.

\textbf{Don’t save dynamic data}

If this option is selected, only the most currently acquired data can be saved and all other previously acquired data will be overwritten and lost. The user should make sure that this box is not checked if dynamic data are to be saved. The advantage of this option is that it will allow the user to view the data without occupying large amounts of memory.

\textbf{Data type}

See ‘Data type’ in the ‘Range’ menu from the Generated Data window, discussed in chapter 8 - ‘The Generated Data Window’.

\textbf{Acquire single scan}

Selecting this button allows the user to collect a single spectrum of ellipsometric data. The data acquired in this way will be displayed as spectroscopic data. This is a very quick way to acquire data in a few seconds or less, and data in the entire designated spectral range may be collected.

\textbf{Update graph, every n points}

During real-time dynamic data acquisition, the data will be continuously plotted in the Graph window if this box is checked. The graph is re-plotted every $n$ measurements.

\textbf{Selected channels}

The 44 wavelengths at which the \textit{M-44}® may acquire data are listed in this box. By default, all of the wavelengths are highlighted (selected) so that data at all wavelengths are displayed in the Graph window. The user may select some of the wavelengths such that only the data at the selected wavelengths will be displayed in the Graph window. This is a very useful feature as it is usually very difficult to make sense of 44 curves on one plot.

Note that even if all of the 44 wavelengths are not selected, data will still be acquired at all 44 wavelengths, but are only displayed at the selected wavelengths. To select one wavelength, simply click the mouse on that wavelength in the listing.
To select more than one wavelength, press and hold the Ctrl key and click on the desired wavelengths, one at a time. If a sequence of wavelengths is to be selected, simply drag the mouse from one end of the sequence to the other.

**Effect on other windows**

The graph in the Graph window will be constantly re-plotted during data acquisition if the “Update graph” option is selected. Also, the data will be shown in tabular form in the Experimental Data window.

### 5.8 Hardware|Signal command

The signal menu allows the user to view the electrical signal from each of the 44 channels. These signals are the “raw” data that the M-44® actually measures. The user may view the signal from any individual channel, or the signals from all 44 channels may be simultaneously viewed. Selecting the Signal menu causes the following dialog box to be displayed.

You can view the signal from a single channel or from all channels simultaneously.

*Figure 5-22. The Signal dialog box.*

**Signal display options**

The following items are present in the Signal dialog box.

**Channel #**

Entering a channel number (0 to 43) to view the signal of that particular channel. Channel numbers 44, 45, 46, and 47 represent the four quadrant alignment detector channels. The signal will be displayed after clicking on the OK button, as shown in figure 5.23. Normally, the signal is a sinusoidal curve. Note that there are two curves displayed in figure 5.23. One of them, the dotted line, is the experimentally measured curve, and the other one is the best-fit curve. The two curves should lie on top of each other if the system is aligned correctly.

Note that the signal is displayed in the Hardware window instead of the Graph window. Other information is also displayed on the top of the Hardware window, such as the number of revolutions per measurements, the electronic gain, and so on. Press the <Esc> to exit this screen.
Detector signal from a single channel.

Figure 5-23. The signal from channel 6 of the detector array.

All channels

Click on this button to view the distribution of signal intensities from all of the channels. A typical intensity distribution is shown in figure 5.24. There are 48 dots across the screen. The one on the very left is from the channel 0 (the first channel) corresponding to the shortest wavelength. The four dots on the right of the screen represent the signal intensities of the four-quadrant alignment detector. If the system is aligned, these four dots should be at the same height (intensity). Note that the signal intensity distribution will depend very strongly on the spectral reflectance of the sample, and may not always resemble figure 5.24.

Detector signal from all channels.

Figure 5-24. A typical distribution of the channel signal intensities.

Gain

Select the electronic gain from this box if the Auto-Gain switch (see below) is not enabled. If the signal on some channels is very small, entering higher gain will help to view the weaker signals.

Auto switching

In order to use a different gain in the “Gain” box, Auto switching must be disabled. When the Auto switching box is checked, WVASE® will set the gain level according to the most intense signal of the 48 (44 + 4 alignment channels) channels. Note that Auto switching must be selected (checked) in order to calibrate the system and to acquire data.
Calc. DC offset

Clicking on this button will cause WVASE® to calculate the DC offset of all of the channel signals, and then subtract the DC offset from the signals. Clicking on this button causes a shutter in the lamp housing to close momentarily and then open again. When the shutter closes or opens, a clicking sound should be heard.

Polarizer

The azimuthal angle of polarizer.

Angle of incidence

This value will be recorded as the angle of incidence when data are saved to a file.
Chapter 6 The Experimental Data Window

6.1 Experimental data window overview

The Experimental Data window is used to store and manipulate experimental data. The Experimental Data window is used to load, save, and select experimental data for fitting. Most commonly the data will have been acquired using the WVASE® program, but it can come from any source as long as the proper format is used. (See Appendix B). The data in the Experimental Data window is not restricted to one type, and the Experimental Data window may contain any combination of ellipsometric, reflection, and transmission data, as well as any other data type supported by WVASE®. The most important function associated with the Experimental Data window is the selection of data for plotting and fitting.

The number of available data points (data rows) is limited by the Maximum # of Data Points as defined using the Memory Allocation button accessed by the |Global|Defaults command.

Features displayed in the Experimental Data window

A snapshot of a typical experimental data window with data present is shown in Figure 6.1.

Figure 6.1. A general Experimental Data window with non time-dependent data.
**Title bar**

If the experimental data has been read from or saved to a disk, the title bar gives the name of the file. However, when acquiring data the last filename will be used as a default until you save it. Thus it is possible to have data in the window that does not correspond to the filename as stored on the disk. Also, different experimental data files can be combined and only the last filename read in will be displayed. In the above example, the data file has been saved as `expdemo1.dat`. This data is also standard non time-dependent (static) data. If the data were time dependent, the title bar would look like Figure 6.2 indicating the presence of time-dependent (dynamic) data.

![Figure 6-2. An Experimental Data window with dynamic data.](image)

**Comment line**

Each data file has an optional comment line which appears above the tabulated data. This is typically used to indicate the sample name and other important measurement considerations.

**Scroll bar**

This is used to change which of the data rows are displayed.

**Selected column**

This column furthest to the left contains either the "#" symbol or nothing. The "#" symbol means that a particular data row is selected. Individual data rows can be deselected or selected, respectively, by clicking on the "#" symbol or clicking where it should be. Most data selection is done in large blocks by the `Exp_Data|Range_Selec` command.

**Type column**

This column contains the code for what type of data is in that particular row. Multiple data types can be mixed in the Experimental Data window. In the above examples, only normal ellipsometric data "E" is shown. The full listing of possible data types is given later (see The Different Experimental Data Types).

**Wavelength column**

This column contains the wavelength applied to this data row. The heading of this column is the current units for wavelength as set by the `|Global|Defaults` command. Data files saved to disk can be in any of the recognized wavelength units, but in an Experimental Data window the current global setting is used. Wavelengths, regardless of units, are rounded to 3 significant digits right of the decimal point.

**Angle column**

This column contains the angle of incidence that was assumed when the data was acquired.
Data columns

For each row two data values and two “error bars” (standard deviations) can be present. The number and meaning of these columns is dependent on the Type Column. For normal ellipsometric data, the first data column is $\psi \pm \sigma_\psi$ and the second data column is $\Delta \pm \sigma_\Delta$.

Time column

This is the time, in minutes, associated with measured data. Only dynamic data files have a time column which is shown to the right of the data column (5).

The Experimental Data window menubar

As shown in Figure 6.3 there are five menus on the main menubar plus the |Window and |Global menus.

![Menu bar when the Experimental Data window is active.](image)

The general functions of these menus are given in the following table. The specific action will be described in succeeding sections.

<table>
<thead>
<tr>
<th>Menu</th>
<th>Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exp_Data</td>
<td>File</td>
</tr>
<tr>
<td>Exp_Data</td>
<td>Range_Select</td>
</tr>
<tr>
<td>Exp_Data</td>
<td>Angles</td>
</tr>
<tr>
<td>Exp_Data</td>
<td>Delete_Data</td>
</tr>
<tr>
<td>Exp_Data</td>
<td>Change_Data_Type</td>
</tr>
</tbody>
</table>

Data from samples with transparent substrates

Samples with transparent substrates require special consideration!

The basic geometry of an ellipsometric experiment is described in chapter 2 - “A Short Course In Ellipsometry”. The simple geometry depicted in chapter 2 (Figure 2.2) ignores the part of the probe beam that is transmitted into the substrate. However, if the substrate is transparent it may not be acceptable to ignore the beam entering the substrate because part of that beam may be reflected from the sample’s back surface and be collected with the primary reflection.
The ellipsometer measurement system will simply convert the measured signal into $\psi$ and $\Delta$ values regardless of how many beams are collected. These effective values are not the same values as defined in the simple geometry and the problem becomes one of modeling the true measurement process. Many of the available WVASE® data types are included to account for these kind of substrate effects.

The reason that these backside reflections can not be treated in the same way as the multiple reflection within the layers on the surface is that the substrate is much thicker. Because the substrate is so thick, light passing through it loses coherence with light reflected from it. Within the layer stack on the surface, all the light from a single incident beam is treated coherently. Thus each of the multiple beams shown in the above figure include the coherent reflections due to interaction with the layered stack, but they do not add coherently from beam-to-beam. The exact mathematical treatment of the substrate effects is given in the chapter covering the Generated Data window.

One of the most direct methods of dealing with substrate effects is to eliminate them from the measurement process by roughening the back surface as shown in Figure 6.5.

This may not be possible for some samples and the substrate effects will have to modeled. In other situations, data can deliberately be acquired through the substrate to increase knowledge about the sample.
The experimental data types

WVASE® supports many types of optical data. The primary data types are standard ellipsometry, reflection intensity, and transmission intensity. These data types can be acquired by J.A. Woollam Co., Inc. VASE® and M-XX systems, however, data from other measurement instruments can also be analyzed. The proper file formats for experimental (and generated) data files are described in Appendix B.

The data type also includes information on how the measurement was performed, so that the proper calculation is performed when model generated data is calculated. The different data types are explained briefly in the following sections. The complete list of currently supported data types is presented, however, the vast majority of sample characterizations will only use three types: (1) Standard Ellipsometry “E”, (2) Backside Corrected Ellipsometry “Eb”, and (3) Intensity Transmission “pT”.

Figure 6-6. Data acquisition modes where data is deliberately taken through the substrate (transmission ellipsometry).

Figure 6-7. Data acquisition mode where the data are deliberately acquired in reflection from the back side of the sample (reverse-direction ellipsometry).
Ellipsometric data types

Users may need to change the data type after data acquisition, prior to modeling and analysis.

At the time of acquisition, the ellipsometer hardware is unable to distinguish among some of the multiple ellipsometric data types and by default will store the data as standard ellipsometric data, type “E” (i.e. Backside Corrected Ellipsometry “Eb” will be stored as Standard Ellipsometry “E”). However, for analysis purposes you may need to change the data type so that the model calculation will simulate the actual measurement process.

The parameters named $\psi$ and $\Delta$ are always used to define the measured complex ratio as:

$$\tilde{\rho} = \tan \psi e^{i\Delta}. \quad (6.1)$$

In the case of standard reflection ellipsometry, this ratio is $\tilde{R}_p / \tilde{R}_s$. For other data types, the ratio is used as described in the preceding section on samples with transparent substrates.

Standard Ellipsometry – types E, Eb Er, Et

The Standard Ellipsometry types are:

<table>
<thead>
<tr>
<th>Type</th>
<th>Mode</th>
<th>Data acquired from sample:</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>E</td>
<td>Reflection</td>
<td>Top side</td>
<td>No substrate backside effects will be included in the model calculations. If a layer with anisotropic optical constants is present, the optical axis for that layer will be assumed to be perpendicular to the surface of the sample.</td>
</tr>
<tr>
<td>Eb</td>
<td>Reflection</td>
<td>Top side</td>
<td>Substrate effects associated with a transparent substrate will be included in the model calculations. If a layer with anisotropic optical constants is present in the model, the optical axis for that layer will be assumed to be perpendicular to the surface of the sample. The calculation is not performed correctly if the substrate is anisotropic.</td>
</tr>
<tr>
<td>Er</td>
<td>Reflection</td>
<td>Back side</td>
<td>Only required when combined with data acquired from the top side of the same sample. Substrate effects will be included in the model calculations. If a layer with anisotropic optical constants is present, the optical axis for that layer will be assumed to be perpendicular to the surface of the sample. The calculation is not performed correctly if the substrate is anisotropic.</td>
</tr>
<tr>
<td>Et</td>
<td>Transmission</td>
<td>Top side</td>
<td>As with all transmission-type experiments, substrate effects will be included in the model calculations. If a layer with anisotropic optical constants is present, the optical axis for that layer will be assumed to be perpendicular to the surface of the sample. The calculation is not performed correctly if the substrate is anisotropic.</td>
</tr>
</tbody>
</table>

%Depolarization: depolE, depolEb, depolEr, depolEt

These data types quantify the %Depolarization of the sample, and are acquired during a “Ellipsometric + Depolarization” measurement. They are only acquired with the standard ellipsometric data types (E, Eb, Er or Et). The various Depolarization data types can be fit using the model non-idealities such as backsurface reflections, non-uniform films, non-zero bandwidth effects, angular spread and patterning.
<table>
<thead>
<tr>
<th>Type</th>
<th>Mode</th>
<th>Data acquired from sample:</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>depolE</td>
<td>Reflection</td>
<td>Top side</td>
<td>No substrate backside effects will be included in the model calculations.</td>
</tr>
<tr>
<td>depolEb</td>
<td>Reflection</td>
<td>Top side</td>
<td>Substrate effects associated with a transparent substrate will be included in the model calculations.</td>
</tr>
<tr>
<td>depolEr</td>
<td>Reflection</td>
<td>Back side</td>
<td>Only required when combined with data acquired from the top side of the same sample. Substrate effects will be included in the model calculations.</td>
</tr>
<tr>
<td>depolEt</td>
<td>Transmission</td>
<td>Top side</td>
<td>As with all transmission-type experiments, substrate effects will be included in the model calculations.</td>
</tr>
</tbody>
</table>

**Generalized Ellipsometry – types AnE, Aps, Asp including types ...b, ...t and ...r**

These Generalized Ellipsometry data types corresponding to three related complex ratios, and are acquired simultaneously using anisotropic measurement options. The Generalized Ellipsometry types calculate ratios from all four of the sample Jones matrix, normalized to \( \tilde{R}_{ss} \):

\[
J_{\text{sample}} = \begin{bmatrix}
\tilde{R}_{pp} & \tilde{R}_{sp} \\
\tilde{R}_{ps} & \tilde{R}_{ss}
\end{bmatrix} = \tilde{R}_{ss} \begin{bmatrix}
AnE & Asp \\
Aps \cdot AnE & 1
\end{bmatrix}
\]

\[
AnE = \frac{\tilde{R}_{sp}}{\tilde{R}_{pp}} = \tan(\Psi_{AnE}) e^{i \Delta_{AnE}} \tag{6.2}
\]

\[
Aps = \frac{\tilde{R}_{ps}}{\tilde{R}_{pp}} = \tan(\Psi_{Aps}) e^{i \Delta_{Aps}}
\]

\[
Asp = \frac{\tilde{R}_{ps}}{\tilde{R}_{pp}} = \tan(\Psi_{psE}) e^{i \Delta_{psE}}
\]

For transmission types \( \tilde{R} \) is replaced with \( \tilde{T} \) in the above equations. All three ratios are complex, so relative phase information is included. AnE is the “normal” ratio, and is equivalent to the standard ellipsometric measurement values for all isotropic and many anisotropic samples. The “p into s” ratio, Aps, is indicative of how p-light is converted into s-light relative to how p-light is reflected as p-light. The “s into p” ratio, Asp, is indicative of how s-light is converted into p-light relative to how s-light is reflected as s-light. The generalized ellipsometry types are:
<table>
<thead>
<tr>
<th>Type</th>
<th>Mode</th>
<th>Data acquired from sample:</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>AnE</td>
<td>Reflection</td>
<td>AnE = $\frac{R_{ss}}{R_{pp}}$</td>
<td>Top side</td>
</tr>
<tr>
<td>Aps</td>
<td>Reflection</td>
<td>Aps = $\frac{R_{ep}}{R_{pp}}$</td>
<td>Top side</td>
</tr>
<tr>
<td>Asp</td>
<td>Reflection</td>
<td>Asp = $\frac{R_{ep}}{R_{pp}}$</td>
<td>Top side</td>
</tr>
<tr>
<td>AnEb</td>
<td>Reflection</td>
<td>AnEb = $\frac{R_{ss}}{R_{pp}}$</td>
<td>Top side</td>
</tr>
<tr>
<td>Apsb</td>
<td>Reflection</td>
<td>Apsb = $\frac{R_{ep}}{R_{pp}}$</td>
<td>Top side</td>
</tr>
<tr>
<td>Aspb</td>
<td>Reflection</td>
<td>Aspb = $\frac{R_{ep}}{R_{pp}}$</td>
<td>Top side</td>
</tr>
<tr>
<td>AnEr</td>
<td>Reflection</td>
<td>AnEr = $\frac{R_{ss}}{R_{pp}}$</td>
<td>Back side</td>
</tr>
<tr>
<td>Apsr</td>
<td>Reflection</td>
<td>Apsr = $\frac{R_{ep}}{R_{pp}}$</td>
<td>Back side</td>
</tr>
<tr>
<td>Aspr</td>
<td>Reflection</td>
<td>Aspr = $\frac{R_{ep}}{R_{pp}}$</td>
<td>Back side</td>
</tr>
<tr>
<td>AnEt</td>
<td>Transmission</td>
<td>AnEt = $\frac{T_{ss}}{T_{pp}}$</td>
<td>Top side</td>
</tr>
<tr>
<td>Apst</td>
<td>Transmission</td>
<td>Apst = $\frac{T_{ep}}{T_{pp}}$</td>
<td>Top side</td>
</tr>
<tr>
<td>Aspt</td>
<td>Transmission</td>
<td>Aspt = $\frac{T_{ep}}{T_{pp}}$</td>
<td>Top side</td>
</tr>
</tbody>
</table>

**Mueller-Matrix Ellipsometry – types mm11, etc. including types …b, …r and …t**

These Mueller Matrix Ellipsometry data types corresponding to the Mueller Matrix elements, and are acquired simultaneously using the Mueller matrix measurement options. The Mueller matrix data types are all real-valued quantities.
that describe how the sample transforms the Stokes vector of the incident light-beam. The Mueller matrix is:

\[
M_{\text{sample}} = \begin{bmatrix}
    m_{11} & m_{12} & m_{13} & m_{14} \\
    m_{21} & m_{22} & m_{23} & m_{24} \\
    m_{31} & m_{32} & m_{33} & m_{34} \\
    m_{41} & m_{42} & m_{43} & m_{44}
\end{bmatrix}.
\]

(6.3)

The \(m_{11}\) element represents the total intensity reflection or transmission of the sample. WVASE records other 15 Mueller matrix quantities “\(m_{jk}\)” normalized to \(m_{11}\), so they always range between -1 and +1.:

\[
m_{jk} = \frac{m_{jk}}{m_{11}}, \quad j, k = 1, 2, 3, 4.
\]

(6.4)

WVASE reports \(m_{12}, m_{13}, \ldots m_{14}\), and they are correctly plotted when the Type|Psi or Type|Delta are selected. The \(m_{11}\) element is only directly recorded during an M-2000® R|T scan, and is plotted using the Intensity Reflection or Transmission Type. See the “Reflected intensity data types” and Transmitted intensity data types” section for further details.

<table>
<thead>
<tr>
<th>Type</th>
<th>Mode</th>
<th>Data acquired from sample:</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>(m_{11}) ... (m_{44})</td>
<td>Reflection</td>
<td>Top side</td>
<td>(m_{12}, m_{13}, \ldots m_{14}) are all normalized to (m_{11}).</td>
</tr>
<tr>
<td>(m_{11b}) ... (m_{44b})</td>
<td>Reflection</td>
<td>Top side</td>
<td>Backside-corrected MM data. (m_{12b}, m_{13b}, \ldots m_{14b}) are all normalized to (m_{11b}). Substrate effects will be included in the model calculations.</td>
</tr>
<tr>
<td>(m_{11r}) ... (m_{44r})</td>
<td>Reflection</td>
<td>Back side</td>
<td>Reverse-side MM data acquired from reverse side of sample. (m_{12r}, m_{13r}, \ldots m_{14r}) are all normalized to (m_{11r}). Only required when combined with data acquired from the top side of the sample. Substrate effects will be included in the model calculations.</td>
</tr>
<tr>
<td>(m_{11t}) ... (m_{44t})</td>
<td>Transmission</td>
<td>Top side</td>
<td>Transmission MM data. (m_{12t}, m_{13t}, \ldots m_{14t}) are all normalized to (m_{11t}). As with all transmission-type experiments, substrate effects will be included in the model calculations.</td>
</tr>
</tbody>
</table>

**Jones Quality factor: \(q_J, q_{Jb}, q_{Jr}, q_{Jt}\)**

The \(q_J\) or “Jones quality factor” data types are always acquired whenever general Mueller Matrix data are acquired. The \(q_J\) data type is a quantitative measure of how closely experimental Mueller matrix data can be described by a Jones matrix. The \(q_J\) value is calculated by finding the Jones matrix which has a Mueller matrix representation closest to the measured Mueller matrix values. The Jones quality factor is the "average" difference (root-mean-square) between the measured Mueller matrix values and the Mueller matrix values for the "closest" Jones matrix representation.

Mathematically all Jones matrices have a particular Mueller matrix representation, but the reverse is not true. For experimental values with measurement noise included, measured Mueller matrix values will not exactly correspond to any particular Jones matrix, even if the sample is essentially describable as a Jones matrix. If a sample is non-depolarizing, it can be described by a Jones matrix.
(isotropic or anisotropic). If a sample produces depolarized light upon reflection or transmission, then a Jones matrix will not completely describe the sample.

- For depolarizing ISOTROPIC samples, WVASE® uses a $\Psi$, $\Delta$, %Depol representation which is similar to the standard non-depolarizing $\Psi$-$\Delta$ representation.
- For ANISOTROPIC samples that depolarize upon reflection or transmission, a general Mueller matrix measurement is probably needed. However, with anisotropic samples there is no simple way to handle depolarization with a single %Depol value as can be done for isotropic samples. This fact also makes it hard to know whether a particular situation only requires anisotropic AnE, Aps Asp measurements, or anisotropic + depolarization – i.e., Mueller Matrix measurements.

If the measured Mueller matrix exactly corresponds to a Jones matrix, then theoretically the $qJ = 0$. With noise included, $qJ$ values are typically similar in magnitude to the noise of the measured Mueller matrix elements. $qJ$ data acquired during a Mueller Matrix measurement of ~25nm thermal oxide on silicon sample suggests that typical instrument errors for $qJ \leq \pm 0.001$. Also, since Mueller matrix elements are effectively bounded by ±1, the maximum $qJ$ value is effectively bounded to something less than 1.

$qJ$ data are not used during the fit process.

Unlike the Depol data for isotropic data, the $qJ$ data are NOT included during fitting, because the calculation speed for $qJ$ data is somewhat slow. If $qJ$ data exists in the experimental window, the final generation of a fit will also place generated $qJ$ data in the generated window. However, misfits between generated and experimental $qJ$ data do not affect the MSE value.

It is generally recommended that if anisotropic data are required for analysis, that general Mueller matrix measurements are used, at least during the initial data acquisition process for a given sample set. Since the general Mueller matrix measurement also reports the Jones matrix values of AnE, Aps and Asp, one gets both sets of data in about the same amount of time. And since the $qJ$ data are included, the user can make a more objective determination about whether the Mueller matrix data is required or whether the Jones matrix data is sufficient.

Please note that if depolarization is required to model the sample, the Jones matrix data (AnE,Aps, and Asp) should NOT be included in the fit because the Jones matrix data measurement assumed (wrongly) that the sample was non-depolarizing.

Unregressed Anisotropic Ellipsometric data types E+45, E-45, E0, and E90

The Unregressed Anisotropic measurement mode was implemented early in the development of generalized ellipsometry. This type can be used if light reaching the detector from the anisotropic sample is an incoherent mixture of light beams. However, it is recommended that you use one of the Mueller-Matrix measurement modes for samples that generate incoherent mixtures of light.

---

2. The detected light beam can be a mixture of incoherent “sources” when, for example: (a) light is reflected from both the back and front sample surfaces, (b) thickness non-uniformity exists on one or more layers on the sample (especially for “thick” films $>1 \mu m$), (c) the instrument spectrometer bandwidth is sufficiently wide that there are significant range of $\Psi$-$\Delta$ values across the band at each wavelength “step”, (d) beam focusing cause sufficient wide angle-of-incidence variation as to produce significant variations in $\Psi$-$\Delta$, and (e) the sample has patterning.
The Unregressed Anisotropic mode is a robust anisotropic measurement mode, but it does not allow the Auto-Retarder to be used and the measured $\Phi$ and $\Delta$ values do not have a direct Jones matrix representation. This anisotropic measurement mode acquires data with the polarizer set at $+45^\circ$, $-45^\circ$, $0^\circ$ and $90^\circ$ and then stores data of types $E_{+45}$, $E_{-45}$, $E_0$, and $E_90$. These stored data are simply direct conversions of the measured $\alpha$ and $\beta$ values to $\Phi$ and $\Delta$ with the polarizer set to the 4 values listed above. (For an explanation of $\alpha$ and $\beta$ and their relationship to $\Phi$ and $\Delta$, see Eqs. (2-27) and (2-28) in the “Jones matrix analysis of the rotating analyzer ellipsometer” section of Chapter 2.) These $E_{+45}$, $E_{-45}$, $E_0$, and $E_90$ data types can be modeled, but they do not have a direct physical significance.

WVASE reports $\Phi_{pol}$ and $\Delta_{pol}$ for each polarizer angle (pol) of $0^\circ$, $+45^\circ$, $-45^\circ$ and $90^\circ$. $\Phi_{pol}$ and $\Delta_{pol}$ are defined by the equation:

$$\tan(\Phi_{pol})e^{i\Delta_{pol}} = \tan \left( \frac{E_{+pol}}{E_{-pol}} \right) e^{i\left( \delta_{pol}^{+} - \delta_{pol}^{-} \right)}, \text{ where} \quad (6.5)$$

$$\begin{bmatrix} E_p \\ E_s \end{bmatrix} = \begin{bmatrix} \hat{R}_{pp} & \hat{R}_{sp} \\ \hat{R}_{ps} & \hat{R}_{ss} \end{bmatrix} \begin{bmatrix} \cos P \\ \sin P \end{bmatrix} = \begin{bmatrix} \hat{R}_{pp} \cos P + \hat{R}_{sp} \sin P \\ \hat{R}_{ps} \cos P + \hat{R}_{ss} \sin P \end{bmatrix}$$

<table>
<thead>
<tr>
<th>Type</th>
<th>Mode</th>
<th>Data acquired from sample:</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_0$, $E_{+45}$, $E_{90}$</td>
<td>Reflection</td>
<td>Top side</td>
<td>Measurements assuming no backsurface or reverse-side effects .</td>
</tr>
<tr>
<td>$E_{0b}$, $E_{+45b}$, $E_{90b}$</td>
<td>Reflection</td>
<td>Top side</td>
<td>Backside-corrected MM data. $m12b$, $m13b$, ... $m14b$ are all normalized to $m11b$. . Substrate effects will be included in the model calculations.</td>
</tr>
<tr>
<td>$E_{or}$, $E_{+45r}$, $E_{90r}$</td>
<td>Reflection</td>
<td>Back side</td>
<td>Reverse-side Unregressed Anisotropic Ellipsometric data. . Only required when combined with data acquired from the top side of the same sample. Substrate effects will be included in the model calculations.</td>
</tr>
<tr>
<td>$E_{ot}$, $E_{+45t}$, $E_{90t}$</td>
<td>Transmission</td>
<td>Top side</td>
<td>Transmission Unregressed Anisotropic Ellipsometric data. . As with all transmission-type experiments, substrate effects will be included in the model calculations.</td>
</tr>
</tbody>
</table>

**Reflected intensity data types**

Reflected intensity (“reflectance”) measurements acquired with M-2000® and VASE® instruments generally use a “straight through no sample” intensity scan (full probe beam) as the baseline. Therefore, when WVASE® calculates intensity reflection values for the model, it works with absolute reflection values from 0 to 1. Other reflection measurement systems may report reflectance relative to another material. For WVASE® to correctly model such data, it must first be converted to absolute reflection data.

It must be remembered that the ellipsometer always acquires polarized reflected-intensity data. That is, the incident beam always has a single, known
polarization state – s, p, or a user-specified. The ellipsometer then detects the intensities for the p, s, or user-specified polarization components of the reflected beam. The detected intensities can be reported as separate quantities, or added all together and reported as the total reflected-intensity.

Reflectance: polarized-incident, total reflected intensity

The table below lists all the data types where the all the polarization components of the reflected beam are added together and reported as total reflected-intensity for a specific input polarization. For example, “pR” means “p-polarized incident, all reflected polarizations added together”. The m11 data type, which can only be recorded by M-2000® ellipsometers, represents the total unpolarized reflected-intensity (sum of all reflected polarizations for an unpolarized incident beam).

Also listed are the backside-corrected and reverse-side data types. At the time of acquisition, the ellipsometer hardware is unable to distinguish between “standard” reflected intensity measurement and a backside-corrected or reverse-side data measurement. Therefore, by default WVASE stores the data a the standard data type – “pR”, for example. For analysis purposes you may need to change the data type so that the model calculation will simulate the actual measurement process – “pR” would become “pRb” or “pRr”, for example.

<table>
<thead>
<tr>
<th>Data Types</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>std</td>
<td>Backside corrected</td>
</tr>
<tr>
<td>pR</td>
<td>pRb</td>
</tr>
<tr>
<td>sR</td>
<td>sRb</td>
</tr>
<tr>
<td>uR</td>
<td>uRb</td>
</tr>
<tr>
<td>xR</td>
<td>xRb</td>
</tr>
<tr>
<td>m11 (iv)</td>
<td>m11b (iv)</td>
</tr>
</tbody>
</table>

Electric field of incident beam is linearly polarized (p, s, u or x). The ellipsometer records the sum of all polarization components of the reflected light.

The ‘b’ postscript indicates backside-corrected data. Substrate effects will be included in the model calculations.

The ‘r’ postscript indicates reverse-side data. This is only required when combined with data acquired from the front side of the same sample. Substrate effects will be included in the model calculations.

m11 can only be measured using M-2000® RT scans, and is plotted using the Intensity Reflection or Transmission Type.

* u = User-defined polarizer azimuth.
* x = u + 90°, u = user-defined polarizer angle.

Reflectance: polarized-incident, polarized reflected intensity

The next table lists the data types where the individual output polarization components are reported. For instance “ARpp” means “p-polarized incident, p-polarized reflected only”. Some of these data types record the reflected intensities of

---

For an M-2000®, the incident polarization state is a known, continuously-varying function of the compensator’s fast axis azimuth as it rotates with time. This means that the sample is illuminated with known values of both p- and s-polarized light during the course of one compensator rotation, and p- and s-incidence reflectance, values such as pR and sR, can be determined.

Because the M-2000® illuminates the sample with both p- and s-polarized light during the course of one compensator rotation, it can record the Mueller Matrix m11 value, which is the “unpolarized” reflectance/transmittance.
light that has been converted from one polarization type to another. For example, “ARps” quantifies the conversion of p-polarized incident light into s-polarized light upon reflection.

<table>
<thead>
<tr>
<th>Data Types</th>
<th>std</th>
<th>Backside corrected</th>
<th>Reverse side</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>ARpp</td>
<td>ARppb</td>
<td>ARppr</td>
<td>Electric field of incident beam is linearly polarized (p, s, $u^a$ or $x^b$). The ellipsometer records only one polarization component (p, s, $u^a$ or $x^b$) of the reflected light.</td>
<td></td>
</tr>
<tr>
<td>ARPs</td>
<td>ARpsb</td>
<td>ARpsr</td>
<td>The ‘b’ postscript indicates backside-corrected data. Substrate effects will be included in the model calculations.</td>
<td></td>
</tr>
<tr>
<td>ARss</td>
<td>ARssb</td>
<td>ARssr</td>
<td>The ‘r’ postscript indicates reverse-side data. This is only required when combined with data acquired from the front side of the same sample. Substrate effects will be included in the model calculations.</td>
<td></td>
</tr>
<tr>
<td>ARsp</td>
<td>ARspb</td>
<td>ARspr</td>
<td></td>
<td></td>
</tr>
<tr>
<td>ARuu</td>
<td>ARuub</td>
<td>ARuur</td>
<td></td>
<td></td>
</tr>
<tr>
<td>ARux</td>
<td>ARuxb</td>
<td>ARuxr</td>
<td></td>
<td></td>
</tr>
<tr>
<td>ARxx</td>
<td>ARxxb</td>
<td>ARxxr</td>
<td></td>
<td></td>
</tr>
<tr>
<td>ARxu</td>
<td>ARxub</td>
<td>ARxur</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

* User-defined polarizer azimuth taken from the ‘Polarizer Angle’ box described below.

Normal-incidence reflected intensity

Normal incidence measurements (incident angle of zero) on isotropic samples and for uniaxial-anisotropic samples with the optic axis oriented normal to the surface reflect the same way regardless of incident polarization. That is, all total reflected intensity and same-polarization reflected intensity measurements ($p_R$, $s_R$, $u_R$, $m_{nl}$, ARpp, ARss, ARuu, ARxx) are equal, since the p- and s-directions are indistinguishable. Furthermore, all cross-conversion reflected intensities (ARps, ARsp, ARux, ARxu) equal zero.

For anisotropic samples with an optic axis not oriented normal to the surface, normal-incidence reflected intensity are polarization dependent, and the cross-conversion reflected intensities do not always equal zero.

Transmission intensity data types

Transmission intensity (“transmittance”) measurements acquired with M-2000® and VASE® instruments generally use a “straight through no sample” intensity scan (full probe beam) as the baseline. Therefore, when WVASE® calculates intensity transmission values for the model, it works with absolute transmission values from 0 to 1. Other transmission measurement systems may report transmittance relative to another material. For WVASE® to correctly model such data, it must first be converted to absolute transmittance data.

Just like reflectance measurements, the ellipsometer always acquires polarized transmission intensity data. That is, the incident beam always has a single, known polarization state $– s$, $p$, or a user-specified. The ellipsometer then detects the intensities for the $p$, $s$, or user-specified polarization components of the transmitted beam. The detected intensities can be reported as separate quantities, or added all together and reported as the total transmission-intensity.
**Transmittance: polarized-incident, total transmitted intensity**

The table below lists all the data types where the all the polarization components of the reflected beam are added together and reported as total transmitted-intensity for a specific input polarization. For example, “pT” means “p-polarized incident, all transmitted polarizations added together”. The m11 data type, which can only be recorded by M-2000® ellipsometers, represents the total unpolarized transmitted-intensity (sum of all transmitted polarizations for an unpolarized incident beam).

<table>
<thead>
<tr>
<th>Data Types</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>pT</td>
<td>Electric field of incident beam is linearly polarized (p, s, u° or x°). The ellipsometer records the sum of all polarization components of the transmitted light.</td>
</tr>
<tr>
<td>sT</td>
<td></td>
</tr>
<tr>
<td>uT</td>
<td>m11 can only be measured using M-2000® R</td>
</tr>
<tr>
<td>xT</td>
<td>As with all transmission-type experiments, substrate effects will be included in the model calculations.</td>
</tr>
<tr>
<td>m11(iv)</td>
<td></td>
</tr>
</tbody>
</table>

a u = User-defined polarizer azimuth.
b x = u + 90°, u = user-defined polarizer angle.

**Transmittance: polarized-incident, polarized transmitted intensity**

The next table lists the data types where the individual output polarization components are reported. For instance “ATpp” means “p-polarized incident, p-polarized transmitted only”. Some of these data types record the transmitted intensities of light that has been converted from one polarization type to another. For example, “ATps” quantifies the conversion of p-polarized incident light into s-polarized transmitted light.

<table>
<thead>
<tr>
<th>Data Types</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>ATpp</td>
<td>Incident beam is linearly polarized (p, s, u° or x°). The ellipsometer records only one polarization component (p, s, u° or x°) of the transmitted light.</td>
</tr>
<tr>
<td>ATps</td>
<td>As with all transmission-type experiments, substrate effects will be included in the model calculations.</td>
</tr>
<tr>
<td>ATss</td>
<td></td>
</tr>
<tr>
<td>ATsp</td>
<td></td>
</tr>
<tr>
<td>ATuu</td>
<td></td>
</tr>
<tr>
<td>ATux</td>
<td></td>
</tr>
<tr>
<td>ATxx</td>
<td></td>
</tr>
<tr>
<td>ATxu</td>
<td></td>
</tr>
</tbody>
</table>

a User-defined polarizer azimuth taken from the ‘Polarizer Angle’ box described below.
b x = u + 90°, u = user-defined polarizer angle.

**Normal-incidence transmitted intensity**

Normal incidence measurements (incident angle of zero) on isotropic samples and for uniaxial-anisotropic samples with the optic axis oriented normal to the surface transmit the same way regardless of incident polarization. That is, all total transmitted intensity and same-polarization transmitted intensity measurements
(pT, sT, uT, m11, ATpp, ATss, ATuu, ATxx) are equal, since the p- and s-directions are indistinguishable. Furthermore, all cross-conversion transmitted intensities (ATps, ATsp, ATux, ATxu) equal zero.

For anisotropic samples with an optic axis not oriented normal to the surface, normal-incidence transmitted intensities are polarization dependent, and the cross-conversion reflected intensities do not always equal zero.

Other data types recognized by WVASE®

These data types were implemented to meet the needs of specific customers, however, they have been made available to all users. These data types cannot be acquired using J.A. Woollam Co., Inc. hardware or software. These data types are included for analysis and simulation purposes only.

N - Neutron reflection

Data acquired in a neutron reflection experiment can also be modeled using WVASE®. This data type cannot be acquired using WVASE®. This feature was added for a particular customer working with neutron reflection data on polymers. For modeling, the neutron.mat layer is used (not described in this manual). If you wish to use this data type for analyzing your neutron reflection data, please contact the J.A. Woollam Co., Inc. directly for more details.

Tph - Transmitted phase

This data type represents the total phase difference of light transmitted through a layer stack relative to transmission through air of the same distance. This data type cannot be acquired using WVASE®. This type of data is usually associated with phase-shifted photomasks. For model calculations, WVASE® calculates the phase difference from only the layers on top of the substrate. The phase difference does not include propagation through the substrate. If acquired on another measurement instrument, data of this type can be used in the fitting process. Alternatively, WVASE® can be used to simulate this data type for a given model, and the model used may be the result of fitting to other ellipsometric and transmission data.

6.2 Exp_Data|File menu

Figure 6-8. The File menu from the Experimental Data window.
**Exp_Data|File|Open_Exp_File item**

This option is used to load a previously saved data file. The loaded data will replace any existing data in the Experimental Data window. A standard windows dialog box is used to select the filename. Only files with the extension .dat and .bdt are considered to be possible WVASE® data files. The .dat extension is used for data files stored using standard ASCII text. This type of file can also be read into most word processing and spreadsheet programs. The .bdt extension designates a binary coded dynamic data file. This type of file usually requires less disk space to save than a corresponding .dat file. However, this file format is specific to WVASE®. Data which has just been opened will automatically be selected for fitting and graphing.

**Exp_Data|File|Append_Exp_File item**

This option is used to add another data file to the end of the data that already exist in the Experimental Data window. For graphing purposes the line connecting the data points follows the order in the Experimental Data window, and when data has been appended sometimes the connecting line will jump abruptly to different spectral ranges. The Experimental Data window’s Title bar and Comment line will reflect the most recently added file. Data which has just been appended will automatically be selected for fitting and graphing.

**Exp_Data|File|Merge_Exp_Data item**

This option is used to add another data file to the end of the data that already exist in the Experimental Data window and then sort that data. The sorting is done by data type, angle of incidence, and wavelength, in that order. If data files covering the same spectral range at the same angle of incidence are merged together, then the graphed data may appear step-like. If you want to compare two data sets covering the same spectral range, you might want to use the Append_Exp_File option described above, because it will produce two separately connected curves. The Experimental Data window’s Title Bar and Comment Line will reflect the most recently added file. Data which has just been merged will automatically be selected for fitting and graphing.

*The result of appending two data files.*

![Graph showing the result of appending two data files.](image)

*Figure 6-9. Two experimental data files appended together in the Experimental Data window.*
The result of merging two data files.

![Graph showing the result of merging two data files.](image)

Figure 6-10. Two experimental data files merged together in the Experimental Data window.

**Exp_Data|File|Sort_Appended_Files item**

This option will sort all the appended files following the same sorting scheme as the Exp_Data|File|Merge_Exp_Data option. The sorting is done by data type, angle of incidence, and wavelength, in that order. If data files covering the same spectral range at the same angle of incidence are merged together, then the graphed data may appear step-like.

**Exp_Data|File|Save_Exp_Data item**

This option is used to save data from the Experimental Data window to a file. Multiple data types can be saved together in a single file. A standard Windows® dialog box is used to select the filename. The file will automatically receive the .dat extension. You are also permitted to input/change the experimental data comment line when you save the file. If a file with the same name already exists, you will be asked for confirmation that you do indeed want to overwrite it. If only part of the data in the window is selected, you will be given the option of saving just the selected data or all of the data.

**Exp_Data|File|CompleteEASE_Data_Transfer menu**

This option allows the user to convert WVASE® and VASEManager® data to CompleteEASE® data, and visa-versa.

**Exp_Data|File|Comment_Data item**

This allows you to manually input text for the experimental data comment line. You are also given the option of commenting the data when you save it.

**Exp_Data|File|Information item**

This item brings up a message box containing the information string attached to the experimental data file. This string contains the software version and information on the acquisition parameters used to acquire the data.

**Exp_Data|File|Copy_to_Clipboard item**

This item allows you to copy the experimental data onto the Windows™ Clipboard. From there it can be pasted into other Windows™ based applications such
as Microsoft Word™. The data is stored on the Windows™ Clipboard as a tab-delimited text table. All the data displayed in the Experimental Data window is copied to the clipboard, not just the selected data. The comment lines, column headers, and error bars are not copied.

6.3 Exp_Data|Range_Select item

When the data in the Experimental Data window is not time dependent (standard spectroscopic data), this command is used to define which data are selected for use in the fitting procedure. Also, only the selected data will be displayed in graphs. When dynamic experimental data is present in the Experimental Data window this command works differently. These two range selection procedures are quite different and are described separately.

Range select for static spectroscopic data

The Exp_Data|Range_Select dialog box is used to define which data are selected for fitting and graphing. Blocks of data based on type, wavelength, and angle of incidence can be added or removed from the currently selected data using the Range Select dialog box.

Angles

These boxes are editable and display the minimum and maximum angles of incidence which define the data block to be worked with. The values in these boxes are maintained for successive executions of this command.
Wavelengths

These boxes are editable and display the minimum and maximum wavelengths which define the data block to be worked with. The units for these boxes are defined by the [Global]Defaults command. The values in these boxes are maintained for successive executions of this command.

Selected data types

This list defines which data types are included in defining the data block. Only data types currently present in the experimental data are available for selection. Multiple data types can be selected by highlighting multiple rows simultaneously. To highlight a single row, click the mouse on it. To change the status of a single row (highlighted to un-highlighted, or un-highlighted to highlighted) <ctrl>-click on it. You can also use the standard Windows® range select commands involving the <shift> and <ctrl>-<shift> modifiers. The highlighted status of this list is maintained for successive executions of this command.

These items are used to define the type of action (add or remove) and the scope of that action:

All data button

This button is used to select all the data in the Experimental Data window. This button simply sets the data selected flag (a pound sign - ‘#’) on each data row regardless of the range settings described above.

Add to button

This button is used to select any data which falls within the defined range.

Remove from button

This button is used to deselect any data which falls within the defined range.

Skip every ____ data point(s)

This box allows the user to ‘shrink’ the data set by skipping data points evenly throughout the data set.

OK button

This button is used to select any data which falls within the defined range and deselect any data which falls outside the defined range. This is equivalent to deselecting all the data and then selecting just the defined range.

Global select box

This box defines the scope of the range select when multiple models are being used. If this box is checked, then the range select action (All, Add, Remove, OK) is performed on the experimental data associated with all 10 models. If this box is not checked, then the range select action applies only to the data in the currently displayed Experimental Data window. The status of this box is maintained for successive executions of this command.

Range select generated data box

If this box is checked, then the range select action (All, Add, Remove, OK) is performed on both the experimental data and generated data. If this box is not
checked, then the range select action applies only to the data in the Experimental Data window.

Range select for dynamic data

Dynamic data can be thought of as a collection of spectroscopic scans, with each scan associated with a different time. Each of these time-dependent spectra are called a time slice. Using an M-XX system, each time slice is a simultaneously acquired multi-wavelength ellipsometric data spectrum. Dynamic data can also be acquired using a VASE® system, but the number of wavelengths in each time slice is small and each wavelength is measured sequentially.

In a dynamic mode, VASE® and M-XX systems can only acquire data as one of the ellipsometric data types, and as such only dynamic ellipsometric data analysis (fitting) has been tested. Analysis of dynamic data of other types (such as intensity reflection), acquired by other instruments might be useable but this feature has not been fully tested. WVASE® is, however, capable of simulating data as a function of time for any of the supported types.

Dynamic data is selected on the basis of time and wavelength only. WVASE® assumes that there will be only one angle of incidence and only one data type within a dynamic experimental data file.

In the case of a VASE®, dynamic data is handled as a single contiguous block of time-dependent data. Data are selected by indicating a wavelength range and a time range. The range select dialog for dynamic VASE® data is shown below. This dialog is exactly the same as the range select dialog for ex situ data with the add boxes for specifying a time range.

![Dialog box used by the Exp_Data|Range_Select command to select or deselect a block of dynamic experimental data acquired with a VASE®.](image)

For an M-XX ellipsometer, dynamic data is handled in two ways: (1) as a single contiguous block of time-dependent data (dynamic mode), or (2) as a set of independent time slices (spectroscopic mode). In the dynamic display mode, the Experimental Data window’s title bar contains the word “Dynamic”, and in the spectroscopic mode it contains “(Spectroscopic Mode)”. The following figures shows the same dynamic data viewed in the two different modes.
Figure 6-14. Simulated dynamic ellipsometric $\psi$ data shown in the dynamic viewing mode.

Each curve corresponds to data for one of the different wavelengths. The vertical lines indicate the time slices which are displayed in the corresponding spectroscopic viewing mode as shown below.

Figure 6-15. Simulated dynamic ellipsometric $\psi$ data shown in the spectroscopic viewing mode.

Each of the $\psi$ spectra shown above correspond to a time slice as designated in the legend. The dialog box for selecting dynamic data and setting the view mode is shown below.

Figure 6-16. The range select dialog box associated with time dependent data acquired by an $M$-XX ellipsometer.
The Dynamic Range Select dialog box looks very different from the one used to select ranges of static experimental data. However, its purpose of selecting the experimental data for fitting and graphing is the same. This box contains the elements listed below.

**Time boxes**

These editable boxes define the beginning and ending times for the data range displayed in the dynamic view mode. Within WVASE® all data times are defined in minutes.

**# of data points to skip**

This editable box defines the number of points to skip between successive selected data times. For many analysis procedures, you do not need to use every data point in the desired time range and including all of them would slow the fitting process. To use every other time slice, set this box to “1”. To use every tenth time slice, set this box to “9”. To use every time slice, set this box to “0”.

**Selected wavelengths list**

This is a standard Windows™ multiple item select box. The selected wavelengths are highlighted, and in this case all wavelengths are selected. An individual wavelength can be selected by clicking. A range can be selected by clicking and dragging, or by clicking and <shift>-clicking. An individual wavelength can be deselected by <ctrl>-clicking, and a range can be deselected by <ctrl>-clicking and <ctrl>-<shift>-clicking. The two selection buttons at the top of the list allow the user to select different wavelength ranges for graphing and fitting. This is useful since you usually want to use a large number of wavelengths for fitting but only a few for graphing so the graph does not appear cluttered.

**OK button**

This button dismisses the dialog box and accepts the currently set time ranges, spectroscopic times, and view mode.

**Select All Data button**

This button selects the data at all times and at all wavelengths, and sets the view to dynamic mode, but does not change the values in the Time boxes or the Selected Wavelength List.

**Spectroscopic Mode Enabled**

When checked, this box indicates that the spectroscopic view mode is in use and data will be displayed as individual spectroscopic time slices. The view mode can also be set directly from the Experimental Data window. If you double-click inside the display portion of the Experimental Data window (not in the title bar), you will cause the display mode to toggle between dynamic and spectroscopic modes.

**Time slice list**

This is the list of times you have selected for use in the spectroscopic view mode. If no times are listed, then no data will be displayed in the spectroscopic view mode. Up to 10 different times can be used. These are the requested times, however, data will only be displayed for times that actually exist in the data file. In the above figure (6.14) showing the spectroscopic view mode, the times displayed in the legend are the actual data times displayed. You can see that these are not exactly
the same times that appear in the dialog box. The data time nearest to, and greater than the requested time is used.

**Add to list button**

This button is used to add the time in the Current Time box to the Time Slice List. In this way very specific times can be added to the list. The more commonly used method of adding times is done directly from the Graph window. If the experimental data is shown in the dynamic view mode in the Graph window, you can use the right mouse button to select a time to add to the Time Slice List. You simply click the right mouse button at the point with the desired time index. You can see the time index of the current mouse location using the left mouse button. When you add a time to the list a new vertical line will be displayed in the dynamic view mode.

**Delete button**

This button is used to remove a single highlighted time from the Time Slice List. The desired time for removal is highlighted by clicking on it.

**Delete all button**

This button removes all times from the time list.

### 6.4 Exp_Data|Angles item

Use this item to specify different angles or fit for angles.

This menubar item brings up a dialog box which displays the angles of incidence that are present in the currently selected data. These angles are compiled from the experimental data associated with all 10 available models.

The primary use of this command is to select an angle of incidence as a fit parameter. For most *in-situ* measurement applications (typical inside a vacuum chamber), a goniometer cannot be used and the angle of incidence must be varied at some point in the analysis.

When using a VASE® system in the *ex-situ* (standard) configuration, WVASE® will automatically record the angles of incidence as specified on the goniometer. The accuracy of the VASE® goniometer is normally better than 0.01° with 0.005° precision. Therefore, assuming your VASE® system is aligned correctly, we do not recommend fitting for the angle of incidence.
The angles of incidence dialog box

![Image of the angles of incidence dialog box]

Figure 6-18. The dialog box used by the Exp_Data|Angles command.

**Nominal angles**

This column of text boxes displays the angle of incidence values that are stored with the original data. These boxes are not editable.

**Actual angles**

This column of text boxes displays the angle of incidence values that are actually used when performing calculations for the model. These values are editable and they can be defined as fit parameters using the associated fit boxes. Note only the first 5 angles in use are displayed and are accessible as fit parameters.

**Global Offset**

This box is used to assign and/or fit for a global angle offset. This offset is added to each of the angles in the experimental data when data is generated. The global offset is intended to be used with horizontal ellipsometer systems, where an alignment error will cause all of the angles to be offset by the same amount. Fitting for a single global offset instead of fitting for each angle reduces the number of fit parameters and reduces the possibility of parameter correlation.

### 6.5 Exp_Data|Delete_Data command

![Image of the delete data option]

*Figure 6-19. The Delete_data option from the Experimental Data window.*

**Use this command to clear the Experimental Data window.**

This menu bar item is used to delete the currently displayed experimental data from memory. Data files already saved to disk will be unaffected. Only the experimental data associated with the currently selected model will be deleted. A caution dialog box is used to confirm your choice of this action.

### 6.6 Exp_Data|Change_Data_Type command

![Image of the change data type option]

*Figure 6-20. The Change_Data_Type option from the Experimental Data window.*
This command is used to change data from one type to another. When a VASE® or a M-XX system acquires ellipsometric data, it first stores the data as standard ellipsometric data, type “E”. If you have a sample with a transparent substrate, then to simulate substrate effects, you may want to convert it to the backside corrected type “Eb”. If you have taken ellipsometric data from both sides of a sample, then to use both data sets simultaneously, you will need to convert one to type “Er”, reverse side ellipsometry. If you acquired transmission ellipsometry data, then you will need to change the type to “Et”. Similar changes are also required for the various anisotropic data types described previously.

Important!

The change type command will change all Range-selected data, regardless of type. Before using this command, make sure that only the desired data type and range are selected. A common mistake is converting all data types into a single data type; for example, the user will inadvertently convert both “E” and “depolE” data into the single data type “Eb”. This problem can be avoided by using the “All: To corresponding …” selections. See following sections for details.

To keep the changes permanently, you will need to save the data with the new type information.

The change data type dialog box

The dialog box used to select the new data type is shown in the figure below.

![Figure 6-21. Dialog box used to select a new data type using the Exp_Data|Change_Data_Type command.](image)

Current data type

This is the data type of the first data row in the window. The change command will be applied to all data in the window regardless of type. This box will not warn you if multiple data types are actually present.

Change to

Under most circumstances, users will want to use one of the three “All: ...” change categories.

- The “All: ...” change categories alter each data type to its associated type in the new category – using “E:” becomes “Eb:”, “pR:” becomes “pRb:”, “depolE:” becomes “depolEb:”, etc.
- The other change categories change all data files to the new category – for instance, “Er:”, “E:”, “pR:” and “depolE:” all become “Er:”

Under most circumstances, users will want to use one of the three “All: ...” change categories.
Figure 6-22. Examples of changing data types: Left “Change to: Eb: Ellipsometric with backside correction”. Right “Change to: All corresponding to backside corrected”. Every data type becomes ‘Eb’!

E’ becomes ‘Eb’, and ‘dpolE’ becomes ‘dpolEb’
Chapter 7 The Model Window

7.1 Model window overview

The Model window is used to build and manipulate the optical model used to fit experimental data.

The Model window is used to specify the layered structure that will be used to simulate the interaction of polarized light with the sample. All models contain at least one layer called the substrate (designated layer #0). Layers can then be added on the top and on the bottom of the substrate to construct the desired structure. This structure is then used to simulate the variety of optical measurements that can be performed on the sample. These include not only normal (top side) ellipsometry but also reverse-side ellipsometry, transmission ellipsometry, transmission intensity, and reflection intensity measurements. The data generated from the model can be used either for simple simulations or for comparison with experimental data when fitting.

The number of layers in the model is limited by the Maximum # of Layers as defined using the Memory Allocation button accessed by the |Global|Defaults command.

Features displayed in the Model window

A general model with two topside layers and one backside layer is shown below.

Model window with two topside layers & one backside layer.

Figure 7-1. Sample Model window.

The following information is displayed in a Model window.

Title bar

If the model has been saved to disk, the title bar gives the name of the model. In this case, the model has been saved as demo1.mod. (Only files with the extension .mod are treated as model files by WVASE®.)
Comment line

Each model also has an optional comment line which appears above the graphical representation.

Layers

Top side layers are numbered starting with 1 nearest the substrate and increasing for each additional layer. Backside layers are numbered starting with -1 nearest the substrate and decreasing for each additional layer. For each layer the thickness is shown on the right.

Current layer

The small arrow to the left of the model drawing indicates what the current layer is. In this case layer #1 is the current layer. The current layer arrow can be moved with the up and down arrow keys. The current layer can be edited by clicking on the layer or by pressing <Enter> when the Model window is active. Editing a layer will cause the dialog box containing the specifications for that layer to appear on the screen. This is the same box that is displayed when the layer is first added to the model.

The Model window menubar

As shown below, there are eight menus on the main menubar plus the Window and [Global menus.

![Menu bar when the Model window is active.](image)

Figure 7-2. Menu bar when the Model window is active.

The general functions of these menus is given in the following table. The specific actions will be described in succeeding sections.

<table>
<thead>
<tr>
<th>Menu</th>
<th>Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model</td>
<td>File</td>
</tr>
<tr>
<td>Model</td>
<td>AddLayer</td>
</tr>
<tr>
<td>Model</td>
<td>DeleteMod</td>
</tr>
<tr>
<td>Model</td>
<td>Superlattice</td>
</tr>
<tr>
<td>Model</td>
<td>Growth</td>
</tr>
<tr>
<td>Model</td>
<td>Select</td>
</tr>
<tr>
<td>[Model]Options</td>
<td>This item is used to simulate certain model non-idealities such as layer non-uniformity and finite light bandwidth.</td>
</tr>
<tr>
<td>[Model]Angles</td>
<td>This item is used to edit or select for fitting the angles of the experimental data. This is equivalent to the Exp_Data</td>
</tr>
</tbody>
</table>
7.2 Model Window Pop menus:

The context sensitive pop-up menus are particularly useful in the WVASE Model window.

General Model Window Pop menus:

Clicking right mouse button in the Model window while the arrow is but outside of the model schematic will bring up a context-sensitive menu that includes all the features available in the pull-down menus at the top of the window, such as Copy Model to Clipboard, File, Addlayer, Recent Layers, DeleteMod, etc.

![General Model Window Pop menus](image)

Figure 7-3. General Model Window Pop menus.

Standard Layer-Related Pop menus:

Clicking right mouse button while holding mouse over a specific standard layer will bring up a context-sensitive menu that includes:

- Operations on the selected layer, such as Edit, Delete, Replace, Optical Constants, & Save.
- Enhanced Add layer options, including
  - Add Above,
  - Add Below,
  - Add Intermix between… If mouse pointer is in upper half of layer, adds intermix between current layer & above layer. If mouse pointer is in lower half of layer, adds intermix between current layer & layer underneath.
- Convert/build Layer operations, such as
  - Convert to Simple Grade
  - Convert to EMA
  - Convert to Function-Based Graded Layer
  - Convert to EMA-Based Graded Layer
  - Add Uniaxial Anisotropy
  - Add Biaxial Anisotropy
  - Convert ‘...’ to GenOsc layer
  - Build GenOsc layer from tabulated ‘...’
  - Make Substrate (turns current layer into substrate, and all layers below current layer into incoherent backside layers).
• All the features normally available in the pull-down menus at the top of the window (Such as File, Addlayer, DeleteMod, Copy to Clipboard, etc.)

Add Uniaxial (or Biaxial) Anisotropy:

The Uniaxial and Biaxial pop-menu items effectively convert the selected layer into an anisotropic layer by creating a combination of biaxial.mat and “dummy” layers (zero-thickness layers that “hold” optical constants used in the biaxial.mat).

These two combinations provide starting anisotropic models that can be altered to suit the user’s own modeling requirements. The various layers created in the conversion are described below.

• Selecting **Add Uniaxial Anisotropy** changes:

  $$\begin{align*}
  &1 \text{ si}_2 \text{ jaw} \\
  &0 \text{ si}_{jaw}
  \end{align*}$$

  into

  $$\begin{align*}
  &4 \text{ Uniaxial} \\
  &2 \text{ Hz} \text{ si}_2 \text{ jaw/1.00%} \text{ (Hz)} \\
  &2 \text{ Hz} \\
  &1 \text{ si}_2 \text{ jaw} \\
  &0 \text{ si}_{jaw}
  \end{align*}$$

Figure 7-6. Changes that occur when “Add Uniaxial Anisotropy” is selected.
- **Uniaxial** is a *biaxial.mat* layer set to uniaxial mode into which \(N_z\), the out-of-plane optical constants, and the in-plane optical constants (*sio2_jaw.mat* in this example) are coupled to the starting layer used when established.

- \(dN_z\) is a *user.mat* layer that parameterizes the difference in optical constant dispersion between the out-of-plane optical constants \((N_z)\), and the in-plane optical constants (*sio2_jaw.mat* here). That is, \(dN_z=sio2_jaw.mat-N_z\).

- \(N_z\) is a refractive index additive layer (same as *sum_nk.mat*) which sums the in-plane optical constants, *sio2_jaw.mat*, and the index-difference layer, \(dN_z\) (i.e., \(N_z=sio2_jaw.mat+dN_z\)). \(N_z\) provides out-of-plane optical constants to the **Uniaxial** layer.

  - Selecting **Add Biaxial Anisotropy** changes:

    | Layer | Description | Thickness |
    |-------|-------------|-----------|
    | 1     | *sio2_jaw* | 26 nm     |
    | 2     | *sio2_jaw* | 1 mm      |

    into

    | Layer | Description | Thickness |
    |-------|-------------|-----------|
    | 7     | **Biaxial** | 26 nm     |
    | 6     | \(N_y\) (\(sio2_jaw\))50% \((dN_{xy})\) | 0 nm |
    | 5     | \(N_x\) (\(sio2_jaw\))50% \((dN_{xy})\) | 0 nm |
    | 4     | \(dN_{xy}\) | 0 nm |
    | 3     | \(N_z\) (\(sio2_jaw\))100% \((dN_z)\) | 0 nm |
    | 2     | \(dN_{xy}\) | 0 nm |
    | 1     | *sio2_jaw* | 0 nm      |
    | 0     | *sio2_jaw* | 1 mm      |

**Figure 7-7. Changes that occur when “Add Biaxial Anisotropy” is selected.**

- **Biaxial** is a *biaxial.mat* layer set to biaxial mode into which \(N_z\), \(N_y\) and \(N_x\) are coupled.

- In this model, *sio2_jaw.mat* actually provides the average in-plane dispersion between \(N_x\) and \(N_y\) (i.e., \(sio2_jaw.mat=(N_x+N_y)/2\)).

- \(dN_{xy}\) parameterizes the difference in optical constant dispersion between \(N_x\) and \(N_y\) \((dN_{xy}=N_x-N_y)\).

- \(dN_z\) parameterizes the dispersion difference between out-of-plane optical constants \((N_z)\) and the average in-plane optical constants.

- \(N_z\), \(N_x\) & \(N_y\) are refractive index additive layers that provide the optical constants used in the **Biaxial** layer.

**Biaxial Layer-Related Pop menus:**

The pop menu for a Uniaxial or Biaxial layer can contains an operation called Convert Uniaxial (Biaxial) to Biaxial2, which converts a Biaxial.mat to Biaxial2.mat. Conversely, a Biaxial2.mat layer can be converted to Biaxial.mat from a similar pop menu. (Biaxial2.mat is described in the Addendum of the WVASE® Software Manual).

**Substrate (Layer 0)-Related Pop menus:**

For substrates, the Context-sensitive menu includes not only some of the operations available in the Standard Layer Pop-menu, but also a Fit Substrate Thickness option. When the Substrate (Layer 0) thickness is already included as a fit parameter, the Pop menu allows the user to deselect the substrate thickness as a fit parameter.
EMA Layer-Related Pop menus:

Context-sensitive menu includes all operations available in standard layer Pop-menu.

In addition, Convert EMA to (layer_name ) is available. This operation will:

- Replace the EMA layer with the EMA’s Material #1, while maintaining the thickness – that is (1st case):

- This

  > 1 EMA 102/80% yield 
  26 mm
  0 Si_yy
  1 mm

  becomes

  > 1 102 26 mm
  0 Si_yy
  1 mm

  Figure 7-10. Changes that occur when “Convert EMA to ‘...’ ” is selected – 1st case.

- OR (2nd case) if the EMA’s Material #1 is coupled to the layer immediately below it, the EMA will be deleted and its thickness entered into the coupled-layer value – that is,
Figure 7-11. Changes that occur when “Convert EMA to ’…”’ is selected – 2nd case.

SimpleGraded Layer-Related Pop menus:

Context-sensitive menu includes operations available in Standard Layer Pop-menu.

Figure 7-12. SimpleGraded -layer Pop-menu.

In addition, Convert to Normal UnGraded Layer is available. This operation will (1st case):

- Replace the SimpleGraded layer with the its Material #1, while maintaining the thickness – that is:

- This

  > 1 SimpleGraded tic2 26 nm
  0 si_x_y
  1 mm

  becomes

  > 1 tic2 26 nm
  0 si_x_y
  1 mm

Figure 7-13. Changes that occur when “Convert to Normal Ungraded Layer” is selected – 1” case.
• OR (2nd case), if the SimpleGraded’s Material #1 is coupled to the layer immediately below it, the SimpleGraded layer will be deleted and its thickness entered into the coupled-layer value—that is,

- This

<table>
<thead>
<tr>
<th>Layer Type</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>SimpleGraded</td>
<td>xx nm</td>
</tr>
<tr>
<td>1 SimpleGraded</td>
<td>0 nm</td>
</tr>
<tr>
<td>0 SimpleGraded</td>
<td>1 nm</td>
</tr>
</tbody>
</table>

becomes

<table>
<thead>
<tr>
<th>Layer Type</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Sin2Vav</td>
<td>xx nm</td>
</tr>
<tr>
<td>0 Sin2Vav</td>
<td>1 nm</td>
</tr>
</tbody>
</table>

Figure 7-14. Changes that occur when “Convert to Normal Ungraded Layer” is selected – 2nd case.

**Function-Based Graded Layer-Related Pop menus:**

Context-sensitive menu includes operations available in Standard Layer Pop-menu.

In addition, Convert to Normal UnGraded Layer is available. This operation will:

- Delete the Function-Based Graded Layer and enter its thickness into the original coupled-layer—that is,

- This

<table>
<thead>
<tr>
<th>Layer Type</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>SimpleGraded</td>
<td>xx nm</td>
</tr>
<tr>
<td>1 SimpleGraded</td>
<td>0 nm</td>
</tr>
<tr>
<td>0 SimpleGraded</td>
<td>1 nm</td>
</tr>
</tbody>
</table>

becomes

<table>
<thead>
<tr>
<th>Layer Type</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Sin2Vav</td>
<td>xx nm</td>
</tr>
<tr>
<td>0 Sin2Vav</td>
<td>1 nm</td>
</tr>
</tbody>
</table>

Figure 7-16. Changes that occur when “Convert to Normal Ungraded Layer” is selected.

**Intermix Layer-Related Pop menus:**

The “Add Intermix between…” menu item is also included in the Context-sensitive menu operations available in Standard Layer Pop-menu.
Figure 7-17. Intermix Layer related pop menu.

Selecting “Add Intermix between…” adds an \textit{intermix.mat} layer between the selected layer and the layer above/or below. If mouse pointer is in upper half of layer, an Intermix layer is added between the current layer & above layer. If mouse pointer is in lower half of layer, an Intermix layer is added between current layer & layer underneath.

Once an intermix layer has been added, the \textit{Convert Intermix to Graded Intermix} is available in the context-sensitive pop menu for the intermix layer. This operation will convert:

- The \textit{intermix.mat} layer

\begin{verbatim}
\begin{verbatim}
2 sio2_vuv  26 mm
1 Intermix  2 mm
0 sio2_vuv  1 mm
\end{verbatim}
\end{verbatim}

into a graded Intermix layer (\textit{intermix2.mat})

\begin{verbatim}
\begin{verbatim}
2 sio2_vuv  26 mm
1 Graded Intermix 2 mm
0 sio2_vuv  1 mm
\end{verbatim}
\end{verbatim}

Figure 7-18. Changes that occur when “Convert Intermix to Graded Intermix Layer” is selected.

\textbf{Graded Intermix-Related Pop menus:}

Context-sensitive menu includes operations available in Standard Layer Pop-menu.

Figure 7-19. Graded Intermix Layer related pop menu.
In addition, *Convert Graded Intermix to Single-Layer Intermix* is available. This operation will convert:

- This a graded intermix layer

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 SiO\textsubscript{2}</td>
<td>26 nm</td>
</tr>
<tr>
<td>1 Graded Intermix</td>
<td>2 nm</td>
</tr>
<tr>
<td>0 Si</td>
<td>1 mm</td>
</tr>
</tbody>
</table>

into a standard intermix layer

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 SiO\textsubscript{2}</td>
<td>26 nm</td>
</tr>
<tr>
<td>1 Intermix</td>
<td>2 nm</td>
</tr>
<tr>
<td>0 Si</td>
<td>1 mm</td>
</tr>
</tbody>
</table>

*Figure 7-20. Changes that occur when “Convert Graded Intermix to Single-Layer Intermix Layer” is selected.*

### 7.3 Layers and optical constants

The optical model consists of one or more layers, for which optical constants and layer thicknesses are specified by the user. Optical constants are stored in files, and may be added or deleted from the model by selecting the appropriate file. Many types of optical constant files are supported by *WVASE\textsuperscript{®}*, and – with the exception of the Genosc\textsuperscript{®} layer – these are discussed later in this chapter. The Genosc\textsuperscript{®} is discussed separately in the chapter that follows.

**Special properties of the substrate**

For model calculations, *WVASE\textsuperscript{®}*, treats the substrate as a special type of layer. *WVASE\textsuperscript{®}* considers the transmission of a light beam through the substrate as being incoherent with respect to other beams. Light beams passing through all other layers are considered to propagate coherently.

This special substrate property is only important if the substrate is transparent or nearly transparent and if part of the light being measured has passed through the substrate before being collected. These conditions are definitely met if transmission measurements are being made. The incoherent nature of the substrate can also be important for reflection measurements if part of the probe beam penetrates surface layers into the substrate, is reflected off the backside of the substrate, returns through the layers on the surface, and is collected along with the primary reflection off the surface layers. A more detailed explanation is given in chapter 13 - ‘VASE\textsuperscript{®} Data Analysis’.

**Ideal and non-ideal models**

The sample, instrument, or model may be non-ideal.

Options are available from the Model window which allow the user to incorporate non-ideality into the optical model to account for both non-ideal samples and non-ideal characteristics of the ellipsometer. These options can be very useful when dealing with non-uniform films, samples on transparent substrates, very thick films, and other non-ideal analysis cases.
Multiple models

For most applications only the primary model (model #1) is used. However, WVASE® is capable of simultaneously analyzing data from more than one sample. Up to 10 separate models can be used. Each of these models work with a different set of experimental data. This can be a very powerful method for determining optical constants. The details of using this technique are left to the advanced analysis techniques section of chapter 13 - ‘VASE® Data Analysis’, in which multiple sample analysis is described.

7.4 Model|File menu

Model|File|Open_Model item

This option is used to load a previously saved model. A standard Windows™ dialog box is used to select the filename. Only files with the extension .mod are considered to be possible WVASE® model files.

A confusing situation may arise when performing this operation if the individual layers can not be found on the disk. When this happens one or more of the layers will be replaced with a ‘dummy’ layer in the model. This can occur if the .mod file or one of the layer’s optical constant files has been moved to a directory not contained in the search path for material files.

Model|File|Save_Model item

This option is used to save the displayed model. A standard Windows™ dialog box is used to select the filename. The file will automatically receive the .mod extension. You are also permitted to input/change the model comment line when you save the model. If a model already exists, you will be asked for confirmation that you do indeed want to overwrite it.

If you have been working with new optical constants for a layer, you will be given the option of saving those optical constants. When the model is saved only the filename is saved for the optical constants of a given layer; the optical constant values themselves are not stored in the model file. When opening a saved model, the saved filenames are in turn opened to import the optical constants.

Model|File|Comment_Model item

This allows you to manually input the text for the model comment line. You are also given the option of commenting the model when you save it.
Model|File|Copy_to_Clipboard item

This item allows you to copy the model in graphical form onto the Windows™ Clipboard. From there it can be pasted into other Windows™ based applications such as Microsoft Word™. The data is stored on the Clipboard as a Windows™ metafile (WMF).

Figure 7-22. Example of model pasted into Microsoft Word™.

7.5 Model|AddLayer command

This item directly executes the command to add a new layer to the model. This layer will be added to the model just above the current layer as indicated by the marker on the left side. If the <shift> key modifier is used (<shift>-<alt>-A or <shift> click on the menu), the layer will be added below the current layer. The only way to add layer #1 is to use the <shift> key modifier with the current layer set on the substrate (layer #0). Only files with the extension .mat can be added as layers.

The primary information included within a layer is a thickness and a set of optical constants. There are many different kinds of layers, but they can be grouped into four principal categories:

1. Tabulated
2. Function Based
3. Composite
4. Anisotropic
5. Specialty

The optical constants for a tabulated layer are described using a wavelength-by-wavelength list. Function-based optical constants are described by a mathematical formula, not a table. Composite layers can include more than one set of optical constants which are mixed together. Anisotropic layers include optical constants for both an ordinary and an extraordinary optical axis. Specialty layers are unique because they do not fall into any of the above categories.

File searching pattern for Model|AddLayer

Several directories are searched for the specified layer name when a layer is added to the model.

When adding a new layer you can always use the dialog box to explicitly define the pathname and filename of the .mat file you want. However, when doing analyses to determine new optical constants it is sometimes inconvenient to continually change directories. WVASE® includes some extra features to make adding layers more convenient. WVASE® keeps a list of the currently loaded materials. You can access this list by selecting “Current Model” from the “List Files of Type:” box. The dialog box used to open .mat files, shown below, is slightly non-standard.
Any time a new layer is added, the “Current Model” list is examined to see if the layer has already been loaded. Even the names of layers that have been deleted may appear in this list indicating that those optical constants are still loaded and they will be used before new information is read from the disk. The only way to clear the “Current Model” list is to delete the primary model (model #1) using the Model|DeleteMod option or to exit WVASE®.

There are also several defined directories that can be accessed using the “List Files of Type” box. These are the “User Directory”, “Current Model”, “Default Materials”, “Metals”, “Dielectrics”, “Semiconductors”, and “Special Materials” folders. These directories can be used to rapidly switch between subdirectories without manually selecting them with the “Folders” and “Drives” boxes. The user can also define additional directories through the |Global|Defaults|Mat_File_Dir item which is discussed in Chapter 2: Navigating WVASE®. If the “Default Materials” directory is selected it will be searched after the “Current Model” list, but before the other directories in the “List Files of Type” box when adding a layer. If the “User Material” directory is selected it will also be searched after the “Current Model” list, but before the directories in the list.

Finally the \wvase\mat directory is always searched. Thus, if you know the file you want is stored in the \wvase\mat directory all you have to do is type the name in the File Name box and click OK (press <enter>).

In summary, when adding a new layer, several lists are looked at when a layer name is selected. First, the “Current Model” directory is searched for the desired file. Next, the selected folder is searched followed by the other directories in the “List Files of Type” list. Finally, the \wvase\mat directory is searched. Only after WVASE® fails to locate the specified file in these four directories will the “File Not Found” error message be displayed.

**Coupling of layers**

The optical constants of layers can be coupled together. Coupling optical constants is primarily used with composite layers which are described later. Coupling can also be used when extracting optical constants for a material which appears more than once in the multiple models. When a new layer is added, WVASE® looks at the existing layers in model #1, starting with the substrate, layer #0. If the same name is found, you will be asked if you wish to couple the optical
constants together. When using multiple models only model #1 is searched for possible coupling opportunities. Therefore all coupled layers must refer back to a layer in model #1.

A coupled optical constant layer is shown with parentheses around the name. The layer to which it is coupled is also shown.

![Image of a model with a coupled layer]

Figure 7-25. Example of a model with a coupled layer. The optical constants for layer #3 are coupled to those of layer #1.

**Quick access to Coupled Layers**

Any coupled layer can be opened directly by double-clicking the left mouse button while holding pointer over the coupled layer name (always in parentheses). The figures on the right illustrate this procedure for the coupled layer “(sio2_vuv)” contained in an EMA.

![Image of double-clicking on a coupled layer]

Figure 7-26. Left: Double-clicking on coupled layers in parentheses, such as “(sio2_vuv)”, will open that layer (Right).

### 7.6 Tabulated layers

A large library of tabulated optical constants of various materials is supplied with WVASE®. All tabulated layers have a wavelength-by-wavelength list of optical constants associated with them. The standard form is the typical list found in reference texts such as Palik’s *Handbook of Optical Constants*. WVASE® can also work with groupings of optical constants to form alloy and temperature dependent optical constant files. These alloy files, such as *algaas.mat* for Al\textsubscript{x}Ga\textsubscript{1-x}As and *gaas_tmp.mat* for temperature dependent GaAs, include some additional information on how to interpolate between compositions and temperatures.

**Standard layers**

Standard layers are defined by a set of optical constants and a thickness. For calculations, WVASE® assumes that the standard layer is homogeneous,
isotropic, and that the interfaces are perfect and parallel. The edit dialog box for a standard layer looks like the following.

![Edit dialog box for a standard layer](image)

Figure 7-27. The edit dialog box for a standard layer with optical constants from si_unl.mat.

Displayed in this edit box are the following items:

**Layer name**

This is the filename containing the tabulated optical constants for this layer. This box cannot be edited.

**Comment**

This is a single line of text describing what this set of optical constants refers to. Typically this line includes a reference to the source of these optical constants. This text box can be edited. Also, if you wish to see part of the comment which does not fit inside the box, you can position the cursor inside the box (click in it or type `<alt>-m`) and then use the right arrow key to scroll to the end.

**Spectral range**

This gives the limiting range on the optical constants contained in the file. If model calculations are performed using wavelengths outside this range, *WVASE®* will extrapolate to the desired value. There are many different operations that will cause *WVASE®* to check the spectral range of the optical constants. If *WVASE®* anticipates that it will have to extrapolate, you will receive a caution message to that effect. Extrapolations performed by *WVASE®* are not very sophisticated and should generally be avoided. Extrapolations to points just outside the spectral range will of course be more reasonable.

**Thickness**

This is the thickness of this layer. The thickness units are set using the [Global]Defaults menu item. The substrate thickness is always represented in millimeters.

**Thickness fit box**

This check box is used to set the thickness as a fit parameter. This box is not enabled for the substrate. If the fit box is checked, the layer name will be displayed in blue in the Model window.
**Opt. con. fit boxes**

These check boxes are used to select either the real part, or the imaginary part, or both parts of the optical constants for fitting. The “n” box is for the real part and the “k” box is for the imaginary part. Even though these boxes are always displayed as “n” and “k,” the actual fit parameter selected depends on the optical constant representation set by the `|Global|Defaults` menu item. If the `|Global|Defaults` setting is for “n and k” then the real and imaginary parts of the complex refractive index will be the fit parameters. If the `|Global|Defaults` setting is for “e1 and e2” then the real and imaginary parts of the complex dielectric function will be the fit parameters. If one or both of these boxes are checked, the layer name will be displayed in blue in the Model window.

**Reset n&k button**

This button will cause the optical constants to revert back to the optical constants stored in the Current Materials list. This is primarily used when trying to fit for new optical constants and the fitting procedure gets lost. The button is enabled only after a fit has been performed for the optical constants.

**OK button**

This button is used to dismiss the layer dialog box and keep changes to the fit boxes and the comment line.

**Cancel button**

This button is used to dismiss the layer dialog box, but does not keep changes to the fit box states and the comment line.

**Replace layer button**

This button is used to replace the current layer with a new one. This button acts just like the `Model|AddLayer` command in the way that the new layer is selected. However, instead of adding a new layer, the layer currently being edited is deleted. The thickness is transferred from the deleted layer to the new layer. All fit boxes for the new layer are turned off. If the layer being replaced has been coupled to by other layers, then those coupled layers will also show a change.

**Delete layer button**

This button is used to delete a layer. This command removes the layer from the current model, but does not remove the optical constants from the Current Materials list. A layer can not be deleted until all layers coupled to it are also deleted. If you wish to maintain the coupling of several layers together but change their optical constants, you might try the Replace Layer button.

**Optical constants>> button**

This button causes another dialog box to appear which displays the optical constants graphically and in tabular form.
On the left is a table of the optical constants at the wavelengths required by WVASE® for generation of data. These wavelengths may not be the same as those in the original .mat file saved on disk, and are usually determined by the wavelengths present in the Experimental Data window. The tabulated data can be examined using the scroll bar control, the up/down arrows, and the page-up/page-down keys. The table headings depend on the |Global| Defaults settings.

Below the graph, the minimum and maximum values for the optical constants in the table are given. A dashed vertical line is drawn in the graph box which corresponds to the one row in the table that is highlighted. The highlighted row can also be set by clicking in the graph window. This feature can be useful in identifying at what wavelength a particular feature in the optical constants is located.

**Edit n&k button**

This button allows you to manually edit the optical constants of the highlighted row. This button is only enabled if one or both of the optical constant fit boxes (‘n’ and/or ‘k’) is checked in the layer dialog box. You might want to edit the optical constants at individual wavelengths if a fit procedure has gotten off on the wrong track.

**Smooth opt. const. button**

This button allows you to perform a polynomial smoothing of the optical constants. When you perform this action you will be given the opportunity to specify the number of points and order of polynomial for smoothing. The smoothing can be performed several times in succession. This option is only enabled if one or both of the optical constant fit boxes is checked in the layer dialog box. You might want to smooth the optical constants if the fit procedure has gotten on the wrong track for a number of wavelengths. By smoothing and restarting a fit you may be able to get the fit procedure to find the correct best-fit optical constants.

**Revert to previous button**

This button is used to undo a smoothing operation. This button is only enabled if a smoothing operation has already been performed while this dialog has been opened. Once this dialog box is dismissed, the smooth operation can not be undone by this button.
Save button

This button is used to save the tabulated optical constant file to a WVASE® compatible material file. The wavelength units and optical constant type displayed in the table will be saved in the file. Only those wavelengths shown in the table will be saved. A standard Windows™ save dialog box is used to get your intended filename. The default filename is the same name and the default directory is the User Materials directory. If the file already exists you will be asked to confirm that you wish to overwrite the values.

Cancel button

This button dismisses the dialog box. Changes made using the Edit n&k and Smooth Opt. Const. buttons are kept.

Alloy layers

This type of layer works with a parameterized set of optical constants which enables WVASE® to calculate the dielectric function of a material as a function of alloy fraction. There are several parameterization schemes that the Alloy layer can use but regardless of the scheme, the Alloy layer appears the same in WVASE®. The simplest parameterization method to implement is described below with the others described in the Appendix B.

The simplest parameterization type in WVASE® works with a group of optical constant tables contained in one file. Each component table represents the optical constants for a specific alloy fraction. In addition to the optical constants, extra information is provided in the file to identify which compositions are present. For alloy layers information for interpolating between the component tables is included. The specifics of the file formats are described in Appendix B.

When WVASE® is asked to calculate optical constants for this type of layer, the alloy fraction is used to find the closest two tabulated alloy fractions stored in the file. Then the optical constant at the specific wavelength is determined by interpolation. For alloy files, this interpolation is not just simple interpolation. Rather, information about the critical point structure of the materials is used to intelligently shift the optical constants before interpolating. This procedure is explained in a published paper (P.G. Snyder et al., J. Appl. Phys., 68, 5925 (1990)). For semiconductors it is especially important to use this type of interpolation scheme. A simpler interpolation scheme can produce a “double peak” effect, where the optical constants for a composition between two tabulated values shows two peaks for a critical point where there should be only one.

Ternary semiconductor alloys, such as AlxGa1-xAs, and pseudo-ternaries, such as (InxGa1-x:As)x(InP)1-x, are the usual kind of materials described by alloy materials. However, any material system that has a systematic progression of optical constants as a function of some parameter can be formed into an alloy file. This can be a very useful way to describe a related set of optical constants and to fit for only one control parameter.

The alloy fraction is usually considered to be in the range from 0 to 1. However, the calculation can be performed for any alloy fraction.

When any alloy file (algaas.mat for example) regardless of the parameterization used is added, the edit dialog box looks like the following.
Figure 7-29. Edit dialog box for the AlGaAs alloy layer.

The Layer Name, Comment, Spectral Range, Thickness, OK, and Delete Layer items are the same as for the standard layer. The new item and other items that behave differently are explained below.

**Alloy fraction**

This box is used to specify the alloy fraction to use when calculating optical constants.

**Alloy fraction fit box**

This check box is used to set the alloy fraction as a fit parameter. Do not try a fit with the Alloy Fraction Fit box and one of the optical constant fit boxes checked. This will generate a ‘Singular matrix error’, as there is not sufficient sensitivity to both parameters at the same time.

**Opt. con. fit boxes**

These boxes work similarly to those in the standard tabulated layer. The difference is that when neither box is checked, the optical constants are derived by interpolation using the alloy fraction. When either one box or both boxes are checked the optical constants are taken from an internally stored list of fitting optical constants. This internal list is started with the interpolated values the first time a fit is performed. However, after the first fit of optical constants, this internal list may be different than the interpolated values.

**Optical constants>> button**

This works exactly the same as for a standard tabulated layer. You just need to be aware where the values displayed in the table and graph are derived from. If one of the optical constant fit boxes is checked, then the displayed values are taken from the internal stored list of fitting optical constants. If neither of the optical constant fit boxes are checked, then the displayed values are interpolated using the alloy fraction value. When you save a set of optical constants you can only do so as a standard tabulated layer. You can not fit the optical constants for a single alloy fraction and then resave the entire alloy file with that new set of optical constants for that composition. To change the components of an alloy file you need to edit the alloy file with a text editor external to WVASE®.

**Temp layers**

Like an alloy layer, this type of layer works with a parameterized group of optical constants, the formats of which are described in Appendix B. The simplest to implement is the use of a group of optical constant tables contained in one file. Each
component table represents the optical constants for a specific temperature. In addition to the optical constants, extra information is provided in the file to identify which temperatures are present. The specifics of the file formats are described in Appendix B.

When WVASe® is asked to calculate optical constants for this type of layer, the temperature is used to find the closest two tabulated file stored in the file. Then the optical constant at the specific wavelength is determined by simple interpolation. This is unlike alloy files which use a more sophisticated interpolation scheme. Typically for semiconductors, the critical point structures change much less with temperature than with composition. Therefore, the “double peaking” phenomenon is much less of a problem.

In other respects the Temp layer behaves just like an alloy layer except that is has a Temperature value box and a Temperature Fit box instead of Alloy Fraction boxes. A typical edit dialog box for a temp layer is shown below.

**Temperature**

This box is used to specify the temperature, in °C, used when calculating optical constants. If more than one temp layer is present in a model, the same temperature will be used for all of them. Therefore, if one is fitting for temperature, the optical constants for all temp layers will change together.

**Temperature fit box**

This check box is used to set the temperature as a fit parameter. Do not try a fit with the Temperature Fit box and one of the optical constant fit boxes checked. Also, if there are other temp layers present in the model, do not check more than one Temperature Fit box. If one box is checked in any of the layers, the temperature in all the layers will track together.

**Alloy-temp layers**

This layer combines the properties of the alloy and temp layers and again several different optical constant parameterizations can be used, all of which are described in Appendix B. Again the simplest is component tables which represent the optical constants for a specific alloy fraction at a specific temperature. There is a list of the included temperatures and compositions. Also included is information for doing the two dimensional interpolation between the component tables. The specifics of the file formats are described in Appendix B.

When WVASe® is asked to calculate optical constants for this type of layer, the alloy fraction and temperature are used to find the closest two tabulated temperatures and the closest two tabulated compositions. Then using four of the
component tables, the optical constant at the specific wavelength is determined by two dimensional interpolation. As for alloy files, this is not done by simple interpolation, rather, information about the critical point structure is used to intelligently shift the optical constants before interpolating. This shifting procedure is performed in both the composition and temperature dimensions.

A representative edit dialog box for an alloy-temp layer is shown below.

![Edit dialog box for an alloy-temp layer.](image)

**Figure 7-31.** Edit dialog box for an alloy-temp layer.

![Graphical representation of the optical constants of the alloy-temp layer as a function of wavelength from 400 to 800 nm.](image)

**Figure 7-32.** Graphical representation of the optical constants of the alloy-temp layer as a function of wavelength from 400 to 800 nm.

The Alloy Fraction and Temperature value boxes and Alloy Fraction and Temperature Fit boxes are the same as for an alloy layer and temperature layer.

### 7.7 Function based layers

Function based layers derive their optical constants from a mathematical expression instead of a wavelength-by-wavelength table. The ability to use functions to describe optical constants comes from the fact that dielectric functions are not random functions of wavelength and that there is a specific relationship between the real and imaginary parts, the Kramers-Kronig (KK) relation. Function based layers have several very useful properties:
1. When fitting for the optical constants, many fewer function parameters are fit for than would be if a wavelength-by-wavelength table of optical constants was used. (Two values per wavelength).

2. Function based optical constants do not have noise associated with them, and they are more easily interpolated and extrapolated.

3. The function can be made to be internally KK consistent.

The only drawback to function based layers is that it is often difficult to find functions that are simultaneously flexible enough to describe the optical constants over a wide spectral range and stable enough when fitting the functional parameters.

Most of the function based layers are described below. Because of its importance and complexity, the Genosco\textsuperscript{®} layer, is described in the next chapter.

### Cauchy layer

Over part of the spectral range for many materials (dielectrics and semiconductors, not metals), the index of refraction $n$ and extinction coefficient $k$ can be represented by a slowly varying function of wavelength, $\lambda$ (converted to $\mu$m), and an exponential absorption tail, respectively:

$$n(\lambda) = A + \frac{B}{\lambda^2} + \frac{C}{\lambda^4}, \quad (\lambda \text{ in } \mu\text{m}) \quad (7.1)$$

$$k(\lambda) = \alpha e^{\beta \left(1.24(\mu\text{m})\left(\frac{1}{\lambda} - \frac{1}{\gamma}\right)\right)}, \quad (\lambda, \gamma \text{ in } \mu\text{m}) \quad (7.2)$$

The six parameters in this dispersion model are $A$, $B$, $C$, the extinction coefficient amplitude $\alpha$, the exponent factor $\beta$, and the band edge $\gamma$. Each of these parameters except for the band edge can be defined as a variable fit parameter in the Cauchy layer dialog box. The default Cauchy layer is \textit{cauchy.mat}. When a Cauchy layer is added or edited a dialog box is used like that shown below.

![Figure 7-33. The edit dialog box for a Cauchy layer.](image)
Figure 7-34. Graphical representation of the optical constants of the Cauchy layer in the previous figure.

The initial values shown in the dialog box are the defaults found in `cauchy.mat`, which are approximately valid for thermal silicon dioxide. The user may enter new values for any of them. The Layer Name, Comment, Thickness, OK, and Delete Layer items are the same as for the standard layer.

**important**

There are no spectral range limits for a Cauchy layer since the function can be evaluated for all wavelengths. However, this does not mean that the optical constants calculated using this formula are correct everywhere, just that they can be calculated everywhere.

**Opt. con. fit boxes**

These boxes work similarly to those of standard tabulated layers. The difference is that when neither box is checked, the optical constants are calculated using the Cauchy and exponential absorption functions. When either one box or both boxes are checked, the optical constants are taken from an internally stored list of fitting optical constants. This internal list is started with the functional values the first time a fit is performed. However, after the first fit of the optical constants, this internal list may be different than the functional values.

**Optical constants>> button**

This works exactly the same as for a standard tabulated layer. You just need to be aware where the values displayed in the table and graph are derived from. If one of the optical constant fit boxes is checked, then the displayed values are taken from the internally stored list of fitting optical constants. If neither of the optical constant fit boxes are checked, then the displayed values are calculated using the Cauchy and exponential absorption functions. When you save a set of optical constants, you have the option of saving them in one of two formats. You can either save the Cauchy parameters into a Cauchy type layer or you can save a tabulated optical constants list into a standard tabulated layer. The `cauchy.mat` file is just the default Cauchy material; you can save a Cauchy type layer under any name you want.

**Lorentz oscillator layer**

The Cauchy layer works well for many transparent materials but does not work at all for metals or for semiconductors above the fundamental bandgap. Lorentz layers, however, can be useful when working with metals, semiconductors above the fundamental gap, and conducting oxides like ITO. The description of the Lorentz layer presented here is primarily a technical one defining the model and
describing the edit box. A more in-depth discussion of the practical application of the Lorentz layer is presented in chapter 13 - ‘VASE® Data Analysis’.

The physical basis for Lorentz oscillators has been discussed in many textbooks, such as Optical Properties of Solids by F. Wooten. A simple description of the Lorentz layer is that it is a collection of absorption peaks which is also Kramers-Kronig consistent. The mathematical model WVASE® uses for a collection of Lorentz oscillators is as follows:

\[ \tilde{e}(h\nu) \equiv \varepsilon_1 + i\varepsilon_2 = \varepsilon_{\infty} + \sum_k \frac{A_k}{E_k^2 - (h\nu)^2 - iB_k h\nu} \] (7.3)

For the \( k \)th oscillator, \( A_k \) is the amplitude, \( E_k \) is the center energy, and \( B_k \) is the broadening of each oscillator. \( h\nu \) is the photon energy in eV. \( \varepsilon_{\infty} \) is an additional offset term defined in the model. Because of the way the function is defined you should note that although \( A_k \) is called the amplitude, it is technically more closely related to the area under the absorption peak. That is, the absorption peak for \( h\nu = E_k \) changes with changes in \( B_k \).

The default Lorentz layer is lorentz.mat. When a Lorentz layer is added or edited a dialog box is used like that shown below.

![Figure 7-35. The edit dialog box for a Lorentz layer with 2 oscillators.](image)

The values shown in the dialog box define a Lorentz layer with 2 oscillators. The optical constants defined by those parameters are shown below. The peaks are at 2 eV (left) and 4 eV (right). Note also the difference in the width of the peaks as defined by the broadening values in the Br column.

![Figure 7-36. The graphical representation of the optical constants from the above Lorentz layer as a function of photon energy from 1 to 5 eV.](image)
The Layer Name, Comment, Thickness, OK, Delete Layer, and Replace Layer items are the same as for the standard layer. The Opt. Con. fit boxes and Optical Constants>> button work just the same as for the Cauchy layer except the Lorentz mathematical model is used instead of the Cauchy model. The edit box items specific to the Lorentz layer are described below.

**# of terms**

This pull down box defines how many of the 7 available oscillators will be used in the calculation. For the case shown above, the # of terms is 2 and therefore only the first 2 oscillators are used and only the first 2 rows of oscillator parameters can be edited.

**Am**

This column of edit boxes and fit check boxes is used to define the oscillator amplitudes (in units of eV^2) and to select an amplitude as a fit parameter.

**Br**

This column of edit boxes and fit check boxes is used to define the oscillator broadenings (in units of eV) and to select a broadening as a fit parameter.

**En**

This column of edit boxes and fit check boxes is used to define the oscillator energy positions (in units of eV) and to select an energy as a fit parameters.

**e1inf**

This parameter defines the (dimensionless) offset ε₁∞ used in the model. The associated check box is used to define this value as a fit parameter.

**User-defined dispersion model layer (user layer)**

The user-defined dispersion model layer (“user layer”, for short) allows great flexibility in defining the functions to describe the dispersion of the optical constants of a given material. You can directly enter functions to describe the real and imaginary parts of either the dielectric function or complex refractive index. The individual functions you define must be real valued; the user layer does not perform complex arithmetic. You can define your own parameter names and select them as fit parameters. The edit dialog box for a user layer is shown below followed by the optical constants defined by this model.
Figure 7-37. The edit dialog box for a user-defined dispersion model. This user layer has been set up to model 7059 glass with some residual absorption.

Figure 7-38. Optical constant spectra calculated from the user-defined dispersion model shown in the previous figure, as a function of wavelength from 3000 to 17000 Å.

**Standard WVASE® buttons & features**

The ‘Comment’, ‘Thickness’, ‘OK’, ‘Replace Layer’, ‘Delete Layer’, ‘Opt. Const. fit’ boxes and ‘Optical Constants>>’ button items are the same as any other WVASE® layers. The unique features of the user layer are described below.

**Defining the optical function**

The user defines an optical function by typing formulas into the ‘n=’ (‘e1=’) and ‘k=’ (‘e2=’) edit boxes (see below). The complete optical function of the user layer is

\[
\begin{align*}
\tilde{n} &= \left[ n = \text{edit box} \right] - i \left[ k = \text{edit box} \right] \\
\tilde{\varepsilon} &= \left[ \varepsilon_1 = \text{edit box} \right] - i \left[ \varepsilon_2 = \text{edit box} \right]
\end{align*}
\]

The “in-line” notation requires that standard operators are placed between the operands and that groupings are defined by parentheses (see ‘e1=’ edit box).

---

\(^{1}\) WVASE® defines \(\tilde{n} = n - i k\) and \(\tilde{\varepsilon} = \varepsilon_1 - i\varepsilon_2\) with the negative signs, as per the Nebraska convention. However, absorbing materials will still have **positive** \(k\) and \(\varepsilon_2\) values.
The user adds new parameter names directly in the equations – parameter names do not need to be predefined. When the ‘OK’ button is selected, any newly defined parameters will be recognized and added to the parameter list immediately prior to exiting the user layer dialog box.

The user layer supports complex functions. This means that complex-valued terms can be included in the ‘n=’ and ‘k=’ (‘e1=’ and ‘e2=’) edit boxes.

The User Layer supports complex functions\(^{ii}\). This means that complex-valued terms (such as the Lorentz and other oscillator functions) can be written into ‘n=’ (‘e1=’) and ‘k=’ (‘e2=’) edit box formulas. A term can be made imaginary by making it the argument of an IMAG() function (for example, see “IMAG(Br2*wvl)” in the ‘e1=’ edit box of the user layer shown in Figure 7.38).

This means that the easiest way to create a complex optical function is to write the entire equation in the ‘n=’ (‘e1=’) box, then set the ‘k=’ (‘e2=’) formula equal to 0. An example of this is shown in Figure 7.38. Note that the ‘e2=’ edit box formula equals zero.

\(\text{Figure 7-39. Left: A user layer with complex-valued Gaussian oscillator and complex Lorentz term written into the ‘e1=’ edit box. Right: the resulting complex dielectric function.}\)

‘In terms of’ selection box
This selection box allows you to choose whether the formulas you are entering should be interpreted as the real and imaginary parts of the complex refractive index (n and k) or if they should be interpreted as the parts of the dielectric function \((\varepsilon_1\text{ and } \varepsilon_2)\).

‘n=’ (‘e1=’) edit box
The function written into this box defines is used to calculate the real part of the refractive index or dielectric function. However since the User layer supports complex equations, both the real and imaginary parts of the optical function can be written into the ‘n=’ (‘e1=’) edit box (see Defining the optical function section above).

‘k=’ (‘e2=’) edit box
The function written into this box is multiplied by \(i\), the square root of -1. Because the User layer now supports complex equations, this function is often set equal to 0 (see Defining the optical function section above).

\(^{ii}\) Available for WVASE\(^\oplus\) versions 2.989 and later.
**Wvl units**

This selection box allows you to pick the units used for wavelength in the user layer functions. The reserved variable “wvl” is assigned the wavelength value in the selected units. This setting is not related to the wavelength units *WVASE*

® uses elsewhere as defined by the [Global|Defaults or |Experimental_window|Range_Select options.

**Parameter name**

This pane lists the parameters *WVASE*

® has recognized in your equations. If you have just entered a new formula you can force *WVASE*

® to recognize the new parameters by using the OK button. When a new parameter is recognized you will be asked to define its value, and given the option to select it as a fit parameter.

**Parameter value**

This list contains the current values for parameters appearing in the formulas.

**Value button**

This button is used to set the value of the highlighted parameter. A parameter name can be highlighted by clicking on its row with the mouse.

**Parameter fit box**

If an asterisk * appears after the parameter value, then that parameter has been selected as an active fit parameter.

**Fit button**

This button is used to select a highlighted parameter name for fitting. If the parameter is already selected for fitting, this button deselects it. A parameter name can be highlighted by clicking on its row with the mouse.

**Delete button**

This button removes the selected parameter from the recognized parameter list. However, if that parameter still exists in one of the formulas, it will be re-added when the ‘OK’ button is selected.

**Operator list>>**

This button brings up a reference list of supported mathematical operations and functions. The user layer currently supports a number of operators and functions. These are listed in the tables that follow.
### Operators

The following operators are supported in the *user.mat* layer.

<table>
<thead>
<tr>
<th>Operator (not case sensitive)</th>
<th>Comments</th>
<th>Operator (not case sensitive)</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>+</td>
<td>Addition</td>
<td>^</td>
<td>Raising to a power</td>
</tr>
<tr>
<td>-</td>
<td>Subtraction</td>
<td>( [</td>
<td>Left Grouping</td>
</tr>
<tr>
<td>•</td>
<td>Multiplication</td>
<td>) ]</td>
<td>Right Grouping</td>
</tr>
<tr>
<td>/</td>
<td>Division</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Functions

The *user.mat* layer now supports the following functions, most of which accept complex arguments.

<table>
<thead>
<tr>
<th>function (not case sensitive)</th>
<th>Comments</th>
<th>function (not case sensitive)</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>exp()</td>
<td>Exponential</td>
<td>erf()</td>
<td>Error Function</td>
</tr>
<tr>
<td>ln()</td>
<td>Natural Logarithm</td>
<td>erfc()</td>
<td>Complimentary Error Function</td>
</tr>
<tr>
<td>log()</td>
<td>Base-10 Logarithm</td>
<td>sqrt()</td>
<td>Square root</td>
</tr>
<tr>
<td>sin()</td>
<td>Sine</td>
<td>sinh()</td>
<td>Hyperbolic Sine</td>
</tr>
<tr>
<td>cos()</td>
<td>Cosine</td>
<td>cosh()</td>
<td>Hyperbolic Cosine</td>
</tr>
<tr>
<td>atan()</td>
<td>Arctangent function</td>
<td>tanh()</td>
<td>Hyperbolic Tangent</td>
</tr>
<tr>
<td>tan()</td>
<td>Tangent function</td>
<td>torad()</td>
<td>*π/180°</td>
</tr>
<tr>
<td>unit()</td>
<td>Unit step function; (=1 for x≥0; =0 for x&lt;0)</td>
<td>todeg()</td>
<td>*180°/π</td>
</tr>
<tr>
<td>edge(x,a,b)</td>
<td>(=a, x&lt;0; =b, x&gt;0)</td>
<td>repart()</td>
<td>Real part</td>
</tr>
<tr>
<td>abs()</td>
<td>Absolute value</td>
<td>impart()</td>
<td>Imaginary part</td>
</tr>
<tr>
<td>sgn()</td>
<td>Sign of value</td>
<td>conj()</td>
<td>Complex conjugate</td>
</tr>
<tr>
<td>max(x,y)</td>
<td>Maximum of two values x &amp; y</td>
<td>imag()</td>
<td>*sqrt(-1)</td>
</tr>
<tr>
<td>min(x,y)</td>
<td>Minimum of two values x &amp; y</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Oscillator Functions

More complete descriptions of the oscillator functions can be found in the “Oscillator model Descriptions” section of the Genosc layer chapter. The User layer also supports many of the functions that are also found in the Genosc layer. The following table provides a brief description of the parameters for each oscillator. For more complete descriptions of the functions, please refer to the “Oscillator Model Descriptions” section of the GenOsc layer Chapter.

<table>
<thead>
<tr>
<th>function</th>
<th>Same as Genosc layer Oscillator function</th>
<th>style type</th>
<th>parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>lorentz(A,E,Br)</td>
<td>Lorentz</td>
<td>Lor.0(eV)</td>
<td>A=Amp</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Lor.5(cm⁻¹)</td>
<td>E= center energy</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Br = broadening</td>
<td></td>
</tr>
<tr>
<td>harmonic(A,E,Br)</td>
<td>Harmonic</td>
<td>Har.0(eV)</td>
<td>A=Amp</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Har.5(cm⁻¹)</td>
<td>E= center energy</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Br = broadening</td>
<td></td>
</tr>
<tr>
<td>gaussian(A,E,Br)</td>
<td>Gaussian</td>
<td>Gau.0(eV)</td>
<td>A=Amp</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Gau.5(cm⁻¹)</td>
<td>E= center energy</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Br = broadening</td>
<td></td>
</tr>
<tr>
<td>gausslor(A,E,Br,Bmix)</td>
<td>Gauss-Lorentz</td>
<td>G-L.0(eV)</td>
<td>A=Amp</td>
</tr>
<tr>
<td></td>
<td></td>
<td>G-L.5(cm⁻¹)</td>
<td>E= center energy</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Br = broadening</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Bmix = Bmix</td>
<td></td>
</tr>
<tr>
<td>cppb(A,E0,Br,Theta,u)</td>
<td>user.mat CPPB function:</td>
<td></td>
<td>A=Amp</td>
</tr>
<tr>
<td></td>
<td></td>
<td>E0=E₀ center energy</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Br= σ, broadening</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Theta=θ, phase projection factor</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>u = μ, μ = ½ for 1-Dimensional CP’s</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>μ = 0 for 2-D CP’s [denominator becomes ln(2E₀ – 2E – iμ)]</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>μ = -½ for 3-Dimensional CP’s</td>
<td></td>
</tr>
<tr>
<td>tauclor(A,E0,C,Eg)</td>
<td>Tauc-Lorentz</td>
<td>T-L.0(eV)</td>
<td>A=Amp</td>
</tr>
<tr>
<td></td>
<td></td>
<td>E0=E₀ center energy</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>C = broadening</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Eg = Bandgap E</td>
<td></td>
</tr>
<tr>
<td>pole(A,E)</td>
<td>Pole</td>
<td>Pole.0(eV)</td>
<td>A=Amp</td>
</tr>
<tr>
<td></td>
<td></td>
<td>E= center energy</td>
<td></td>
</tr>
<tr>
<td>drude(A,Br)</td>
<td>Drude</td>
<td>Drd.0(eV)</td>
<td>A=Amp</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Drd.5(cm⁻¹)</td>
<td>E= center energy</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Br = broadening</td>
<td></td>
</tr>
<tr>
<td>CPM0(A,E,Br)</td>
<td>CPM0</td>
<td>CPM0.0(eV)</td>
<td>A=Amp</td>
</tr>
<tr>
<td></td>
<td></td>
<td>E= center energy</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Br = broadening</td>
<td></td>
</tr>
<tr>
<td>CPM1(A,E,Br)</td>
<td>CPM1</td>
<td>CPM1.0(eV)</td>
<td>A=Amp</td>
</tr>
<tr>
<td></td>
<td></td>
<td>E= center energy</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Br = broadening</td>
<td></td>
</tr>
<tr>
<td>CPM2(A,E,Br)</td>
<td>CPM2</td>
<td>CPM2.0(eV)</td>
<td>A=Amp</td>
</tr>
<tr>
<td></td>
<td></td>
<td>E= center energy</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Br = broadening</td>
<td></td>
</tr>
<tr>
<td>CPM3(A,E,Br)</td>
<td>CPM3</td>
<td>CPM3.0(eV)</td>
<td>A=Amp</td>
</tr>
<tr>
<td></td>
<td></td>
<td>E= center energy</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Br = broadening</td>
<td></td>
</tr>
<tr>
<td>function (not case sensitive)</td>
<td>Same as Genosc layer Oscillator function</td>
<td>style type</td>
<td>parameters</td>
</tr>
<tr>
<td>-------------------------------</td>
<td>-----------------------------------------</td>
<td>------------</td>
<td>------------</td>
</tr>
<tr>
<td><code>tanguy(A,Eg,B,R,ln(g))</code></td>
<td>Tanguy</td>
<td></td>
<td>A = Amp, Eg = bandgap, B = broadening, R = Unscreened bind. energy, ln = ln(screening factor)</td>
</tr>
<tr>
<td><code>codylorentz(A,E0,B,Eg,Ep,Et,Eu)</code></td>
<td>Cody-Lorentz</td>
<td>C-L.0(eV)</td>
<td>A = Amp, E0 = center energy, B = broadening, Eg = bandgap, Ep = Cody to-Lor transition, Et = Urbach transition, Eu = exp rate</td>
</tr>
<tr>
<td><code>ionic(ET,eDC,einf,B)</code></td>
<td>Ionic1</td>
<td>ion1.0(eV), ion1.5(cm⁻¹)</td>
<td>ET = E₇(transverse phonon energy), eDC = εₑ, einf = εᵣ, B = broadening</td>
</tr>
<tr>
<td><code>ionic2(Eto,elo,eDC,B)</code></td>
<td>Ionic2</td>
<td>ion2.0(eV), ion2.5(cm⁻¹)</td>
<td>Eto = E₇(transverse phonon energy), elo = E₇(longitudinal phonon energy), eDC = εₑ, B = broadening</td>
</tr>
<tr>
<td><code>TOLO(Eto,elo,Bto,Blo)</code></td>
<td>TOLO(eV)</td>
<td>TOLO.0(eV)</td>
<td>Eto = E₇(transverse phonon energy), elo = E₇(longitudinal phonon energy), Bto = E₇(transverse phonon broad.), Blo = E₇(longitudinal phonon broad.)</td>
</tr>
<tr>
<td><code>TOLOCM(Eto,elo,Bto,Blo)</code></td>
<td>TOLO(cm)</td>
<td>TOLO.5(cm⁻¹)</td>
<td>Eto = E₇(transverse phonon energy), elo = E₇(longitudinal phonon energy), Bto = E₇(transverse phonon broad.), Blo = E₇(longitudinal phonon broad.)</td>
</tr>
</tbody>
</table>

**Sto(#,x) and Rcl(#) Functions**

The user layer has available the `sto(#,x)` and `rcl(#)` functions that allow some pre-calculations to be performed once and then reused to produce the final result.

<table>
<thead>
<tr>
<th>function (not case sensitive)</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>sto(#,val)</code></td>
<td>Store(#0 … 19, value). (See example below).</td>
</tr>
<tr>
<td><code>rcl(#)</code></td>
<td>Recall(#0 … 19). (See example below).</td>
</tr>
<tr>
<td><code>;</code></td>
<td>Expression separator (see example below).</td>
</tr>
</tbody>
</table>

In the example below, both the ‘n’ and ‘k’ equations produce the same final functional output. The ‘n’ equation first calculates 1/wvl and stores the results in slot#1 (“sto(1,1/wvl”)”. The slot# for the ‘sto’ function can be from 0 to 19. The ‘;’ is used to start a new calculation. The final output for ‘n’ is defined by the section on the right-side of the final ‘;’ in the equation. Next, 1/(wvl*wvl) is calculated using the previous results stored in slot#1 with the new result stored in slot#2 (“sto(2,rcl(1)^2”). Similarly, 1/(wvl*wvl*wvl*wvl) is calculated and stored in slot#3. The final ‘n’ value for output is then calculated using the results from slot#2 and slot#3 (“A+B*rcl(2)+C*rcl(3)”) to produce the standard Cauchy function.
In the example above, the use of the ‘sto’ and ‘rcl’ functions is certainly not required – this is only a simple demonstration of the functions. However, there may be situations where a more complicated equation can be simplified by pre-calculation and reuse of certain terms. Please note, that the values stored by one equation are NOT available to any other equation. In this example, the results of slots#1-3 are NOT available in ‘k’ equation; they must be re-entered in ‘k’ equation if they are needed.

Physical constants

The following physical constants have also been included for convenience.

<table>
<thead>
<tr>
<th>function</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>pi(0)</td>
<td>π</td>
</tr>
<tr>
<td>epsz(0)</td>
<td>ε₀</td>
</tr>
<tr>
<td>musz(0)</td>
<td>μ₀</td>
</tr>
<tr>
<td>ev(0)</td>
<td>Electron charge</td>
</tr>
<tr>
<td>sol(0)</td>
<td>Speed of light</td>
</tr>
<tr>
<td>plank(0)</td>
<td>h, Plank’s constant</td>
</tr>
<tr>
<td>hbar(0)</td>
<td>ħ</td>
</tr>
<tr>
<td>plank(1)</td>
<td>h, Plank’s constant</td>
</tr>
<tr>
<td>hbar(1)</td>
<td>ħ</td>
</tr>
<tr>
<td>boltz(1)</td>
<td>Boltzman’s constant</td>
</tr>
</tbody>
</table>
layereps, layernk, user & usertime functions

The following functions return values originating from outside the user.mat layer; either from another layer or from the “user” data columns.

<table>
<thead>
<tr>
<th>function</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>layereps(layer#)</td>
<td>( \varepsilon_1, \varepsilon_2 ) of specified layer</td>
</tr>
<tr>
<td></td>
<td>(see section entitled “layereps &amp; layernk functions”)</td>
</tr>
<tr>
<td>layernk(layer#)</td>
<td>( n, k ) of specified layer</td>
</tr>
<tr>
<td></td>
<td>(see section entitled “layereps &amp; layernk functions”)</td>
</tr>
<tr>
<td>user(0)</td>
<td>Data point User1 value (e.g., temperature values acquired during data</td>
</tr>
<tr>
<td></td>
<td>acquisition using HTC 100 HeatCell or cryostat options)</td>
</tr>
<tr>
<td>usertime(0)</td>
<td>Data point Time value (for data acquired during dynamic data scan)</td>
</tr>
</tbody>
</table>

The user can also include optical constants from other layers by using the layereps(layer#) and layernk(layer#) functions. The argument “layer#” MUST be specified as the layer number of the referenced layer that appears on the left-side of each layer in the model window (circle in figure below).

Figure 7-41. Model window showing locations of the layer numbers in a model schematic.

The figure below illustrates an example of these commands in a user layer. Note that the operator arguments are specifically defined as “-1” and “-2”. In this example, only \( \varepsilon_1 \) needs to be defined, since the User layer accepts complex expressions.

Figure 7-42. User.mat layer dialog box showing layeps commands.
NOTE #1: The layereps(layer#) function would only be valid for dielectric function equations. Therefore, the user should select the “e1,e2” radio button in the lower left corner of the user.mat layer dialog box.

NOTE #2: The user must manually update “layer#” if the number of the referenced layer has been changed in the model.

This particular User layer produces the same optical constants as are found in sum_eps.mat substrate (the sum_eps.mat layer is described in WVASE® summation layers application note, which can be obtained from Applications group of J.A. Woollam Co., Inc.).

The user(0) and usertime(0) functions return parameters usually recorded during dynamic data acquisition. As the first figure below illustrates, the time parameter is recorded in a column immediately to the right of the last data column (the Δ data column for ellipsometric data types). The User1 parameter is placed in the right-most column. For the HeatCell data illustrated in the two figures below, the User1 value is the heat stage thermocouple temperature.

![User time and User1 Value](image1)

*Figure 7-43. Experimental data window of real-time Dynamic Scan data from HeatCell showing locations of the Usertime and User1 value. These same data are plotted in the next Figure.*

![Graph window](image2)

*Figure 7-44. WVASE® Graph window of real-time Dynamic Scan data from HeatCell.*
Parametric semiconductor layer

This is the most sophisticated and correspondingly most complicated function-based optical constant layer. This model was principally designed to work with semiconductor optical constants, however it is not limited to that application.

Semiconductors typically have the most complicated optical constants to work with because of their sharply defined critical point structure and the presence of direct bandgaps where the absorption can abruptly go to zero. The parametric semiconductor layer can, without compromising the quality of data fits, replace the usual tabulated optical constant lists while using a reasonable small set of adjustable parameters. The model is Kramers-Kronig consistent and can correctly describe semiconductor dielectric functions, below, above, and through the fundamental bandgap. The model is flexible enough to describe the complicated critical point structures, but is stable enough to describe dielectric functions grouped by compositional alloys, temperature dependence, and doping. This model allows the integration of data sets acquired using different measurement techniques and covering different spectral ranges to be simultaneously analyzed, providing wide spectral coverage.

The details of using this layer are described in chapter 13 - “Analysis of Static Optical Data”. Only a representative edit box is presented here.

![Figure 7-45. The edit box for a parametric semiconductor layer used to model the optical constants of GaAs.](image)

7.8 Composite layers

Composite layers combine information from more than one set of optical constants. They are typically used to model interface roughness and layers with optical constants that change as a function of position.

Effective Medium Approximation (EMA) layer

The effective medium approximation (EMA) layer provides a method to mix 2 or 3 sets of optical constants together. The usual interpretation of the EMA theory is that small particles of one material are suspended in a matrix of the host material. Under that approximation the optical constants can be mixed in a way that satisfies certain electromagnetic equations. (For a review of effective medium
theory, see D.E. Aspnes, Thin Solid Films 89, 249 (1982).) In practice it is just a reasonable way to mix optical constants together.

An EMA is most often used to simulate a small amount of interfacial intermixing or surface roughness. It can also be used to simulate small index shifts by including a small fraction of voids. For these applications, the EMA layer is very useful. However, if the materials you want to intermix form a true alloy system like AlGaAs, do not use an EMA layer to model an intermediate set of optical constants for a thick layer.

To define an EMA layer, two parts are needed:

1. The optical constants to be mixed together
2. The manner in which the mixing is to occur.

The default EMA layer in WVASE® is ema.mat. The edit box for a fully specified three-constituent EMA layer is shown below. When an EMA layer is first added the material names will be blank, and the constituent materials must be selected by the user before the EMA layer dialog box may be closed.

The # of constituents box

This pull down box sets the number of constituents for the EMA. If the # of Constituents is set to 1, then the layer becomes 100% material #1.

Material #1 button

This button allows you to select the material to use as the “host” material. The component fraction of this material is calculated as 100% minus the fractions of the other materials. If possible you want this material to have the highest component fraction. (This helps with the numeric calculation of the effective optical constants.) You can put any material type you want in this slot from a standard tabulated material, to an alloy type material, to a function based material like a Cauchy, or
even another EMA layer. However, if you use something other than a standard material you should probably include this as a coupled layer. You do this by first putting the desired EMA constituent in the model below the EMA layer. If the material would not normally appear below the EMA layer, put it below the EMA layer and give it a thickness of zero. (A zero thickness layer appears in the model but does not effect model calculations.) Then use the Material button to include that material again and answer “yes” when asked if you want to couple to the existing layer. In the example above, the gaas_unl material in the EMA layer is coupled to the gaas_unl substrate layer. Only by coupling the layers together will you have access to the edit box for the component materials.

**Material #2 button**

This button allows you to select the material to use as the second constituent of the EMA. It is operationally equivalent to the Material #1 Button.

**Fraction #2 box**

This box defines the component fraction for material #2 and the associated fit box allows you to select this fraction as a fit parameter.

**Material #3 button**

This button allows you to select the material to use as the third constituent of the EMA. It is operationally equivalent to the Material #1 Button.

**Fraction #3 box**

This box defines the component fraction for material #3 and the associated fit box allows you to select this fraction as a fit parameter.

**EMA type setting**

This box allows you to select exactly how the EMA is calculated. The Bruggeman and Maxwell-Garnett formulations use slightly different approximations. For most applications the differences are very small. The Linear option performs a simple weighted average of the optical constants.

**Depolarization factor box**

This factor is used to describe the microstructure of the constituents in the EMA mixture. It is only used with the Bruggeman and Maxwell-Garnett models, and only when there are 2 material constituents. The default depolarization factor of 1/3, assumes that material #2 is incorporated as small spheres within the “host” material #1. The depolarization factor can also be defined as a fit parameter by using the fit box next to it. However, to avoid correlation effects, it is usually best to fix it at one value. The default value of 1/3 usually works just fine.

A depolarization factor of 1 means maximum screening of the electric field and a factor of 0 means no screening of the electric field. Under the assumption that the light travels through the film at normal incidence, a factor of 1 represents a needle-like or columnar microstructure and a factor of 0 represents flat disks or a laminar microstructure. However, since most ellipsometer data are acquired at non-normal incidence angles, the standard EMA.mat layer is incorrect for depolarization factors that are not equal to 1/3. Instead, a layer with uniaxial or biaxial character is required to model this form of shape anisotropy. Nevertheless, in many instances the ellipsometric measurement will not be very sensitive to the anisotropy, and the standard ema.mat layer is an adequate approximation.
Some types of structured layers (e.g., porous silicon), require a complete
anisotropic treatment. In those cases, you may want to use the Bruggeman Biaxial
EMA layer. Contact the Woollam Co. for details about this rarely-used layer.

EMA layer applications

The following is a short list of the general applications for EMA layers.

Simulate interfacial intermixing

Create an EMA layer that mixes the material above and below the interface.
Set the fraction for material #2 to 50%. Then fit the thickness only.

Simulate surface roughness

Create an EMA layer that mixes the top most material with void (void, mat,
\(n=1, k=0\)). Set the fraction for material 2 to 50%. Then fit the thickness. In rare
cases fitting the constituent fraction will also help, but if the fraction goes above 80%
or below 20% you probably don’t have sensitivity to the value and it should be set
back to 50%. In most cases fitting for the constituent (void) fraction along with the
roughness layer thickness yields a very strong correlation between these two
parameters.

Simulate oxidized surface roughness

For some materials, especially semiconductors and metals, a native oxide
with very different optical constants will be formed. If just a native oxide layer does
not seem sufficient, you might try a three constituent EMA that mixes the uppermost
material with void and with the oxide optical constants. Set fractions #2 and #3 to
33%. Then fit the thickness. If you also fit the fraction values you might be able to
determine whether you have any sensitivity to those parameters.

Simulate index shifts

The index of some transparent materials can be affected by small dopant
levels or deposition process variations. Thus the optical constants from one film to
the next may vary slightly in absolute magnitude but change little in dispersion
(shape). In this case, the optical constants from one film can be used to approximate
the optical constants of another film by shifting the index up or down. This could be
done by using a Cauchy layer and allowing the Cauchy ‘A’ parameter to vary, but it
can also be done by forming an EMA layer that mixes the original optical constants
with the void optical constant spectra (index of unity, extinction coefficient of zero).
In this case, the void fraction is not included to imply that there are actually holes in
the material. Rather, this is just a convenient way to model an optical constant shift.
A positive void fraction implies a slightly lower index, and a negative void fraction
implies a slightly higher index.

Model partially crystallized silicon (polysilicon)

In silicon semiconductor manufacturing one often encounters silicon films
that are neither totally crystalline nor totally amorphous. To model this type of layer,
a three constituent EMA of amorphous silicon, crystalline silicon, and voids can
often be used. It will usually be necessary to fit for both composition fractions.
Most good quality poly-silicon can be fit with a two-constituent EMA of crystalline
and amorphous silicon, although both the two- and three-constituent models tend to
work best when the film is either mostly crystalline or mostly amorphous.
Surface roughness layer

The surface roughness layer (*srough.mat*) is a special type of EMA layer. This layer automatically forms a 50% EMA layer between the top layer in the model and the ambient material. This layer can also be used in growth rate analyses because it can “float” on top of the growing layer (See “Dynamic Data Analysis” chapter).

![Edit dialog box for a surface roughness layer (*srough.mat*).](image)

**Figure 7-47.** Edit dialog box for a surface roughness layer (*srough.mat*).

Intermix Layer (*intermix.mat*)

The intermix layer\(^{iii}\) is an EMA layer that can model interfacial mixing or interface “roughness” by mixing the layers above and below the interface in 50:50 Bruggeman EMA. It can be confusing because the layer subtracts thickness from the surrounding layers to add to its own thickness. This design allows the intermix layer to change thickness without changing the interference structure in the data.

The intermix layer can be converted into a Graded intermix layer by right-clicking on the intermix layer and selecting ‘Convert ‘Intermix’ to ‘Graded Intermix’. The details of the graded-intermix layer are described below in the “Graded-intermix Layer” section.

To understand the intermix layer, consider an intermix layer of thickness \(C\) inserted between layers of Mat1 (thickness \(A\)) above and Mat2 (thickness \(B\)) below (see figure below). The intermix is expanded as three layers as follows:

- Sublayer\#1 thickness is \(-C/2\) with optical constants of Mat1,
- Sublayer\#2 has thickness \(C\) with optical constants from a 50:50 EMA of Mat1 and Mat2, and
- Sublayer\#3 has thickness \(-C/2\) with optical constants of Mat2.

By expanding the intermix layer model, we can see that the intermix layer can be inserted into an existing model to simulate interface roughness without significantly changing the overall interference pattern from the layer stack. An intermix layer can be placed anywhere in a model (topside or backside). The similar surface roughness layer (*srough.mat*) only works as the top layer in a model.

\(^{iii}\) Available for WVASE versions 2.989 and later.

![Intermix layer model and equivalent Bruggeman EMA layer model.](image)

**Figure 7-48.** Intermix layer model and equivalent Bruggeman EMA layer model.
7.9 Graded layers

Graded layers work by creating a series of homogenous layers with optical constants that change slightly in each layer. Each of these piecewise constant layers is called a “slice” (see figure below). The more slices you use the closer the model approximates a true grading. However, increasing the number of slices rapidly increases the computing time required to calculate data from the graded model. Generally not many slices are needed, because optical measurements are not very sensitive to the fine details of the grading as long as the thickness of each individual slice is much smaller than the measurement wavelengths. Finally, there is a limit on how many layers you can use (see |Global|Defaults) and each slice counts against that limit.

The # Sublayers determines the number of sublayers (slices) will make up the graded layer. Odd integer values are generally preferred. One way to determine the right number is to increase the # Sublayers just until the MSE no longer decreases.

The following sections describe the Simple Graded layer (gradedsimple.mat), the Graded Intermix layer (intermix2.mat), the Function-based Graded layer (graded2.mat), and the old graded.mat layer.

Simple Graded Layers (gradedsimpleINDEX.mat & new gradedsimpleEMA.mat)

The Simple Index Graded layer and the new Simple EMA Graded layer (WVASE® vers. 3.736 and later) makes it easier to model layers with relatively small amounts of vertical grading. When the grading range is small, the Simple Index and Simple EMA layers will produce equally good fits to the same data.

However, the %Variation of the Index graded layer will generally be different from %Void range for a similar MSE result. This is because of the following:

- The Index grading directly grades the complex refractive index, while EMA grading effectively grades the dielectric function via the EMA %Void fraction.
- A positive %Variation of the Index grading increases the index; while a positive %Void of the EMA grading decreases the index.
- Even if the Exponent value is the same (e.g., equal to 1), the two versions will produce a different index profile shape, since $\hat{n} = \sqrt{\varepsilon^*}$.

Under certain circumstances the simple index grade will not work well for large %Variation values. For one thing the large variations index in some positions in graded layer can extend to un-physical values (e.g., $n < 1$).

Simple Index Graded Layer (gradedsimple.mat or gradedsimpleINDEX.mat)

Any non-substrate layer can be converted to a Simple Graded layer model by right-clicking with the mouse while the cursor is on the target layer. When the context-sensitive pop menu appears, select the “Convert to Simple Index Grade” menu item. WVASE® will automatically do the following:

- It adds a Simple Index Graded layer on top of the target layer.
- It transfers the target layer thickness to the Simple Index Graded Layer, and sets the target layer thickness to zero (it is now a dummy layer that is coupled into the Simple Graded Layer).
• It opens the Simple Index Graded Layer dialog box (see Figure 7-49 below).

![Simple Index Graded Layer dialog box](image)

**Figure 7-49. Left: Simple Index Graded Layer conversion process. Right: Simple Index Graded Layer dialog box.**

Equations (7.4) – (7.6) define the grading profiles of the Simple Index Graded layer. In the equations, $x$ is a normalized depth:

\[ 0 < x < 1 \]

- $C$ is the %Variation range
- $A$ is the Exponent

For the Asymmetric case, the refractive index (real or complex) is a function of normalized depth

\[
\hat{n}_{\text{simplegrad}}(x) = \hat{n}_{\text{mat}} \cdot \left[ \frac{C}{100} \cdot \left( x^A - \frac{1}{A+1} \right) \right]
\]

(7.4)

\[
\int_0^1 \frac{C}{100} \cdot \left( x^A - \frac{1}{A+1} \right) dx = 0
\]

For the Symmetric case:

\[
\hat{n}_{\text{simplegrad}}(x) = \hat{n}_{\text{mat}} \cdot \left[ \frac{C}{100} \right] \cdot \left\{ \begin{array}{ll}
\frac{1}{2} (2x)^A - \frac{1}{2}, & x \leq 0.5 \\
\frac{1}{2} - \frac{1}{2} (2 - 2x)^A, & x > 0.5
\end{array} \right.
\]

(7.5)

\[
\int_0^{0.5} \frac{1}{2} (2x)^A - \frac{1}{2} dx = \frac{1}{2} \left( \frac{1}{A+1} - 1 \right), \quad \int_{0.5}^1 \frac{1}{2} (2 - 2x)^A + \frac{1}{2} dx = \frac{1}{2} \left( - \frac{1}{A+1} + 1 \right)
\]

In both cases,

\[
\int_0^1 \hat{n}_{\text{simplegrad}}(x) dx = 0
\]

(7.6)

The various sections and parameters of the Simple Graded Layer dialog box are described below. The dialog box is shown in Figure 7-49.

**Material 1**

Use this button to enter the material file that is to be graded. The material file will contain the average values for the graded film. If you want to vary the average values, then Material 1 should be a coupled layer. In this case, the layer must exist...
below the Simple-graded layer in the model. If a material file is coupled, it will be shown with parentheses around the name in the simple-graded dialog box.

**%Variation Range box**

The range of variation is set by the %Variation Range box. This value refers to the index variation from top to bottom of the film. The reference material provides the average index with variation above and below the average dependent on the exponent and symmetry specifications. Since the average index is effectively independent of the details of the grade profile, the positions of interference oscillations will not change appreciably as the profile changes. This helps the fitting algorithm stay locked onto the proper average index and thickness values while testing the shape parameters to see if a better fit can be obtained.

**Exponent and Symmetric Profile**

The shape of the grading profile can be adjusted using the Exponent Box and the Symmetric Profile Checkbox. The default profile shape is a linear grade (exponent = 1). The following figures show the profiles for various exponent values.

![Effect of Exponent, Symmetric Profile](image)

**# Sublayers**

The # Sublayers determines the number of sublayers (slices) will make up the Simple Graded layer. *Odd integer values are generally preferred*. The default # Sublayers = 5. For films greater than about 100nm, this number should be increased to at least 9 or 11. One way to determine the right number is to increase the # Sublayers just until the MSE no longer decreases.

![Effect of Exponent, NOT Symmetric](image)

*Figure 7-50. Index profiles for Simple Graded layers with different Exponent values.*
Graph

The graph shows the shape of the profile at the user-specified wavelength in the Wavelength box. Click on the graph to redraw the updated profile after changing any of the parameters. The graph values can be copied to the clipboard by selecting the “Data to Clipboard” button. The graph will show the index variation versus the default thickness, with the correct thickness of this layer used to define the graph range.

Simple EMA Graded Layer (gradedsimpleEMA.mat)

Any non-substrate layer can be converted to a Simple EMA Graded layer model by right-clicking with the mouse while the cursor is on the target layer. When the context-sensitive pop menu appears, select the “Convert to Simple EMA Grade” menu item. WVASE® will automatically do the following:

- It adds a Simple Graded EMA layer on top of the target layer.
- It transfers the target layer thickness to the Simple Graded Layer, and sets the target layer thickness to zero (it is now a dummy layer that is coupled into the Simple Graded Layer).
- It opens the Simple Graded EMA Layer dialog box (see Figure 7-49 below).

%Void Range box

All of the parameters and sections of the Simple EMA graded layer dialog box is the same as the Simple Index graded layer box, except for the %Void range, which is the range of void fraction in the EMA of the sublayers. Material #1 provides the other constituent of the EMA, and the void mixture with this material depends on the exponent and symmetry specifications.

Equations (7.7) through (7.9) define the grading profiles of the Simple EMA Graded layer. In the equations, \( x \) is a normalized depth:

\[
0 < x < 1
\]

\( C \) is the %Void range

\( A \) is the Exponent

For the Asymmetric case, the refractive index (real or complex) is a function of normalized depth:
\[ f_{\text{void}}(x) = \frac{C}{100} \cdot \left(x^A - \frac{1}{A+1}\right) \]  
\[ \int_0^1 C \cdot \left(x^A - \frac{1}{A+1}\right) dx = 0. \]  
\[ (7.7) \]

For the Symmetric case:

\[ f_{\text{void}}(x) = \frac{C}{100} \cdot \begin{cases}  
\frac{1}{A} (2x)^A - \frac{1}{A}, & x \leq 0.5 \\
\frac{1}{A} - \frac{1}{A} (2-2x)^A, & x > 0.5 
\end{cases} \]
\[ \int_0^{0.5} \frac{1}{A} (2x)^A - \frac{1}{A} dx = \frac{1}{A} \left( \frac{1}{A+1} - 1 \right) \quad \int_0^{0.5} \frac{1}{A} (2-2x)^A + \frac{1}{A} dx = \frac{1}{A} \left( \frac{1}{A+1} + 1 \right) \]
\[ (7.8) \]

In both cases,

\[ \int_0^1 f_{\text{void}}(x) dx = 0. \]
\[ (7.9) \]

**Graded-Intermix Layer (intermix2.mat)**

The Graded Intermix layer is similar to the Intermix layer in that it performs an EMA mixing of the layers above and below it, and it also ‘subtracts’ from the thickness of the surrounding layers. However; Intermix2 supports multiple slices and grading profiles similar to the Simplegraded material file. Click on the graph to redraw the updated profile after changing any of the parameters. The ‘Depth Profile’ plot has been modified to correctly show the behavior of the Intermix2 layer (and now also Intermix and Srough layers). *(Discussed in later section.)*

![Image](image.png)

Figure 7-52. Intermix layer model and equivalent Bruggeman EMA layer model.

The # Sublayers determines the number of sublayers (slices) will make up the graded layer. Odd integer values are generally preferred. One way to determine the right number is to increase the # Sublayers just until the MSE no longer decreases.

**The Function-based graded layer (graded2.mat)**

The function-based graded layer *(graded2.mat)* is a more powerful and flexible version of the older graded.mat layer. The function-based graded layer allows the user to grade the parameters of the referenced (coupled) layer, while the simple-graded layer *(gradedsimple.mat)* simply grades optical constants at every wavelength \((n(\lambda)\) and \(k(\lambda)\), or \(\varepsilon_1(\lambda)\) and \(\varepsilon_2(\lambda)\))*.
Any user-fittable parameter (except $n$ and $k$) in the referenced layer (sometimes called the “coupled” or “dummy” layer) can be graded. Example parameters might include the $An$ term of a Cauchy layer, the $\rho$ (resistivity) term of a Drude oscillator, or the amplitude of a Tauc-Lorentz oscillator (see figure below).

The next figure shows the optical constants $n(\lambda)$ and $k(\lambda)$ from the top and bottom of the graded layer shown in the figure above.

Using the Function-based graded layer

Converting to function-based graded layer using standard Layer-Related Pop menu

The easiest way to convert a layer to a function-based graded layer is to place the cursor over the layer you wish to convert, then press right mouse button. This will open a context-sensitive menu that includes a number of options such as Edit, Delete, etc. That menu will include a “Convert to Function-Based Graded Layer” option (see next figure).
The function-based graded layer dialog box is shown in the figure below. Note that it has the usual options found in all WVASE® layers, including a Thickness box, as well as a “Replace Layer”, “Delete Layer”, “Save” and “OK” buttons. The additional features are discussed in the following sections.

Parameter List & Add/Edit Grade Profile

Each parameter in the coupled layer can have its own grading profile, by selecting the parameter in the leftmost listbox and clicking ‘Add/Edit Grade Profile’.

Material Name (Material 1, 2)

The user can specify 1 or 2 material files, but both layers must be coupled from existing layers in the WVASE model. If 2 materials are used, they must be of the same type (e.g., both CAUCHY layers).
**Add/Edit Grade Profile**

Each parameter in the coupled layer can have its own grading profile, by selecting the parameter in the leftmost listbox and clicking ‘Add/Edit Grade Profile’. This will open the Grade Profile dialog box (see below).

**Return to Default Grade**

If a parameter is not to be graded, selecting this button will return to the parameter value to that found in the coupled reference layer.

**Grade Profile Dialog Box**

After you press the “Add/Edit Grade Profile” for a parameter, the Profile dialog box appears (see figure below). This allows the variation of that parameter to be set.

As before, grading profiles can be node based or use a continuous equation (Compare next two figures). The parameter profiles and the optical constant profiles can be graphed and copied to the clipboard. Mouse Click on the graph to redraw the updated profile after changing any of the parameters.

![Profile dialog box, showing a 2-node profile.](image)

When using the continuous equation mode, nodes are still used to define the density of slices across the film. This is illustrated by this figure. Only three slices define the first 60% of the film depth, where the profile is almost flat. Narrower slices define the elbow in the profile (60% – 90%), and even narrow slices define the upper 90% – 100% region of the film.
Figure 7-58. Profile dialog box, showing Continuous equation profile.

Note equation (lower left portion of Profile dialog box) includes two user-defined parameters (A and B) as well as “d”, which represents the depth in the layer and is reserved by the program.

**Fit, Value & Delete buttons**

The “Fit”, “Value” and “Delete” buttons provides control of the user-created parameters. They appear only when the “Continuous Equation” radio button is selected (see Figure above).

**Operator List**

The Operator List provides a list of all the functions available to the user when creating a continuous equation. It appears only when the “Continuous Equation” radio button is selected (see Figure above).

**Match Ends**

When “Match ends” is checked, the profile is “sliced up” using the same algorithm as the older graded.mat layer (see Figure below). However, the ‘unchecked’ behavior provides a more accurate representation of the grading profile.

Figure 7-59. Profile dialog box, showing Continuous equation profile.
Examples of Continuous Equation Profiles for the Function-based graded layer

Several continuous equation examples are illustrated below. All of them are based on 2500 nm thick Function-based graded layer coupled to a Cauchy layer.

Figure 7-60. Left: Model used for all Continuous Equation examples. Right: Function-based graded layer dialog box, showing exponential grading profile for the Cauchy An parameter.

**Exponential function examples (base value defined at bottom of layer)**

The first example is a simple exponential function for the Cauchy parameter $A_n$. The equation is shown in the figure below. The equation has two fittable parameters, $A_0$ and rate. $A_0$ defines the value at the bottom of the layer. The Parameter $d$ is reserved by WVASE and refers to the normalized Depth. ($d = 0$ at bottom of layer, $d = 1$ at top of layer).

Figure 7-61. Profile dialog box, showing an exponential Continuous equation profile. Top Left circle indicates equation, Bottom left circle indicates definition of $d$ parameter. Right circle indicates fit parameter and arrow indicates exponential profile curve.
The next figure shows two exponential profiles: \( A_n = [A_0 + A \exp(d/rate)] \) and \([A_0 - A \exp(d/rate)]\). The base value \((A_0)\) is defined for the bottom of the layer, and the \(A\) and \(rate\) define the magnitude and rate of change.

**Exponential function examples (base value defined at top of layer)**

Replacing the dependent variable \(d\) with \((1 - d)\) effectively places the function’s origin at the top of the layer. This allows the base value to define the quantity at the top of the layer. For the functions \([A_0 \exp((1 - d)/rate)]\) and \([A_0 + A (1 - \exp((1 - d)/rate))]\) shown in the figure below, the parameter \(A_0\) defines the base value found at the layer surface.
**Multiplying d by graded layer thickness**

The depth parameter \( d \) represents normalized layer thickness, which means that all parameters related to thickness are also normalized. The rate parameter in figures below is an example of such a parameter. Sometimes, it is desirable to configure the equation so that these parameters explicitly relate to a depth location in the layer, with the same units of length as the layer thickness.

This can be accomplished by multiplying the depth parameter \( d \) (or \([1 – d]\)) by the film thickness. With this modification, rate parameter explicitly to the thickness, and directly refers to a specific location within the depth of the film. The profiles shown in the figure below are identical to those found in the previous figure, except that \((1 – d)\) has been multiplied times a parameter called thickness.

**When using this method, it is important that internal grading profile parameter thickness equals the thickness of the graded layer.** This can be accomplished in two ways:

- Coupling the thickness parameter used in the depth profile to the graded layer thickness, using the Edit Fit Parameters dialog box (Edit Parms menu item). (Fit Parameter coupling is described in The Fit Window chapter of the Guide to Using WVASE®.)
- Fixing the layer thickness and the internal grading profile’s thickness parameter to the same value.

![Figure 7-64](image)

Figure 7-64. Similar functions as shown in the previous figure, except the variable \( d \) has been multiplied times the parameter thickness, which equals the graded layer thickness. Note that the rate parameter is now explicitly tied to the layer thickness.

**Thickness \( \times d \) example: variable layer thickness**

In this example, the graded layer thickness is allowed to vary, with \( An = [Amin + (Amax – Amin)\exp(- (1 – d)*thick\text{ness}/rate)]\). At the top of the graded layer, \( An = Amax \), and at the bottom \( An = ~Amin \). The details of the coupling in the Edit Parameters dialog box are shown in the next figure. (Fit Parameter coupling is described in The Fit Window chapter of the Guide to Using WVASE®.)
**Thickness \times d example: fixed layer thickness, (exponentially graded surface layer)**

In this example, the exponentially graded layer represents a modified surface of a much thicker layer – in this case, a bulk substrate. We will also stipulate that the modified optical properties of the surface region must smoothly change in a way such that they are identical to the bulk optical properties at the bottom interface of the graded layer.

In this model, the depth exponential decay of the surface modification is described by the rate parameter, which equals the depth from the surface at which surface modification has by to $e^{-1}$.

In the next figure, a bulk substrate index is represented by a Cauchy layer with active fit parameters $A_n$ and $B_n$. The surface modification is represented by $A_n = [A_{bulk} + (A - A_{bulk}) \exp(-(1 - d)\times\text{thickness/rate})]$. $A_n = A$ the top of the graded layer, and $A_n = A_{bulk}$ at the bottom. The model forces the $A_n$ at the bottom of the graded layer to be identical to the bulk $A_n$ value Coupling the $A_{bulk.1}$ to $A_{n.0}$ (Layer 0 is the substrate). The details of the coupling in the Edit Parameters dialog box are shown in the figure below.

In order to assure that the function varies smoothly at the graded-layer-bulk substrate, the graded layer thickness is fixed at value that is sufficiently large to guarantee that the slope of the exponential function is relatively flat at the bottom of the graded layer. Care must be taken not to make the layer too thick. Otherwise, there will be insufficient number of slices to adequately represent the steepest part of the exponential, which occurs at the surface. The number of Slices per node can also be increased, but remember that additional slices will increase the generated data calculation time.
Figure 7-66. Left: Edit Fit Parameters Dialog Box showing coupling of Abulk.1 parameter to An of substrate (An.0). Note graded layer thickness and profile. Thickness parameter are fixed at 2500nm. Right: Model and Profile.

**Thickness x d example: fixed layer thickness, (Gaussian graded surface layer)**

In this example, the Gaussian graded layer represents a modified surface of a bulk substrate. As in the last example, the Gaussian profile varies smoothly and is identical to the bulk optical properties at the bottom interface of the graded layer.

The profile equation is:

\[ An = (A_{max} - A_{bulk}) \times \exp\left(-\frac{1}{2}\left\{\frac{(1 - d) \times \text{thick} - \text{mean}}{\text{sigma}}\right\}^2\right) + A_{bulk} \]

In this model, the mean and sigma parameters explicitly describe depth of the Gaussian peak and its standard deviation, respectively.

By coupling Abulk.1 from the graded layer with the bulk An.0 from the substrate, the model forces the An at the bottom of the graded layer to be identical to the substrate An. value. The details of this coupling in the Edit Parameters dialog box are shown in the next figure.

The graded layer thickness is fixed at a value that is sufficiently large to guarantee that the slope of the Gaussian function is relatively flat at the bottom of the graded layer, but not so thick that the Gaussian is not sufficiently defined by the grading slices.
EMA-Based Graded Layer

The EMA-based Graded Layer is simply a graded2.mat layer (described above) coupled to an EMA layer. This allows the user to vary the EMA fraction. This reproduces the functionality of the EMA option in the old graded.mat layer. We can convert any un-graded layer by selecting “Convert to EMA-Based Graded Layer” from the context-specific pop menu. This is done by clicking the right-mouse button while placing the mouse pointer over the layer in the model. The thickness of the Cauchy layer is transferred into the Graded layer, and two “dummy” zero-thickness layers are created. See the figure below.

Figure 7-68. EMA-based Graded layer model, which consists of a graded2 layer (Function-based graded layer) combined with an EMA layer.

The next figure shows the function-based graded layer dialog box after the conversion. In the list box on the left, you will want to select the EMA fraction you wish to grade – usually EMA2_EMA. If you have a three-constituent EMA, you can also choose EMA3_EMA. Then choose ‘Add/Edit Grade Profile’ to grade the profile either using nodes or a continuous equation (described in Function-based graded layer section above).
Figure 7-69. Function-based Graded layer dialog box after EMA-Based Graded Layer conversion.

Please note: you can also choose to grade parameters from whatever layers are coupled into the EMA file. In this case, the $A_n$, $B_n$, $C_n$, $A_k$ and $B_k$ parameters from the original Cauchy layer.

An example of a node-based grading of EMA2 is shown in the next figure. Note that there are 10 slices for each node, and the 2nd node is positioned 35% from the bottom of the film. One could also choose to make a continuous equation profile as well.

Figure 7-70. Function-based Graded layer dialog box after EMA-Based Graded Layer conversion.
Graded.mat layer

It is generally recommended that you use the simple graded and function-based graded layers rather than the older graded.mat layer.

The Graded.mat layer was the first WVASE® graded layer. In many instances, users will find that the newer simple graded layer (gradedsimple.mat) and Function-based graded layer (graded2.mat) are easier to use and more readily adaptable to the modeling situations. The simple graded and function-based graded layers are described in earlier sections of this chapter.

This type of layer is used to simulate a layer which is inhomogeneous in the direction perpendicular to the sample surface.

There are two parts in the definition of a graded layer:
1. The optical constants and optical constant grading technique:
   - EMA, Alloy, or Parametric
2. The grading profile definition:
   - Discrete nodes or Continuous equation

The grading can be accomplished by using a 2 constituent EMA where the component fraction for material #2 is graded through the layer, using an Alloy layer where the alloy fraction is graded through the layer, or using a function based (parameterized) layer (Lorentz oscillator, Cauchy, etc.) where one or two of the layer parameters are graded through the layer. In turn, the profile definition can be defined in two ways. Either a set of discrete nodes can be used or a continuous equation can be entered to describe the profile.

As a first look at a graded layer, we will consider a discrete node grading using an EMA optical constant model. The graded optical constants use a Cauchy layer mixed with voids. The optical constant mixing is done using a linear EMA. In this case, the profile is defined by 3 discrete nodes. In this case a negative void fraction is used indicating that the optical constants will grade to a higher index near the surface. The graded layer edit box, the model containing the graded layer, and a depth profile are shown below. Note in the model that a zero thickness Cauchy layer has been used to allow editing access to the optical constants being graded.

![Figure 7.71. The edit dialog box for a discrete node, EMA graded layer.](image)

![Figure 7.69. The model containing the graded layer shown in the previous figure. Note the use of the zero thickness Cauchy layer to model the optical constants of one constituent of the graded layer.](image)
Figure 7-72. Depth profile of the index of refraction of the graded layer shown in the previous two figures.

The Spectral Range, Thickness, OK, and Delete Layer items work the same as for the standard layer. From this dialog box, there is no option to look at or save the optical constants since each slice is different. The new features for this layer type are discussed below.

Opt. const. calc.

This section is used to define the method for grading the optical constants. In this example the grading is accomplished through the component fraction of an EMA layer.

Material #1 button

This button works just like the Material #1 button described in the EMA layer section previously. This material is the “host” material and its component fraction is calculated to be 100% minus the fraction of material #2.

Material #2 button

This button works just like the Material #2 button described in the EMA layer section previously. This material is the incorporated material and its component fraction is determined by the Value % in the profile definition.

EMA type

This selection box determines what style of EMA calculation is used. For more information see the discussion in the EMA layer section previously.

Profile definition

This section is used to define the grading profile. In this example 3 discrete nodes are used.

# of nodes box

This selection box allows you to define how many of the eight available nodes are in use.

Node position % box

This column of parameters determines where the nodes are located within the layer. The bottom (0%) and top (100%) node positions can not be adjusted. For this example, a third node is located at 25% of the way from the bottom of the layer to the top. You can fit for the position of all nodes except for the top and bottom value.
**Value % box**

This column of parameters defines the EMA component fraction for material 2 at each node. In this case the component fraction is -10% voids at the surface and -5% voids at the 25% position. You can fit for the component fraction of all nodes. As a word of caution, if you were fitting for the optical constants of the Cauchy layer in the above examples then you should not fit for all the node values. In this situation, you must leave one of the component fractions at a fixed value or there will be complete correlation between the node values and the optical constants. If you are using discrete nodes with an alloy layer for the optical constants, then the numbers used in the Value % are actually the alloy fractions as would be used in normal alloy layer. That is you would use 0.1, not 10% to model the optical constants for an alloy fraction of 0.1.

**Slices per node box**

This selection box allows you to define how many slices will be placed between adjacent nodes. If you are using several nodes and many slices, the total number of layers can become large very rapidly.

As a second example of a graded layer, we will consider a continuous grading using an alloy parametric model for an alloy semiconductor. In this case we are modeling a parabolically graded composition of Al$_x$Ga$_{1-x}$As. The graded layer edit box, the model containing the graded layer, and a depth profile of the index of refraction at a wavelength of 1000 nm are shown below.

![Figure 7-73. The edit dialog box for a discrete node, EMA graded layer.](image)

![Figure 7-74. A model containing the graded layer shown in the previous figure.](image)

![Figure 7-75. Depth profile of the index of refraction of the graded layer shown in the previous two figures.](image)
The Spectral Range, Thickness, OK, and Delete Layer items work the same as for the standard layer. From this dialog box, there is no option to look at or save the optical constants since each slice is different. The new features for this layer type are discussed below.

**Opt. const. calc.**

This section is used to define the method for grading the optical constants. In this example the grading is accomplished through the alloy fraction of an alloy layer (algaas.mat) defined by the Material Button.

**Material button**

This button is used to select the alloy material for the grading. Only parametric alloy layers can be used here. Do not couple this layer to another AlGaAs layer. A layer coupled to an alloy material uses only the optical constants for the specific alloy fraction of the original layer.

**Profile definition**

This section is used to define the grading profile. In this example a continuous equation is used.

**Operators list>>**

This button brings up a reference list of supported mathematical operations. Currently addition (+), subtraction (-), multiplication (*), division (/), raising to a power (^), the exponential (EXP), the natural log (LN), the sine (SIN), the cosine (COS), and the unit step function (UNIT) are supported. Also the reserved variable “d” accesses the position within the layer given in the range from 0 (bottom) to 1 (top).

**%= box**

This is the edit box where the continuous grading formula is specified. The “in-line” notation is used which places the standard operators between the operands and uses parentheses to define groupings. This function is used to calculate the real part of the dielectric function or refractive index. You add new parameter names directly in the equations. You do not have to predefine what your parameters are. When you go to leave the box (use the OK button) any newly defined parameters will be recognized and added to the parameter list. If you are using a parametric alloy model for shifting the optical constants then you need the equation to return values that correspond to an alloy fraction, not a percentage. If you are using an EMA for shifting the optical constants you would need the function to calculate in percent.

**Parameter name**

This lists the parameters WVASE® has recognized in your equations. If you have just entered a new formula you can force WVASE® to recognize the new parameters by using the OK button. When a new parameter is recognized you will be asked to define its value. Valid parameter names are a maximum of three characters long and contain only letters, not numbers.

**Parameter value**

This list contains the current values for parameters appearing in the formulas.
Parameter fit

If an asterisk * appears after the parameter value, then that parameter has been selected as an active fit parameter.

Fit button

This button is used to select the highlighted parameter name for fitting. If the parameter is already selected for fitting, this button deselects it. A parameter name can be highlighted by clicking on its row with the mouse.

Value button

This button is used to specify or modify the value of the highlighted parameter. A parameter name can be highlighted by clicking on its row with the mouse.

Delete button

This button removes a parameter from the recognized parameter list. However, if that parameter still exists in one of the formulas, it will be re-added when you use the OK button. A parameter name can be highlighted by clicking on its row with the mouse.

Slices per layer

This selection box allows you to define how many slices will be used to model the grading. The optical constants for each slice are determined using the calculated composition at the center of the slice.

7.10 Biaxial layer

The new anisotropic modeling features of WVASE® software versions 2.84 and higher allow modeling of uniaxial and biaxial materials with any set of optical constants.

These features are a significant improvement over the ACAUCHY.MAT layer, which is no longer supported. All anisotropic layer modeling is now accomplished using the BIAXIAL.MAT layer. The dialog box for this layer is shown below.

![Biaxial Anisotropic Layer](image)

*Figure 7-76. Biaxial.mat layer dialog box.*

The user must choose the Anisotropy Type by selecting one of 3 radio buttons, (left side of figure above):

- Isotropic
The user also specifies a material file to represent each set of optical constants (Ex, Ey, Ez). Any WVASE® material file may be used – so you are not restricted to modeling anisotropic materials with Cauchy equations only. Fixed optical constants can be used, but you can also use dispersion relations such as Cauchy, Genosc® Lorentz, parametric semiconductor, or your own user-defined dispersion relation with User layer.

Also note that the BIAXIAL layer allows the optical axis to be tilted in an arbitrary direction by adjusting the Euler angles. The tilt angles can also be selected as model fit parameters. This is another improvement over the old acauchy.mat layer which did not allow the axis to be tilted. Euler angles are described in more detail below.

Building a BIAXIAL model for a thin film

When modeling an anisotropic thin film on a substrate it is necessary build a model using BIAXIAL.MAT. The user inputs the nominal film thickness, and selects from one to three materials depending on the anisotropy type. The Euler angles may also need to be adjusted somewhat. It is a very instructive exercise to experiment with the Euler angles and notice the effects on the generated ellipsometric data. This is a feature that can only be learned properly by experimentation.

The following shows how the BIAXIAL.MAT layer can model a uniaxial anisotropic film of MgF2 on a silicon substrate.

```
1 biaxial 1000 Å
0 si 1 mm
```

*Figure 7-77. Uniaxial MgF2 layer on Si using Biaxial.mat layer.*

The corresponding Biaxial layer dialog box is shown in the figure below. Note that the ‘Uniaxial’ radio button is selected.

*Figure 7-78. Biaxial.mat dialog box for uniaxial MgF2 layer.*

Only the film thickness is being varied. The ordinary and extraordinary sets of optical constants are fixed tabulated values. With the optical constants fixed, the user could fit the Euler angles to determine the direction of the optic axis.
Varying Optical Constants in \textit{biaxial.mat}

In the above example, the optical constants of Materials \#1 and \#2 are fixed. Also note that there are no boxes to directly fit \( n \) and \( k \). Often the optical constants of the anisotropic material are unknown, and the goal is to determine the dispersion curves of each component of the biaxial layer’s dielectric function.

It is possible to add dispersion equations to the model, but they are not directly added to \textit{biaxial.mat}. Instead, they are placed as layers of zero thickness below the biaxial layer as shown in the following example.

![Figure 7-79](image)

The model contains two Cauchy layers of zero thickness. These “dummy” layers are used to define the equation used for each set of optical constants, and provide a way to define the dispersion (shape) of each function. Do not fit the thickness of these dummy layers, as the entire film thickness is represented by BIAXIAL.MAT. The dummy layers are used only to define a set of optical constants. The dispersion model parameters for each dummy layer can be edited and selected as fit parameters in the model.

It important to add the dummy layers below BIAXIAL.MAT since we want to “couple” these optical constants into the BIAXIAL layer. Coupling optical constants between layers allows the optical constants to vary in the dummy layer, and these variations are simultaneously used by the BIAXIAL layer. The parentheses around the material names cauchy and cauch2 above indicate that the optical constants are coupled to the dummy layers below. WVASE will use the following dialog box to determine if coupling is desired.

![Figure 7-80](image)
Important!

The optical constants from the dummy layer must be coupled into biaxial.mat if the optical constants are to be varied. If coupling is not chosen, the default values for the material (stored on disk) will be used and held fixed during the data fits. If the dummy layer is a dispersion model such as the Cauchy, the default parameter values will be used. Always check for parentheses around the material name to indicate coupling.

Using biaxial.mat for bulk samples

The biaxial layer can also be used as the substrate. However, dummy layers must still be used if the optical constants are to be varied. Furthermore, coupling requires that the dummy layers be placed below the substrate. For a bulk substrate this is accomplished by adding the dummy layers on the back side of the substrate as shown below.

![Figure 7-81. Left: Model schematic for anisotropic substrate, with two “dummy” user layers placed below the substrate for coupling. Right: biaxial layer dialog box.](image)

In this case the substrate is 1 mm thick and the dummy layers each contain a user-defined dispersion equation. Building the above model requires several steps:

1. Delete any existing model
2. Add BIAXIAL.MAT as the substrate. The biaxial dialog box should appear.
3. Enter the appropriate thickness for the substrate.
4. Enter the appropriate file names for Materials #1-3. Close the dialog box by selecting OK.
5. Add the first dummy layer to the back side by depressing the <Shift> key while selecting “Add Layer” with the mouse. Another way is by simultaneously selecting <Shift> + <Alt> + <A> on the keyboard.
6. Repeat step 5 for the second and (if applicable) third dummy layers.
7. Activate the BIAXIAL dialog box and reenter the file names for Materials #1-3. WVASE will now allow coupling to the dummy layers. (Coupling was not possible at step 4 since the dummy layers were not present in the model.)

Euler angles

This new layer in WVASE can be used to model uniaxial and/or biaxial materials, with an arbitrarily oriented optical axis (however, if the optical axis is not oriented normal to the sample, or not in the sample plane and parallel or
perpendicular to the plane of incidence, an ‘anisotropic’ ellipsometric measurement is required to quantitatively measure the non-zero off-diagonal Jones matrix elements of the sample).

**WVASE® Experimental Coordinate system**

To understand this, it is important to correctly identify the Experimental coordinate system used by WVASE® (see diagram below):

- **x-axis** is in the sample plane, *aligned parallel to the plane of incidence*. It is in the p-direction, when the beam angle of incidences approaches 0°.
- **y-axis** is in the sample plane, *aligned perpendicular to the plane of incidence* (corresponds with s-direction).
- **z-axis** is normal to the sample surface, *but it points into the sample*, consistent with a right-handed coordinate system.
- **The surface normal** points along the *negative z-axis*.

With the Euler angles all set to zero, the optical constants \( n_x, n_y, \) and \( n_z \) of the biaxial layer match the WVASE® x-y-z experimental coordinate system as shown in the diagram below.

In the figure below, the beam transverses from left to right; this corresponds to *positive* angles of incidence. *Negative* angles of incidence correspond to beams which propagate in the opposite direction.

![Figure 7-82. Experimental coordinate system. It is defined by the sample surface (x-y plane) and the plane of incidence (x-z plane). The \( \varepsilon_{11}, \varepsilon_{22}, \) and \( \varepsilon_{33} \) directions shown correspond to Euler angles \( (\phi, \psi, \theta) = (0°, 0°, 0°) \).](image)

**Euler Angles Rotations**

The Euler Angles\( (\phi, \psi, \theta) \) define the orientation of sample dielectric tensor relative to the experimental coordinate system (Laboratory Frame of reference). To define the sample dielectric tensor, the Euler angles rotate the principle dielectric functions \( \varepsilon_{xx}, \varepsilon_{yy}, \) and \( \varepsilon_{zz} \) using rotation matrix \( A \) defined below.

\[
\tilde{\varepsilon} = \begin{bmatrix}
\varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\
\varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} \\
\varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33}
\end{bmatrix} \quad \text{(7.10)}
\]
\[
\tilde{e} = \tilde{A} \begin{bmatrix}
\varepsilon_{xx} & 0 & 0 \\
0 & \varepsilon_{yy} & 0 \\
0 & 0 & \varepsilon_{zz}
\end{bmatrix} \tilde{A}^T
\]

(7.11)

Following the figure below, the Euler angle rotation rules are defined as:

- **1st rotation (Phi 'φ')** is about the z-axis (resulting in new x' and y' axes, while z' = z)
- **2nd rotation (Theta 'θ')** is about the x'-axis (resulting in y'' and z'' axes, while x'' = x')
- **3rd rotation (Psi 'ψ')** is about the z''-axis (resulting in new x''' and y''' axes, while z''' = z'').

*Euler Rotations must be performed in the order shown.*

Note that the Euler Angles are not unique: Adding integral multiples of 360° results in the same transform, and for films with certain symmetry (e.g., uniaxial), additional sets of Euler angles (e.g., by adding integral multiples of 180°) can often be found. However, following the above transform rules can **always** specify the resulting crystal axis rotation for orthorhombic crystals.

**Euler Angle Examples**

The three Euler angles specify the orientation of the principle dielectric functions with respect to the sample and plane of incidence. Below are some examples for a uniaxial material. The orientation of uniaxial materials only requires the first two Euler angles to completely specify the orientation of the material’s optic axis.
In the following examples, the principle dielectric functions for the following examples are shown in the next figure.

**Uniaxial Film on Silicon**

<table>
<thead>
<tr>
<th>Layer Type</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>bi axial</td>
<td>250.00 nm</td>
</tr>
<tr>
<td>cauchy_e</td>
<td>0.00 nm</td>
</tr>
<tr>
<td>cauchy_o</td>
<td>0.00 nm</td>
</tr>
<tr>
<td>si_jaw</td>
<td>1 mm</td>
</tr>
</tbody>
</table>

**Cauchy_ordinary, Cauchy_extraordinary**

\[
\begin{bmatrix}
E_{11} & E_{12} & E_{13} \\
E_{21} & E_{22} & E_{23} \\
E_{31} & E_{32} & E_{33}
\end{bmatrix}
= \begin{bmatrix}
0 & 0 & 0 \\
0 & E_o & 0 \\
0 & 0 & E_e
\end{bmatrix}
\]

**Optical Constants**

**Uniaxial Layer (Biaxial.mat) dialog box**

\[(\phi, \theta, \psi) = (0^\circ, 0^\circ, x) : Optic axis perpendicular to surface\]

In this example, the principle dielectric functions are parallel to \((x, y, z)\) of experimental coordinate system. Due to the alignment of principle dielectric functions with the experimental coordinates, the ‘off-diagonal’ ellipsometric values Aps and Asp equal 0 (\(\Psi = 0^\circ\) and \(\Delta = 0\) or “undefined”). Note that setting the Euler angles to \((0, 0, x)\) aligns the optical axis of a uniaxial material normal to the surface.

**Generated Data**

\[
\begin{align*}
\phi & = 0^\circ \\
\theta & = 0^\circ \\
\psi & = 0^\circ
\end{align*}
\]
\((\phi, \theta, \psi) = (90^\circ, 90^\circ, x)\):

\(\phi = 90^\circ\) first rotates \(x\) and \(y\) about the \(z\)-axis by \(90^\circ\), then \(\theta = 90^\circ\) rotates the new axes \(y'\) and \(z'\) about \(x'\) by \(90^\circ\). This is equivalent to rotating \(e_x \rightarrow e_{11}, e_o \rightarrow e_{22}\) and \(e_z \rightarrow e_{33}\). The two Biaxial layer dialog boxes shown in the next figure are equivalent models. On the left, the Uniaxial button is selected; \(\text{Mat1}(Ex) = e_o, \text{Mat2}(Ez) = e_e\); and \((\phi, \theta, \psi) = (90^\circ, 90^\circ, 0^\circ)\). In the biaxial equivalent definition on the right, the Biaxial button is selected; \(\text{Mat1}(Ex) = e_e, \text{Mat2}(Ez) = e_o, \text{Mat3}(Ey) = e_o\); with \(\phi = \psi = \theta = 0^\circ\).

As before, the principle dielectric functions are aligned with the experimental coordinates, so the ‘off-diagonal’ ellipsometric values \(A_{ps}\) and \(A_{sp}\) equal 0 (\(\Psi = 0^\circ\) and \(\Delta = 0\) or “undefined”).

**Definition:**

**Biaxial equivalent:**

\[
\begin{bmatrix}
\varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\
\varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} \\
\varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33}
\end{bmatrix} =
\begin{bmatrix}
e_e & 0 & 0 \\
0 & e_o & 0 \\
0 & 0 & e_o
\end{bmatrix}
\]

**Below: Principle dielectric functions \(e_o\) and \(e_e\)**

**Optical Constants**

- \(\text{cauchy}_o\)
- \(\text{cauchy}_e\)

**Generated Data**

- \(\Phi\) in degrees
- \(\Delta\) in degrees

**Figure 7-86.** 250nm biaxial film on silicon. Euler angles \((\phi, \theta, \psi) = (90^\circ, 90^\circ, 0^\circ)\).
The Euler angles \((\phi, \theta, \psi) = (60^\circ, 90^\circ, x)\):

The Euler angles \((\phi, \theta, \psi) = (60^\circ, 90^\circ, x)\) will first rotate \(x\) and \(y\) \(60^\circ\) about the \(z\)-axis, then rotate \(y'\) and \(z'\) \(90^\circ\) about \(x'\). The \(\theta = 90^\circ\) rotation causes \(\varepsilon_{33} = \varepsilon_o\) (note the factor of \(\frac{1}{4}\) in front of the matrix on the right). In the biaxial equivalent definition on the right, the Biaxial button is selected; \(\text{Mat1}(E_x) = \varepsilon_o\), \(\text{Mat2}(E_z) = \varepsilon_o\), and \(\text{Mat3}(E_y) = \varepsilon_e\); with \(\phi = 60^\circ\), \(\theta = \psi = 0^\circ\).

Because the off-diagonal elements of the dielectric tensor are no longer zero, the ‘off-diagonal’ ellipsometric values \(A_{ps}\) and \(A_{sp}\) are also non-zero (see next figure).

**Definition:**

**Biaxial equivalent:**

\[
\begin{bmatrix}
\varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\
\varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} \\
\varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33}
\end{bmatrix} = \frac{1}{4} \begin{bmatrix}
\varepsilon_o + 3\varepsilon_e & \sqrt{3}(\varepsilon_o + \varepsilon_e) & 0 \\
\sqrt{3}(\varepsilon_o + \varepsilon_e) & 3\varepsilon_o + \varepsilon_e & 0 \\
0 & 0 & 4\varepsilon_e
\end{bmatrix}
\]

\[
\begin{align*}
\text{Biaxial Optical Constants} \\
\text{Wavelength (nm)} & \quad \begin{array}{c}
200 \\
400 \\
600 \\
800 \\
1000
\end{array} \\
\varepsilon_{11} & \quad \begin{array}{c}
\text{Re(\varepsilon_{11})} \\
\text{Re(\varepsilon_{12})} \\
\text{Re(\varepsilon_{13})} \\
\text{Re(\varepsilon_{21})} \\
\text{Re(\varepsilon_{22})} \\
\text{Re(\varepsilon_{23})} \\
\text{Re(\varepsilon_{31})} \\
\text{Re(\varepsilon_{32})} \\
\text{Re(\varepsilon_{33})}
\end{array}
\end{align*}
\]

**Figure 7-87.** 250nm biaxial film on silicon. Euler angles \((\phi, \theta, \psi) = (90^\circ, 0, 0)\).
7.11 Specialty layers

WVASE® recognizes some additional layers that do not fall into the previous categories. These layers are described in the following sections.

Kramers-Kronig layer

The layer kk.mat may be used to check the Kramers-Kronig (KK) consistency of a set of optical constants. For a specified material, the KK integral (equation 7.4) is numerically evaluated to calculate $\varepsilon_1$ values. The model then adds the contribution from two zero-width oscillators and a fixed offset to account for absorption outside the range of available $\varepsilon_2$ values. Because this model does a complete numerical integration for each calculated $\varepsilon_1$ value, it can be quite slow in its calculation.

$$
\varepsilon_{1 KK}^E(E) = \varepsilon_{1 \infty} + \frac{A_1}{E_1^2 - (E)^2} + \frac{A_2}{E_1^2 - (E)^2} + \frac{2}{\pi} P \int_0^\infty \frac{E_2^{\text{meas}}(E) \, dE'}{E_1^2 - (E)^2} \nonumber
$$

The edit box shown below was used to check the KK consistency of optical constant spectra measured for InP.

![Edit dialog box for the Kramers-Kronig layer, kk.mat.](image)

The Spectral Range, OK, Cancel, Replace Layer, Delete Layer items work similar to those for the standard tabulated layer. The Optical Constants>> button allows you to graphically display the optical constants and to save the values as a standard tabulated .mat file. You can not fit for the optical constants in a wavelength-by-wavelength manner using a KK layer.

Material button

The $\varepsilon_2$ values that are integrated come from the material chosen using this button.
**Integration range boxes**

These two parameters define what spectral range the $\varepsilon_2$ values will be integrated over. The integration is performed using the original values stored in the .mat file on disk. The integration range and density of points does not depend on which wavelengths are in use according to the Optical Constants>> graphical display.

**Step size box**

This is the step size for the numeric integration. This can be, and often is, set less than the separation of points in the .mat file.

**$e_1$ offset box**

This is the constant value added to the model $\varepsilon_1$ values.

**Pole #1 position**

This is the energy location of a zero width oscillator which is added to simulate absorption outside the integration range.

**Pole #1 magnitude**

This is the magnitude of the zero width oscillator located at Pole #1 Position.

**Pole #2 position**

This is the energy location of a zero width oscillator which added to simulate absorption outside the integration range.

**Pole #2 magnitude**

This is the magnitude of the zero width oscillator located at Pole #2 Position.

To use this layer to check the KK consistency of a set of optical constants, you will need to do the following things:

1) Build a model with a substrate that has the optical constants you want to check for KK consistency.

2) Generate ellipsometric data at one angle over the spectral range of the .mat file. Copy these values in to the Experimental Data window. (see Gen_Data|Copy_to_Exp) In the above example this was 0.75 to 6.0 eV by 0.01 eV steps.

3) Replace the model with the kk.mat layer as the substrate.

4) Use the Material Button to select the .mat file you are working with. (The one used in step 1.)

5) Set the integration range to cover the spectral range of the .mat file where $\varepsilon_2$ is non-zero. In the above example this was 1.0 to 6.0 eV. You do not need to integrate a region where $\varepsilon_2 = 0$. Therefore, the integration range did not need to include 0.75-1.0 eV because $\varepsilon_2 = 0$ in that range.

6) Set the experimental data range (see Exp_Data|Range_Select) to cover as much of the data range as possible without being too close to an edge where the $\varepsilon_2$ values are non-zero. In the above example this was 0.75 to 5.0 eV.
The experimental range could extend to 0.75 eV because $\varepsilon_2$ is zero at that end of the experimental range. However, the experimental range should not be set close to 6.0 eV, because the model will be inaccurate near that end.

7) Change the fit defaults to $<\varepsilon_1>$ only. (see Fit|Defaults)

8) Fit the offset and pole parameters as needed to obtain the best fit between the model $\varepsilon_1$ values and the $<\varepsilon_1>$ in the experimental window. If the $\varepsilon_1$ values match up you can say the optical constants are KK consistent

**Drude Layer (Drude.mat)**

This layer adds Drude absorption “tail” on to any other material file; multiple parameterizations of the Drude tail parameters are supported. for details about the Drude oscillators see the Drude oscillator section of the Genosc layer chapter.

A combination of the sum_eps.mat and a GenOsc.mat, lorentz.mat or user.mat layer could also provide this functionality, but the Drude layer is more convenient to use.

![Figure 7-89. Drude.mat layer dialog box.](image)

**Delay layer**

This layer (delay.mat) is used only when modeling dynamic (time dependent) data. It is used to specify a period of time during a dynamic data analysis when nothing is happening to the sample. This layer is used exclusively in the modeling of dynamic data using a growth rate model. The use of this layer is examined fully in the chapter 17 - “Dynamic Data Analysis”.

![Figure 7-90. Edit box for a Delay layer (delay.mat).](image)

Note that there are no optical constants and no thickness associated with this layer.
**Delay time box**

The length of time for which the model did not change. The can be selected as a fit parameter by using the associated fit box.

**Ok button**

This button dismisses the dialog box.

**Delete layer button**

This button removes the layer from the model.

**Virtual interface layer**

Like the delay layer, the virtual interface layer (virtual.mat) is used exclusively with dynamic data. This layer is an implementation of the common pseudo-substrate approximation. Simply put, this assumption is that everything below a certain level in a multi-layer stack can be replaced by an effective, semi-infinite substrate that has optical constants equal to the pseudodielectric values for the stack below that level. This approximation works amazingly well for semiconductors and other high index materials, but does not work for low index transparent materials, like glass.

A virtual interface should always be placed as the substrate layer (layer #0) and as such there should only be one virtual interface in a model. When WVASE® encounters a virtual interface layer in a model, it uses the experimental $\psi$ and $\Delta$ data for the virtual time and converts them into pseudodielectric values. These values become the optical constants for the effective substrate.

![Virtual interface dialog box](image)

*Figure 7-91. Edit dialog box for the virtual interface layer (virtual.mat).*

The OK and Delete Layer buttons work as expected.

**Virtual type setting**

The type of virtual interface used is set as either a fixed time interface or a running interface. The virtual time does not change for a fixed time interface regardless of what time the data is being analyzed for. A fixed time virtual interface is used to determine the thickness of a growing layer. The virtual time for a running interface moves in conjunction with what time the data is being analyzed for. A running virtual interface is used to model just the near-surface material, and is primarily used to model the near-surface composition of an alloy material.

**Fixed at time box**

This box specifies the virtual time for a fixed time interface. This is not a fitable parameter.
# of pts to average box

This box specifies how many data behind (less than) the fixed time should be averaged when calculating the pseudovalues. It is common to put a virtual interface at the end of a “dwell” period in which the sample has not changed.

Running separation box

This box specifies the number of data points the virtual interface lags behind the data time currently being analyzed.

Opt. const. fit boxes

These boxes are used when the pseudovalues are to be fit instead of using the directly inverted pseudovalues from the data. Note the internally stored fitting pseudovalues are not filled until at least one data generation has been performed. Thus if a virtual interface is added and the Opt. Const. fit boxes are checked before any generation is performed, the fitting pseudovalues will start as \( n=1, k=0 \).

Pseudo opt. constants

This brings up a graphical display of the pseudovalues being used in the model. This is the same as for a standard tabulated layer. The pseudovalues can be saved to a standard tabulated .mat file.

7.12 Model|DeleteMod command

![Image](image_url)

*Figure 7-92. The DeleteMod (delete model) option from the Model window.*

This menubar item is used to delete the currently displayed model from memory. Models already saved to disk will be unaffected. If the model number is from #2 to #10, then only that model will be deleted. If the primary model (model #1) is deleted then the remaining models #2 through #10 will also be deleted. Additionally when the primary model is deleted, the loaded optical constants in the Current Materials list are also deleted.

![Image](image_url)

*Figure 7-93. Confirmation dialog box when deleting the primary model (model #1).*

7.13 Model|Superlattice item

![Image](image_url)

*Figure 7-94. The Superlattice option from the Model window.*

Use the superlattice option for repeated periodic structures.

This menubar item is used to create repeating patterns of layers (a superlattice) within the model. The dialog box for setting the superlattice parameters and the corresponding model representation are shown below.
Figure 7-95. Superlattice definition box.

Figure 7-96. Model containing the superlattices defined in the previous figure.

In this example both superlattices are enabled. The first superlattice causes layers 1 and 2 to be repeated 20 times. The coupling range and number of periods are shown on the right side of the model. In this case a series of alternating GaAs and Al$_{0.3}$Ga$_{0.7}$As layers are modeled. When calculations are performed using this model, a total of 61 layers will be included in the calculation. The repeated layers in a superlattice do not count against the total number of layers specified by |Global|Defaults. The second superlattice is used to produce a similar repeated pattern of layers 4 and 5.

**Superlattice #1/#2 enabled**

When checked, these boxes cause the corresponding superlattice definition to be applied to the model.

**Start layer**

This box selects the first of the layers to be repeated.

**End layer**

This box selects the last layer in the repeated sequence.

**# of periods**

This box defines how many times to repeat the sequence when performing a model calculation. This value must be an integer value.

### 7.14 Model|Growth item

Figure 7-97. The Growth option from the Model window.
This option is used to model dynamic data, usually acquired in situ.

This option is used only for growth rate analyses of dynamic data. This command opens a dialog box that allows you to enter growth rates for the first 10 layers. The growth rates are specified in Å/sec regardless of the thickness units specified by |Global|Defaults. A sample dialog box is shown below along with a corresponding model.

![Layer Growth Rates](image)

Figure 7-98. The growth rate parameter edit box.

The growth rates can be defined as fit parameters by checking the fit box next to them. When modeling dynamic data, WVASE® assumes that the growth rate is constant during the deposition of the entire layer. If the growth rate of one model layer is not constant, you may have trouble performing a growth rate analysis. Delay layers are often used when performing growth analyses and they will appear in the growth rate edit box. However, do not define the growth rate of a delay layer as a fit parameter because it will cause the fitting procedure to fail.

### 7.15 Model|Select item

This option is used for multiple sample analyses or analysis of dynamic optical data.

When the data in the experimental window is not time dependent (standard spectroscopic data), this command is used to select which of the 10 available models are active in the fit and which one is selected. When dynamic experimental data is present in the experimental window and the experimental data view is in the dynamic-spectroscopic mode, this option is used to work with the fit parameters at the selected data times. These two modes of operation are quite different and are described separately.

#### Select model in standard mode

For each of the 10 available models there is a corresponding set of experimental and generated data. Furthermore, the Graph window also works with the currently displayed model. Thus changing the currently displayed model will
also change the views in the Experimental Data window, Generated Data window, and Graph windows. The standard Select Model dialog box is shown below.

![Select Model dialog box](image)

*Figure 7-101. Standard Select Model dialog box.*

**Current model**

This column is used to select which of the 10 models will be displayed in the Model window. In this case, model #1 will be displayed. There is a short cut to selecting which model is displayed that does not require you to use the Model Select command. You can move between models using the <alt> key in combination with a single digit. For example, <alt>-1 will cause model #1 to be displayed, <alt>-2 will cause model #2 to be displayed, and so forth up to <alt>-0 which causes model #10 to be displayed. The models do not have to be used in order. You can use models #1 and #10 without using any of the models from #2 through #9. (Model #1 is special with regard to coupling optical constants between layers, see the advanced modeling techniques section of chapter 13 - ‘VASE Data Analysis’). Anytime the displayed model changes, the Experimental Data window, the Generated Data window, and the Graph window will also change correspondingly.

**Active in fit**

This column is used to select which of the models will actually be used when fitting the data. You can create other models for generating simulated data or comparing optical constants which are not used for fitting.

**Model present**

This column indicates which of the 10 models actually has a model present.

**Exp. data present**

This column indicates which of the 10 models actually has experimental data present. If both a model and experimental data are present the model can be included in the fitting process.

In the above example, the Select Model box indicates that there are 3 models present and that each has an associated set of experimental data. Also shown is that only models #1 and #2 will be included in the fitting process. Finally model #1 is selected, so when this box is dismissed (OK button), model #1 will be displayed in the Model window.
Multiple models in dynamic-spectroscopic mode

Performing multiple model fits on this type of data is complicated. A representative dialog box for this operation is shown below.

![Model Options dialog box](image)

Figure 7-102. Dialog box for working with multiple model fit parameters in the dynamic-spectroscopic data mode.

The functionality of these features is best explained by examples. The details of using this fitting mode are described later in chapter 17 - “Dynamic Data Analysis”.

7.16 Model|Options item

![Options option from Model window](image)

Figure 7-103. The Options option from the Model window.

The Model|Options command provides access to parameters that describe extra information needed for certain special data types and that are used to model certain sample non-idealities. These parameters are contained within the Model|Options dialog box shown in the next figure.

![Default Model Options dialog box](image)

Figure 7-104. The default Model|Options dialog box.
Ideal ellipsometric measurements

Ideal ellipsometric measurements are defined as measurements where the light collected by the analyzer/detector consists of a single polarization state, which can be described as a single Jones vector. Furthermore, the sample can be modeled as a single 2x2 Jones matrix:

\[
J = \begin{bmatrix}
E_p \\
E_s
\end{bmatrix} = \begin{bmatrix}
\tilde{r}_{pp} & \tilde{r}_{ps} \\
\tilde{r}_{sp} & \tilde{r}_{ss}
\end{bmatrix} \begin{bmatrix}
E_{p}^{in} \\
E_{s}^{in}
\end{bmatrix}
\] (7.13)

where \( E_p = E_{p0}e^{i\phi_p} \), \( E_s = E_{s0}e^{i\phi_s} \), \( E_{p0}^{in} = E_{p0}e^{i\phi_{p0}} \), and \( E_{s0}^{in} = E_{s0}e^{i\phi_{s0}} \). The 2x2 Jones matrix represents a sample and/or other optical element(s) that transform the input E-fields \( E_{p0}^{in} \) and \( E_{s0}^{in} \) into the output fields \( E_p \) and \( E_s \). The Fresnel coefficients \( \tilde{r}_{pp} \), \( \tilde{r}_{ps} \), \( \tilde{r}_{sp} \), and \( \tilde{r}_{ss} \) are, in general, complex-valued (for transmission, replace \( \tilde{r} \) with \( \tilde{t} \)).

Non-ideal ellipsometric measurements

For non-ideal ellipsometric measurements, the light collected by the analyzer/detector consists of an incoherent mixture of two or more polarization states. Stokes vectors, which describe polarized intensities rather than complex-valued electric field quantities, are more useful descriptions of an incoherent mixture of polarization states. The Stokes vector is described below:

\[
S = \begin{bmatrix}
I \\
Q \\
U \\
V
\end{bmatrix} = \begin{bmatrix}
I_{total} \\
I_{p-pot} - I_{s-pot} \\
I_{45^\circ} - I_{-45^\circ} \\
I_R - I_L
\end{bmatrix} = \begin{bmatrix}
E_p E_p^* + E_s E_s^* \\
E_p E_p^* - E_s E_s^* \\
2 \text{Re}(E_p E_s^*) \\
2 \text{Im}(E_p E_s^*)
\end{bmatrix}
\] (7.14)

- \( I_{total} \) = the total intensity of the light.
- \( I_p \) and \( I_s \) are the intensities measured with a linear polarizer oriented in the p- and s-orientation, respectively.
- \( I_{45^\circ} \) and \( I_{-45^\circ} \) are the intensities measured with a linear polarizer oriented + and – 45° with respect to the p-plane, respectively.
- \( I_R \) and \( I_L \) are the intensities measured with a right- and left-circular polarizer, respectively.

Note that a Stokes vector can be calculated from any Jones vector by entering \( E_p \) and \( E_s \) from equation (7.13) into equation (7.14). However the reverse is not always true. A Jones vector can be calculated from a Stokes vector only if the Stokes vector is completely polarized (\( Q^2 + U^2 + V^2 = I^2 \)).

The 4x4 Mueller matrix represents a sample and/or other optical element(s) that transform the input Stokes vector into the output Stokes vector. The elements of the Mueller matrix are real-valued quantities.

\[
S = \begin{bmatrix}
I \\
Q \\
U \\
V
\end{bmatrix} = \begin{bmatrix}
m_{11} & m_{12} & m_{13} & m_{14} \\
m_{21} & m_{22} & m_{23} & m_{24} \\
m_{31} & m_{32} & m_{33} & m_{34} \\
m_{41} & m_{42} & m_{43} & m_{44}
\end{bmatrix} \begin{bmatrix}
I^{in} \\
Q^{in} \\
U^{in} \\
V^{in}
\end{bmatrix}
\] (7.15)

The Mueller matrix of a sample contains all of the information about how that sample alters the polarization of the incident light. That would include isotropic values \( \Psi, \Delta \), the generalized ellipsometric quantities \( \text{AnE}, \text{Aps} \) and \( \text{Asp} \), and information about depolarization. However, a detailed discussion of the Mueller Matrix is beyond the scope of this brief description.
Any 2x2 Jones Matrix can be converted into a 4x4 Mueller matrix via a procedure described in Azzam and Bashara\textsuperscript{iv} and elsewhere. However, a depolarizing Mueller matrix cannot be converted to a Jones Matrix.

In summary:

- For ideal ellipsometric measurements, a single Jones vector is sufficient to describe the electric field components of the light entering the analyzer/detector.
- An ideal sample can be modeled as a single Jones matrix.
- For non-ideal ellipsometric measurements, the combinations of polarized intensities of the light beam entering the detector can be described by a Stokes vector, since it can also describe any light ranging from total polarized, to partially polarized, to completely unpolarized light.
- A non-ideal sample can be modeled using a Mueller matrix.

**Modeling Non-ideal ellipsometric measurements**

For non-ideal ellipsometric measurements, the light beam collected by the analyzer/detector consists of an incoherent mixture of two or more polarization states after interacting with the sample. For example, this occurs when:

- The light beam reflects from a sample with a film that has thickness non-uniformity as shown in Figure 7-105 a),
- When the sample induces significantly different polarization states depending upon which wavelength is present within the bandwidth of the instrument’s spectrometer, as shown in Figure 7-105 b),
- When there is a range of incident angles because of beam focusing or curvature of the sample surface, creating a range of polarization states in across the reflected beam, as shown in Figure 7-105 c),
- When backside reflections of a transparent substrate are collected by the detector along with front surface reflections, as shown in Figure 7-105 d), and
- When the sample has “patterning”; that is, when the sample consists of two or more distinctly different areas. If the lateral dimensions of the areas are much-much greater than the measurement wavelengths, the light from the different regions mix incoherently at the detector. See Figure 7-105 e), as well as the Large Scale Patterning section on page 7-84.

These different polarization states mix incoherently at the detector. Therefore, the light from a non-ideal measurement is modeled as a summation of intensities (Stokes vectors) rather than instantaneous electric fields (Jones vectors). Each of outgoing beams is considered to be incoherent with respect to all of the other outgoing beams. Within each beam there are p- and s-polarized components, and they are considered to be internally coherent.

To model non-ideal ellipsometric measurements, WVASE\textsuperscript{®} generates several sample Jones matrices by varying the particular parameter, then converts those Jones matrices into Mueller Matrices. The Mueller Matrices are then added together as a weighted sum. The Mueller matrix summation represents a collection of different Jones matrices that, for any given totally polarized incidence beam, will produce a Stokes vector with an average polarization state with a certain amount of

depolarization. The level of depolarization depends upon the distribution of polarization states that enter the detector.

Figure 7-105. Non-ideal samples: a) Film of non-uniform thickness. b) Finite bandwidth. c) Angular spread. d) Backside reflections (detector aperture collecting ~1.5 backside reflections). e) Patterning. $S_1 \ldots S_m$ represent the Stokes vectors for light collected by the analyzer/detector from different portions of the reflected beam.

The model options dialog box

The Model|Options dialog box with default settings is shown in Figure 7-106. Starting at the top and working down, this dialog box contains the items listed in the following sections.
Figure 7-106. The default Model|Options dialog box.

### # of backside reflections box

This box is used to define one of the parameters needed to simulate the backside-corrected data types. This value refers to how many secondary reflections through the substrate are collected. For example, the number of backside reflections entering the detector aperture in Figure 7-105 d) is approximately 1.5 (parameter BackRefl = ~1.5). This value has an associated fit check box. For more details, see Chapter 9, “Calculations performed for the different data types” page 9-3.

### Top layer is ambient

This option is used to model data acquired with the sample immersed in an ambient that is not air or vacuum.

This check box is used to change the ambient optical constants used when generating data from the model. The ambient is the material above all the topside layers and below all the backside layers. By default WVASE\textsuperscript{®} uses an ambient with the free space optical constants ($n=1$, $k=0$). However, if you were making measurements on a sample immersed in a liquid (perhaps an electro-chemical deposition cell) then you would need to use a different ambient. In this case you would add one additional layer containing the ambient optical constants and then check this box. A model with water.mat specified as the ambient medium is shown below.

```
<table>
<thead>
<tr>
<th>AMBIENT: water</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 sio2</td>
</tr>
<tr>
<td>1000 Å</td>
</tr>
<tr>
<td>0 si_uni</td>
</tr>
<tr>
<td>1 mm</td>
</tr>
</tbody>
</table>
```

Figure 7-107. Model with water defined as the ambient medium.

### % of first reflection collected box

This box is also used to define the other parameter needed to simulate backside-corrected data types. In some instances you may only collect part of the primary (first surface) reflection (WVASE\textsuperscript{®} parameter 1stRefl ). This value has an associated fit check box.
**Polarizer angle for polarized refl./trans. box**

This box defines the polarizer setting (relative to the plane of incidence) that is used when calculating user-specified polarization intensity reflection and transmission measurements. The WVASE® parameter is Pol. For more details on this data type see Chapter 9 “Reflected intensity data types” on page 9-15, and “Transmission intensity data types” on page 9-17.

**Wavelength shift box**

This parameter is used to simulate an offset error in wavelength. The WVASE® parameter is WvlShift. This shift is applied at the time of calculation. If the experimental data point wavelength is \( \lambda_1 \) and the shift is \( s \), then the model will be calculated using a wavelength of \( \lambda_1 + s \). If the model uses optical constants which are known to be correct in wavelength and the final fitted shift values is greater than zero, then that may indicate that the experimental data wavelengths should be shifted to a larger value, i.e. the monochromator wavelength may be reading low. As a word of caution, a wavelength shift may also correlate to model thicknesses and other parameters. Finding a non-zero wavelength shift may indicate a possible monochromator calibration error, but it is not a conclusive test.

**Window effects button**

This button opens the Window Effects dialog box, which is used to model the In-plane and Out-of-plane birefringent retardation of windows placed in the optical path between the ellipsometer components and the sample. Contact the Woollam Company for further information regarding modeling of window effects.

![Figure 7-108. The default Window Effects dialog box.](image)

**Delta Offset**

These boxes define the Delta offsets that are the result of in-plane window effects. They usually have a Cauchy-like dispersion as a function of \( 1/\lambda \). Contact the Woollam Company for further information regarding modeling of window effects.
Non-Ideal Model Options

Thickness non-uniformity option

When this sample non-ideality option is selected, this parameter is used to simulate layers which do not have parallel interfaces. This non-ideality is simulated by calculating data for the structure using a series of slightly different thicknesses for all layers in the model. The number of different structures calculated is set by the # of points in the Convolution Profile section. The maximum change in thickness from the model thickness is determined by the Thickness Non-Uniformity %. This value defines maximum and minimum percentage deviations from the model thicknesses at the edges of the convolution profile. The weighting each structure receives in the calculation is determined by the Convolution Profile Shape. The WVASE® parameter is ThkUni.

Light bandwidth option

This type of instrument non-ideality simulates the finite bandwidth of the probe beam. This non-ideality is simulated by calculating data from the model using a series of slightly different wavelengths. Whereas the Thickness Non-Uniformity option used a convolution of layer thickness, this option uses a convolution of wavelengths. The Light Bandwidth parameter defines the range of wavelengths used relative to the center wavelength. The Convolution Shape and # of points define the weighting and sampling density used. The WVASE® parameter is BndWdth.

Angular spread option

This type of non-ideality simulates the effect that occurs when using a focused probe beam, and is also useful for describing curved or warped sample surfaces or measurements performed with a highly decollimated probe beam. In all of these cases, the light collected by the detector struck the sample at a range of angles of incidence, rather than at a single well defined angle of incidence. This option is just like the light bandwidth option except that the convolution is performed on the angle of incidence for the model. The WVASE® parameter is AngSprd.

Convolution profile shape setting

These selection boxes determine the convolution profile used for averaging non-idealities based on layer thickness, light bandwidth, and incident angle. Experience indicates that most models are insensitive to the choice of the convolution profile shape. Users can always try different profiles during fitting to see if the profile type significantly affects the MSE.

Convolution # of points box

This box defines how many points are used for the convolution. This number should be an odd integer. Experience indicates that 5 points generally works for most models. The exception would be Ψ-Δ spectra that have a large number of interference oscillations. Users can always try increasing the number of points and refitting until no there are no longer any improvements in the MSE.

All 3 non-idealities option

This option allows the model to simultaneously include Thickness Non-Uniformity %, Light Bandwidth, and Angular Spread parameters as part of the fit. Users can include any two of the three options by fixing its value at zero. In a practical sense, it is often not possible to ascertain the type of non-ideality present in
the measured data by fitting the data alone, and some knowledge of the sample structure and measurement geometry is often required to deduce the appropriate choice of model non-ideality.

**IR Res (cm⁻¹) box**

This box allows the model to account for bandwidth effects specific to IR-VASE® data types. When IR-VASE® data files are opened WVASE® will automatically enter the correct resolution into this box and will also enter the correct value into the Bandwidth box. Those entries are based on information stored directly in IR-VASE® data files during data acquisition.

**Ellipsometer Type**

WVASE® calculates the model-generated ellipsometric data based the ellipsometer type selected from this list. Information on the ellipsometer type is stored directly in WVASE data files during data acquisition, and the correct ellipsometer type is automatically selected from this list whenever those data files are opened.

**Min Delta**

The value entered in this box defines the minimum Δ value allowed during plotting and calculation. This is an arbitrary choice, and does not alter the mathematical meaning of Δ, since it describes the phase difference between two complex values. The maximum Δ value plotted will always be the minimum value plus 360°.

**Global Model Options checkbox**

When the Global Model Options box is checked, these options are simultaneously applied to all of the available models. The Global Model Options checkbox is located in bottom right of dialog box, see Figure 7-106.

**Large Scale Patterning**

**Single Model Large Scale (“Layer #” box)**

This selection simulates a layer that only has partial coverage – for example, see Figure 7-110 top. For Large Scale patterning, the generated ellipsometric data represent an incoherent mixture of light from the covered and uncovered regions of the illuminated area on the sample.

In the figure, model “a” includes the specified layer, and model “b” is identical to the first except the patterned layer is not present. To model patterning, the software first calculates two Jones matrices:

\[ J_a = \text{Jones matrix for sample with designated layer} \]

\[ J_b = \text{Jones matrix for sample without designated layer} \]
Figure 7-110. Single-model pattern schematic with WVASE® models and patterning options.

$J_a$ and $J_b$ are converted into Mueller Matrices $M_a$ and $M_b$, and then each Mueller Matrix is multiplied by a weighting factor that represents its contribution to total light beam reflected or transmitted from the sample. The two Mueller Matrices are then added together to form a weighted sum $M_{sample}$ which represents a patterned sample that incoherently mixes light from the two regions of the sample surface.

$$J_a = \text{Jones matrix for sample with designated layer}$$

$$J_b = \text{Jones matrix for sample without designated layer}$$

$$J_a \rightarrow M_a \quad M_{sample} = \left(1 - \frac{P_l}{100}\right) M_a + \frac{P_l}{100} M_b \quad (7.16)$$

The “Layer #” box specifies which layer has partial coverage. $P_l$ is the “Patterned Large Scale %” parameter (WVASE® parameter name PercPat). $P_l$ is the fraction (%) of the illuminated area where the specified layer that is not present.

Using $M_{sample}$, the program calculates the generates the desired data type: $\Psi$, $\Delta$, %Depolarization, $R_p$, $R_s$, etc. The figure below illustrates Large Scale patterning.

Figure 7-111. Large Scale patterning generated data, various Percent Patterning values.
**Multiple Models Option**

Selecting the “Multiple Models” option will simulate samples with two or more regions, each region having a different layer structure. For every region, a layer structure is created in a different model window (to select different model windows, enter <Alt-1>, <Alt-2>, <Alt-3>, etc., or choose the “Select” option from the Model Window pull-down menus).

For the Multiple Model Option, the “Patterned Large Scale %” parameter $P_{Ln}$ (WVASE® parameter name PercPat-[model#]; for example, PercPat-2) is related to the percentage of total illuminated area that is covered by the specified model. The measurement parameters are calculated by adding the light collected from each region incoherently, using the following formula:

$$
\left(1 - \sum_{n} \frac{P_{Ln}}{100}\right) \cdot M_1 + \sum_{n} \frac{P_{Ln}}{100} M_n, \quad n = 2,3,4,...(\text{total # models}) \tag{7.17}
$$

where $M_1$ and $M_n$ are the Mueller Matrices for each model. The model therefore calculates and performs a weighted average to determine the effective simulated measurements. When the Multiple Model Option is selected, the “Patterned Large Scale %” parameter box for the 1st model ($P_{L1}$), is not active. Instead,

$$
P_{L1} = \left(100\% - \sum_{n} P_{Ln}\right), \quad n = 2,3,4,...(\text{total # models}) \tag{7.18}
$$

Figure 7-112 shows an example of a two-region pattern, with the WVASE® models along with the Patterning section of Model Options dialog box. Figure 7-113 shows the resulting $\Psi$, $\Delta$ and %Depolarization curves generated by the model.

![Two-region pattern schematic with WVASE® models and patterning options.](image)

Figure 7-112. Two-region pattern schematic with WVASE® models and patterning options.
Figure 7-113. \( \Psi \), \( \Delta \) and \%Depolarization generated from Multiple Models pattern models shown in previous figure.
Chapter 8 General Oscillator Layer

Introduction to the General Oscillator Layer

The General Oscillator Layer, or “GenOsc® layer”, (genosc.mat) was developed to simplify modeling material optical constants in WVASE® software. The GenOsc® layer allows the user to choose from a large variety of oscillator models and dispersion equations, all in a single material layer. Furthermore, a large number of oscillators (of the same or different types) are easily added together in an ensemble capable of describing extremely complicated dielectric functions.

Not only does the GenOsc® layer make it easy to combine a number of oscillators to model a layer’s dielectric function; it also allows the user to compare and fit that dielectric function directly to the optical constants of a reference material. The ease of use and flexibility of the GenOsc® layer means users will rarely need any other model in the WVASE® library.

Adding the Genosc® Layer to a model

One can add the general oscillator layer to a model by typing “genosc.mat” in the “File name:” space after selecting Model|Add Layer in the “Model” window. Figure 1 shows the genosc layer dialog box once it has been opened in WVASE®.

General Oscillator Theory: sum of parametric terms

The Genosc layer models the dielectric function of a film or substrate as a linear summation of real or complex terms (or “oscillators”), each of which is a function of
wavelength (nm or μm), inverse wavelength (in cm\(^{-1}\)), or photon energy (in eV). An example of such a sum is shown in Eq. (1) below.

\[
\varepsilon = \varepsilon_1 + i\varepsilon_2 = \text{Offset} + \frac{A_1}{E_1^2 - E^2} + \frac{A_2}{E_2^2 - E^2 - iB_2E} = \text{Gaussian}(E, A_1, E_3, B_3)
\]

The reader may recognize several of the terms. The Offset term is purely real constant, equivalent to \(\varepsilon_{\infty}\) that is often seen in scientific literature. The second and third are Pole or Sellmeier terms, and the fourth is a Lorentz oscillator term. The last term is a Gaussian term. It is a complex function in which the imaginary part models a Gaussian absorption and the real part is its Kramers-Kronig transform. All of these functions are described in more detail below. Currently, 24 different functions are available to the user of a Genosc layer. They are listed below, and described in detail in the Oscillator Types section:

1) **e1 Offset**
   Purely real constant added to \(\varepsilon_1\).

0

**Sellmeier & Pole**
Lorentz Oscillators with zero broadening.

3) **Cauchy**
Standard Cauchy with Urbach absorption.

4) **Lorentz**
Classic Lorentz Oscillator.

5) **Harmonic**
Classic Harmonic Oscillator.

6) **Ionic1 & Ionic2**
phonon absorption with \(\varepsilon_{dc}, \varepsilon_{\infty}, E_{TO}, E_{LO}\), & broadening as

7) **TOLO**
Factorized model for phonon absorption uses broadening for both TO & LO.

8) **Drude, rho-tau Drude & N-mu Drude**
Zero resonance energy Lorentz oscillators, used to represent free carrier effects.

9) **Tauc-Lorentz & Egap Tauc-Lorentz**
Tauc-Lorentz model for amorphous materials

10) **Cody-Lorentz**
Cody-Lorentz model for amorphous semiconductors.

11) **Gaussian**
Gaussian absorption model.

12) **Gauss-Lorentz**
Gaussian-Lorentzian absorption combination model.

13) **GLAD**
Gaussian-Lorentz Asymmetric Doublet oscillator.

14) **Psemi-(M0, M1, M2, M3 & Tri**
Parameterized Semiconductor oscillator model for modeling crystalline semiconductors.

15) **CPPB**
Critical Point Parabolic Band Oscillator for semiconductors.

16) **CPM0, CPM1, CPM2 & CPM3**
Adachi models for critical point functions M0, M1, M2, & M3.

17) **Tguy (Tanguy model)**
Provides an analytical expression of Wannier excitons.

18) **Lorentz-PB & Lorentz-LB**
Parabolic & Linear JDOS Band of Lorentz Oscillators.
Description of Genosc Layer Dialog Box

Figure 8-2. Various sections of genosc layer window.

The various sections of the Genosc.mat dialog box are listed in the table below. Their locations are shown Figure 2. Details are presented in the pages that follow.

<table>
<thead>
<tr>
<th>1. Standard features: Layer Name, Comment, Thickness, Delete Layer, Replace Layer, Optical Constants, &amp; OK (exit box). These buttons are found in most WVASE® layers.</th>
<th>8. Dielectric Function Display window. Displays ε1 and ε2 of model (and Reference Material, if selected).</th>
</tr>
</thead>
<tbody>
<tr>
<td>2. Position (eV) and “Magnitude: Center energy (position) and strength (magnitude) of two zero-width oscillators.</td>
<td>9. Ref. Material: Displays optical constants from an existing “reference” material file.</td>
</tr>
<tr>
<td>3. ε1 Offset: Purely real offset to ε1.</td>
<td>10. Fit to Ref.: Fits selected oscillators’ parameters directly to reference material.</td>
</tr>
<tr>
<td>4. Type &amp; Style: Pull-down menus select the oscillator type and exact functional form, respectively.</td>
<td>11. x-axis range, steps &amp; units: Selects x-axis range, steps and units (eV or cm⁻¹) for Dielectric Function display.</td>
</tr>
<tr>
<td>5. Active: Determines if corresponding oscillator is included optical model.</td>
<td>12. Graph/Fit ε1 &amp; ε2: Allows ε1 to be both displayed and fit along with ε2.</td>
</tr>
<tr>
<td>6. Oscillator Parameters: Parameter values of selected oscillator</td>
<td>13. Add (Delete) Oscillator Adds “NEW” oscillator to Oscillator List. If an active oscillator is selected, selecting this button will delete the oscillator from the list.</td>
</tr>
<tr>
<td>7. Oscillator List: List of all oscillators currently defined in model</td>
<td>14. Osc Up &amp; Osc Down Moves position of selected oscillator in Oscillator List</td>
</tr>
</tbody>
</table>
The various sections of the Genosc.mat dialog box are described in more detail below. Their locations are shown Figure 2.

1. **Standard WVASE® layer Feature:**

   Name, Comment, Thickness, Delete Layer, Replace Layer, Optical Constants >>, Opt Const Fit, & OK (exit box). These are the same features that are found in most WVASE® layers. The layer-thickness value is included as a fit parameter when the Fit check box next to the Thickness window is selected. The optical constants are fit at every wavelength when the Opt Const Fit (n & k) boxes are selected.

   ![Standard WVASE® layer selection](image)

   **Figure 8-3.** Standard WVASE® layer selections.

2. **Poles #1 & #2 Position (eV) and “Magnitude:**

   The user can define the position (center energy) and magnitude (strength) of two zero-width Lorentz oscillators (or poles). These simulate the dispersion in ε1 created by absorption that occurs outside the measured spectral range. Each position and magnitude can be included as a fit parameter by selecting check box next to it. These oscillators are called Pole oscillators, and are functionally equivalent to Sellmeier oscillators. The Pole and Sellmeier oscillator types are described in the Oscillator types section.

   ![Poles #1 & 2](image)

   **Figure 8-4.** Poles #1 & 2.
3. **e1 Offset:**
   The user can enter a purely real offset to e1 in this box. The offset term can be included as a fit parameter by selecting the check box directly to its right.

4. **Type and Style:**
   The user can select the type of oscillator from the **Type** pull-down menu (Fig. 6 left). Certain types of existing oscillators can be freely converted from one to another (e.g. Lorentz⇒Harmonic⇒Gaussian). Irreversible conversion from one type to another is also possible and you will be prompted to confirm that you really want to make the change (e.g. Lorentz ⇒ Gauss-Lorentz). Some conversions are not possible (e.g. a Pole cannot be converted to a Lorentz). Descriptions of the different types of terms are described in the Oscillator types section.

   The “**Style**” pull-down menu (Fig. 6 right) allows the user to select the exact functional form of each oscillator type. Most oscillator types have more than one style. The style defines whether the oscillator is a function of Energy (eV), inverse wavelength (cm\(^{-1}\)), or wavelength (nm or μm). Depending on the circumstances, one functional form might work better than another. In addition, the styles of some oscillators provide direct access to “physical” fit parameters that might be included in a particular functional form (e.g., see **rho-tau** oscillator description). The aspects of the various Styles, as well as oscillator descriptions, are discussed in a later section.

---

**Figure 8-5. e1 Offset.**

**Figure 8-6. Oscillator model “Type” (Left) and “Style” (right) pull down menus.**
5. **Active:**
   This check box determines if an oscillator is included in optical model (Fig. 7).

6. **Oscillator Parameters:**
   The parameters and their values corresponding to the selected oscillator term will be displayed in the area directly below the **Type** and **Style** menus. Each parameter can be allowed to vary in the fit by selecting the check box next to the parameter (Fig. 7).

![Oscillator Parameters](image)

**Figure 8-7.** *Active check box & Oscillator Parameters.*

7. **Oscillator List:**
   The **Oscillator List** at the bottom left of the dialog displays all oscillators included in the model (with the exception of **New Osc**, see next paragraph).

   The **New Osc** is always the first oscillator listed. It is used to add new oscillators to the model. **New Osc** is **never** active in the model. To add new oscillators to the model, the user highlights the **New Osc** line, selects the desired oscillator **Type** and **Style**, then adds the **New Osc** to the model by selecting the **Add Oscillator** button (Section 8).

   The parameters of any oscillator can be manually varied by selecting it in the **Oscillator List**. The selected oscillator will be highlighted in blue, and its corresponding **Type**, **Style** and **Oscillator Parameters** will be displayed in the boxes above (Fig. 8). Furthermore, the selected oscillator contribution to $\varepsilon_2$ will be shown as a blue curve in the **Dielectric Function Display window** (Fig 8).

   Multiple oscillators can be selected from the list and the $\varepsilon_2$ for each selected oscillator will be displayed as blue curves in the **Dielectric Function Display window**. Multiple oscillators are selected by clicking on the desired oscillators in the list while holding down the “Ctrl” button. The parameters for the last oscillator highlighted will be displayed in **Oscillator Parameters**. Figure 9 shows a dispersion model for gallium arsenide. Note that two oscillators are selected and their $\varepsilon_2$ are displayed in the graph window.
8. **Add Oscillator (Delete Oscillator) button:**

This button adds the *New oscillator* to the *Oscillator List*. When another oscillator is highlighted in the *Oscillator List*, the button becomes a *Delete Oscillator* button, which allows the user to remove oscillators from the list.

9. **Dielectric Function Display window:**

Displays the real and imaginary parts of the dielectric function, $\varepsilon_1$ and $\varepsilon_2$, of model and reference material (if a reference material has been selected). The curves are displayed as a function of energy (in eV) or wavenumbers (in cm$^{-1}$) (See Section 10).

The amplitude, broadening, and center energy of many oscillators (*Lorentz*, *Gaussian*, *Harmonic*, *Tauc-Lorentz*, etc.) can be varied interactively from within the graph window by first highlighting the desired oscillator in the *Oscillator List* (Section 7 and Fig. 8). When the individual oscillator is displayed in the *Dielectric Function Display window*, there will be small squares that provide a means of interactively adjusting the amplitude, broadening, and center energy (Fig. 9). To adjust parameters, use the mouse to click and drag the squares.

Moving the cursor anywhere over the *Dielectric Function Display window* will display the energy and optical constant values under the arrow.

**NOTE:** Many ‘New Osc’ oscillators can be added to the model by holding down the shift key and clicking the left mouse button (shift left-click). Not all oscillators can be added graphically (e.g. a Drude oscillator cannot be added this way). The amplitude and energy of the new oscillator will be adjusted to match the energy and $\varepsilon_2$ value of the cursor where the user just clicked.
Figure 8-9. Dielectric Function Display window. Model $\varepsilon_1$ and $\varepsilon_2$ are displayed as black lines. $\varepsilon_2$ of selected individual oscillators are highlighted in blue.

10. **x-axis units, steps & range:**
    These windows and pull-down menu allow the user to select x-axis units (eV or cm$^{-1}$), steps and range in the Dielectric Function Display window. Fig. 9 shows the x-axis parameters set for 0.1 to 6 eV by .0295 eV steps. (maximum of 5000 wavelengths). The drop-down menu allows one to select the wavelength units in either electron volts (eV) or wavenumbers (cm$^{-1}$). The units in terms of eV works well for the UV to NIR spectral range and cm$^{-1}$ works well for viewing IR data. The steps and range are automatically updated when a tabulated Ref Material is loaded. When the Reference Material is a parameterized model, the user must set the range and step size manually. **NOTE:** the range should not exceed the valid energy range of the reference material file.

11. **Ref. Material button:**
    This button allows the user to display the dielectric function for an existing “reference” material file in the Dielectric Function Display window. An example is shown in Fig. 10, where the file gap.mat is being displayed. $\varepsilon_1$ and $\varepsilon_2$ of reference material dielectric function are displayed as a green line and a red line, respectively. The reference material file name is displayed directly below the Ref. Material button.
    When a tabulated Ref Material file is loaded, the energy steps and range are automatically updated to values found in that file.
12. **Fit e2 only, Fit e1 only, & Fit Both** buttons:

   Allows user to select whether \( \varepsilon_2, \varepsilon_1 \), or both will be and enabled for fitting. When **e2 only** is selected, only \( \varepsilon_2 \) is displayed the Dielectric Function Display window. Otherwise, both \( \varepsilon_1 \) and \( \varepsilon_2 \) are displayed. In cases where the \( \varepsilon_2 \) fit is not very good, or the reference spectra is not precisely Kramers-Kronig consistent, it might be useful to fit the \( \varepsilon_1 \) spectra separately.

13. **Fit to Ref.** button:

   This button allows the user to fit the selected model parameters directly to the reference material. The user selects the desired oscillator, \( \varepsilon_1 \) offset, & pole fit parameters and then clicks the **Fit to Ref.** button. This is a very powerful and simple way of fitting dispersion models to existing optical constants (from other parametric models, literature or point-by-point fits).

14. **Reset** button:

   Resets all fit parameters to original values.

15. **Osc Up & Osc Down** buttons:

   These buttons move the position of the selected oscillator in Oscillator List.

---

**Style numbers in the Generalized Oscillator Layer**

The Lorentz, Harmonic, and Gaussian Oscillator Types in the Generalized Oscillator Layer each allow six different styles: .0, .1, .2, .5, .6, and .7. The first three styles listed are in eV units, while the last three are in cm\(^{-1}\) units. Although all six styles produce equivalent dielectric functions, their amplitude term \( A_n \) is multiplied by combinations of \( B_r \) and \( E_n \) such that the amplitude is directly related to either the \( \varepsilon_2 \) peak height or peak area, or the amount of offset in \( \varepsilon_1 \) (or \( \delta\varepsilon_1 \)) induced by the Oscillator. (The quantity \( \delta\varepsilon_1 \) should not be confused with \( \varepsilon_{1\_offset} \), which is a constant that is added to \( \varepsilon_1 \) at all photon energies).
The table below shows the formulas for the examples of style "0.0" using Gaussian Oscillators. The $\varepsilon_2$ peak heights equal $A_n$, regardless of the Broadening ($B_{rn}$). ("0.5" is similar to "0.0").

<table>
<thead>
<tr>
<th>Style #</th>
<th>Lorentz example</th>
<th>$\varepsilon_2$ at $E_n$</th>
<th>$A_n$</th>
<th>Units of $A_n$</th>
</tr>
</thead>
<tbody>
<tr>
<td>.0 (.5)</td>
<td>$\varepsilon = \frac{A_n B_{rn} E_n}{E_n^2 - E^2 - iB_{rn} E}$</td>
<td>$A_n$</td>
<td>Is the peak height of $\varepsilon_2$ at center Energy ($E_n$)</td>
<td>Dimensionless</td>
</tr>
<tr>
<td>.1 (.6)</td>
<td>$\varepsilon = \frac{A_n E_n}{E_n^2 - E^2 - iB_{rn} E}$</td>
<td>$A_n B_{rn}$</td>
<td>Is proportional to Area</td>
<td>eV (cm$^{-1}$)</td>
</tr>
<tr>
<td>.2 (.7)</td>
<td>$\varepsilon = \frac{A_n E_n^2}{E_n^2 - E^2 - iB_{rn} E}$</td>
<td>$A_n E_n / B_{rn}$</td>
<td>Is $\delta \varepsilon_1$, where $\delta \varepsilon_1 = \varepsilon_1 (E &lt; E_n) - \varepsilon_1 (E &gt; E_n)$</td>
<td>Dimensionless</td>
</tr>
</tbody>
</table>

The figure below shows examples of style "0.0" using Gaussian Oscillators. The $\varepsilon_2$ peak heights equal $A_n$, regardless of the Broadening ($B_{rn}$). ("0.5" is similar to "0.0").

![Image of Gaussian Oscillators](image1)

**Figure 8-11.** $\varepsilon_2$ for plots for three Gaussian-style0 (Gau.0) oscillators.

The next figure shows examples of style "1.1" using Gaussian Oscillators. The areas under each curve are proportional to $A_n$, regardless of the Broadening ($B_{rn}$). (Style "1.6" is similar to style "1.1").

![Image of Gaussian Oscillators](image2)

**Figure 8-12.** $\varepsilon_2$ for plots for three Gaussian-style1 (Gau.1) oscillators.

Examples of style "2.2" using Lorentz Oscillators. The $\varepsilon_1$ offset generated by the oscillator equals $A_n$, regardless of the Broadening ($B_{rn}$), [i.e., $A_n = \delta \varepsilon_1 = \varepsilon_1 (E < E_n) - \varepsilon_1 (E > E_n)$]. (Style "2.7" is similar to style "2.2").

![Image of Lorentz Oscillators](image3)
Styles for the Gauss-Lorentz, GLAD, CPPB & TOLO

Similar styles are available with the Gauss-Lorentz, GLAD, CPPB and TOLO Oscillator Types. The only difference between these four oscillator types and the Lorentz, Harmonic, and Gaussian oscillators is that $A_n$ is proportional to the peak height, not equivalent to it.

Other oscillator styles

The styles Pole, Sellmeier, Cauchy and Drude, rho-tau Drude and $N$-mu Drude are described in the “Oscillator Function Descriptions” section below.

Some of the specialty oscillators such as Tanguy and CPM0, CPM1, CPM2 and CPM3, are constructed with only the one style representing the form described in original reference(s). Refer to the oscillator description below for more details.

Oscillator Function Descriptions

Every Genosc layer models the dielectric function of a film or substrate as a linear summation of real and complex terms (or “oscillators”), each of which is a function of wavelength (nm or $\mu$m), inverse wavelength (in $\text{cm}^{-1}$), or photon energy (in eV). For example, the Genosc oscillator list shown in the figure below consists of three oscillator types – a Lorentz, Gaussian, and Tauc Lorentz. In addition, every Genosc layer has are the Pole #1, Pole #2, and $e1$ Offset terms. The resulting mathematical formula for the layer as displayed is:

$$
\varepsilon = \varepsilon_1 - i\varepsilon_2
$$

$$
= e_1 \text{ Offset} + \text{Pole #1}(\text{Pos, Mag}) + \text{Pole #2}(\text{Pos, Mag}) +
\text{Lorentz}(A_n, E_n, B_r) +
\text{Gaussian}(A_n, E_n, B_r) +
\text{Tauc Lorentz}(A_n, E_n, E_g, B_r)
$$

Although the Pole #1, Pole #2, and $e1$ Offset terms are included in every Genosc layer, they can be effectively disabled by setting their amplitudes equal to zero. The Lorentz, Gaussian, and Tauc Lorentz terms are complex functions of energy.
Figure 8-14. Genosc dialog box configured to represent equation above.

Oscillator functions

Currently, 27 different functions are available to the user of a Genosc layer. All of these functions are described in more detail in the following sections:

1) **e1 Offset**
   Purely real constant added to $\varepsilon_1$.

2) **Sellmeier & Pole**
   Lorentz Oscillators with zero broadening.

3) **Cauchy**
   Standard Cauchy with Urbach absorption.

4) **Lorentz**
   Classic Lorentz Oscillator.

5) **Harmonic**
   Classic Harmonic Oscillator.

6) **Ionic1 & Ionic2**
   Phonon absorption with $\varepsilon_{\text{dc}}$, $\varepsilon_{\text{ex}}$, $E_{\text{TO}}$, $E_{\text{LO}}$, & broadening as

7) **TOLO**
   Factorized model for phonon absorption uses broadening for both TO & LO.

8) **Drude, rho-tau Drude & N-mu Drude**
   Zero resonance energy Lorentz oscillators, used to represent free carrier effects.

9) **Tauc-Lorentz & Egap Tauc-Lorentz**
   Tauc-Lorentz model for amorphous materials

10) **Cody-Lorentz**
    Cody-Lorentz model for amorphous semiconductors.

11) **Gaussian**
    Gaussian absorption model.

12) **Gauss-Lorentz**
    Gaussian-Lorentzian absorption combination model.

13) **GLAD**
    Gaussian-Lorentz Asymmetric Doublet oscillator.

14) **Psemi-(M0, M1, M2, M3 & Tri**
    Parameterized Semiconductor oscillator model for modeling crystalline semiconductors.

15) **CPPB**
    Critical Point Parabolic Band Oscillator for semiconductors.

16) **CPM0, CPM1, CPM2 & CPM3**
    Adachi models for critical point functions M0, M1, M2, & M3.

17) **Tguy (Tanguy model)**
    Provides an analytical expression of Wannier excitons.

18) **Lorentz-PB & Lorentz-LB**
    Parabolic & Linear JDOS Band of Lorentz Oscillators.
1) e1 Offset

Purely real constant added to $\varepsilon_1$. $e1$ Offset is equivalent to “$\varepsilon_\infty$”, which is often seen in scientific literature.

2) Sellmeier & Pole oscillators

**NOTE:** The center energies (or wavelengths) chosen for Pole and Sellmeier oscillators must be outside the valid spectral range of the model.

Sellmeier and pole terms\(^{iii}\) are Lorentz oscillators with zero broadening, and so they only affect the real part of the dielectric function ($\varepsilon_1$). They can accurately describe dispersion in spectral regions with **no absorption**. The various Sellmeier and Pole styles use different parameter values to produce identical curves.

Sellmeier dispersion models a material as a collection of atoms whose electron clouds are displaced by the oscillating electric fields of the light\(^{iii}\). The resulting oscillating atomic dipoles have a resonant frequency (energy) but no absorption, so each Sellmeier term is a Lorentz oscillator with zero broadening. The Sellmeier model works quite well in regions were there is no absorption – i.e., $\varepsilon_2 = 0$.

**Sellmeier Styles:**

<table>
<thead>
<tr>
<th>Style</th>
<th>Equation/asymptotic value &amp; (applications)</th>
<th>Fit Parameters ($n = \text{osc#}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sell.0 (nm) Sell.5 (µm)</td>
<td>$\varepsilon_{n,\text{sellmeier}} = \frac{A_n \cdot \lambda^2 \lambda_n^2}{\lambda^2 - \lambda_n^2}$ $\rightarrow -A_n \lambda^2$ when $\lambda \ll \lambda_n$ (model NIR-dispersion)</td>
<td>$Amp_n = A_n (\text{nm}^{-2})$, $Wvl_n = \lambda_n (\text{nm})$ $Amp_n = A_n (\text{µm}^{-2})$, $Wvl_n = \lambda_n (\text{µm})$</td>
</tr>
<tr>
<td>Sell.1 (nm) Sell.6 (µm)</td>
<td>$\varepsilon_{n,\text{sellmeier}} = \frac{A_n \cdot \lambda^2 \lambda_n}{\lambda^2 - \lambda_n^2}$ $\rightarrow A_n \lambda_n$ when $\lambda_n \ll \lambda_n$</td>
<td>$Amp_n = A_n (\text{nm}^{-1})$, $Wvl_n = \lambda_n (\text{nm})$ $Amp_n = A_n (\text{µm}^{-1})$, $Wvl_n = \lambda_n (\text{µm})$</td>
</tr>
<tr>
<td>Sell.2 (nm) Sell.7 (µm)</td>
<td>$\varepsilon_{n,\text{sellmeier}} = \frac{A_n \cdot \lambda^2}{\lambda^2 - \lambda_n^2}$ $\rightarrow A_n$ when $\lambda &gt;&gt; \lambda_n$ (used to model Schott glass &amp; other optical materials)</td>
<td>$Amp_n = A_n (\text{dimensionless})$, $Wvl_n = \lambda_n (\text{nm})$ or $Wvl_n = \lambda_n (\text{µm})$</td>
</tr>
</tbody>
</table>

### Pole Styles (including Poles #1 & #2 in upper-left corner of Genosc® dialog box):

<table>
<thead>
<tr>
<th>Style</th>
<th>Equation/asymptotic value &amp; (applications)</th>
<th>Fit Parameters (n = osc#)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pole.0 (eV)</td>
<td>( \varepsilon_{n_pole} = \frac{A_n}{E_n^2 - E^2} )</td>
<td>( \text{Amp}_n = A_n (nm^-2), , \text{Wvl}_n = \lambda_n (nm) )</td>
</tr>
<tr>
<td>Pole.5 (cm(^{-1}))</td>
<td>( \rightarrow -A_n/E^2 ) when ( E &gt; &gt; E_n )</td>
<td>( \text{Amp}_n = A_n (\mu m^{-2}), , \text{Wvl}_n = \lambda_n (\mu m) )</td>
</tr>
<tr>
<td>Pole.1 (eV)</td>
<td>( \varepsilon_{n_pole} = \frac{A_n \cdot E_n}{E_n^2 - E^2} )</td>
<td>( \text{Amp}_n = A_n (eV), , \text{En}_n = E_n (eV) )</td>
</tr>
<tr>
<td>Pole.6 (cm(^{-1}))</td>
<td>( \rightarrow A_n/E_n ) when ( E &lt;&lt; E_n )</td>
<td>( \text{Amp}_n = A_n (cm^{-1}), , \text{En}_n = E_n (cm^{-1}) )</td>
</tr>
<tr>
<td>Pole.2 (eV)</td>
<td>( \varepsilon_{n_pole} = \frac{A_n \cdot E_n^2}{E_n^2 - E^2} )</td>
<td>( \text{Amp}_n = A_n ) (dimensionless), ( \text{En}_n = E_n (eV) ) or ( \text{En}_n = E_n (cm^{-1}) )</td>
</tr>
<tr>
<td>Pole.7 (cm(^{-1}))</td>
<td>( \rightarrow A_n ) when ( E &lt;&lt; E_n )</td>
<td>( \text{PoleMagn}_n = A_n (eV^2) ), ( \text{PolePosn}_n = E_n (eV) ) ( n = 1, 2 )</td>
</tr>
<tr>
<td>Pole #1 &amp; #2</td>
<td>( \varepsilon_{n_pole} = \frac{A_n}{E_n^2 - E^2} )</td>
<td>( \text{PoleMagn}_n = A_n (eV^2) ), ( \text{PolePosn}_n = E_n (eV) ) ( n = 1, 2 )</td>
</tr>
</tbody>
</table>

**Figure 8-15.** \( \varepsilon_1 \) plot showing the dispersion obtained from two Pole terms. Please note that the center energy \( (E_n \text{ or } \lambda_n) \) is **outside** the model’s valid spectral range.

### 3) Cauchy

The **Cauchy** function\(^{iv}\) can describe dispersion for a material that is essentially non-absorbing over the measured wavelength range. Like the **Sellmeier** and **Pole** oscillators, the **Cauchy** function provides a means to curve-fit dispersion. However, the **Cauchy** term is most effective when curve fitting normal dispersion (n

decreasing with wavelength). Note that the Cauchy equation, which is given below, is described in terms of refractive index $n$ (Re$\sqrt{\varepsilon}$). The GenOsc Cauchy term also includes Urbach absorption, which is used to describe the exponential absorption tail that occurs below the bandgap of many materials – the same as Cauchy.mat.

**Cauchy Styles:**

<table>
<thead>
<tr>
<th>Style</th>
<th>Equation</th>
<th>Fit Parameters ($n = \text{osc#}$)</th>
</tr>
</thead>
</table>
| Chy.0 | $N_n = A_n + B_n/\lambda^2 + C_n/\lambda^4$ | $An = A_n$ (dimensionless)  
$Bn = B_n$ ($\mu$m$^2$)  
$Cn = C_n$ ($\mu$m$^4$)  
$\lambda$ ($\mu$m)  
$Akn = \alpha$ (dimensionless)  
$Bkn = \beta$ (eV$^{-1}$)  
$Ckn = \gamma$ (eV) (user adjustable but not fitable*). |
| Chy.1 | $N_n = A_n + B_n/\lambda^2 + C_n/\lambda^4$ | $An, Bn, Cn$ and $\lambda$ same as above  
$Akn = \alpha$ (dimensionless)  
$Bkn = \beta$ (eV$^{-1}$)  
$Ckn = \gamma$ (eV) (user adjustable but not fitable*). |

*Completely correlated with $Akn(\alpha)$

When using the Cauchy term in the GenOsc layer, you will normally want to set the $e1$ Offset value equal to zero. This will guarantee that only the Cauchy terms will contribute to the index.

In the Cauchy equation, the $A_n$ term describes the long-wavelength asymptotic index value, while the $B_n$ and $C_n$ are the dispersion terms that add upward slope to the index curve as wavelengths become shorter ($B_n$ and $C_n \geq 0$). The Cauchy dispersion relation was design to model the normal dispersion seen in transparent materials.

An exponential function models an Urbach absorption tail. In the model, $K_n = \alpha$ when $E - \gamma = 0$. Therefore, $\gamma(Ckn)$ is completely correlated with $\alpha(Akn)$. Also note that $K_n = \alpha e^{-1}$ when $E - \alpha = \beta^{-1}$ ($\beta = Bkn$). The effects of the various parameters on a Cauchy dispersion model are illustrated in the figure below.

![Figure 8-16. $n(\lambda)$ and $k(\lambda)$ for a Cauchy term ($A_n=1.5$, $B_n=0.05$, $C_n=0.0$, $K_n=1.7$).](image)
The limitations of the Cauchy and Urbach parameterization of the optical response of strongly absorbing materials are detailed in Chapter 13 of the WVASE® software manual.

4) Lorentz

This is the classic Lorentz oscillator, which is described in more detail in chapter 13 of the WVASE® software manual (See also Optical Properties of Solids by F. Wooten⁷). The complex dielectric function Lorentz Oscillator model is shown in Figure 8-17. Note that the low-energy portions of the ε₁ curves are most strongly effected by area under of the curve (Area is proportional to $A_n \times Br_n$). Also note that the peak shifts to lower energies as broadening increases.

**Lorentz Styles:**

<table>
<thead>
<tr>
<th>Style</th>
<th>Equation</th>
<th>Fit Parameters ($n = osc#$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lor.0 (eV)</td>
<td>$\varepsilon_{n,Lorentz} = \frac{A_n Br_n E_n}{E_n^2 - E^2 - iBr_n E}$</td>
<td>$Amp_n = A_n \ (\text{dimensionless}), \ E_n = E_n \ (eV), \ Br_n = Br_n \ (eV)$</td>
</tr>
<tr>
<td>Lor.5 (cm⁻¹)</td>
<td>$\varepsilon_{n,Lorentz} = \frac{A_n E_n}{E_n^2 - E^2 - iBr_n E}$</td>
<td>$Amp_n = A_n \ (\text{dimensionless}), \ E_n = E_n \ (eV), \ Br_n = Br_n \ (eV)$</td>
</tr>
<tr>
<td>Lor.1 (eV)</td>
<td>$\varepsilon_{n,Lorentz} = \frac{A_n E_n}{E_n^2 - E^2 - iBr_n E}$</td>
<td>$Amp_n = A_n \ (\text{eV}), \ E_n = E_n \ (eV), \ Br_n = Br_n \ (eV)$</td>
</tr>
<tr>
<td>Lor.6 (cm⁻¹)</td>
<td>$\varepsilon_{n,Lorentz} = \frac{A_n E_n}{E_n^2 - E^2 - iBr_n E}$</td>
<td>$Amp_n = A_n \ (\text{cm}^{-1}), \ E_n = E_n \ (cm^{-1}), \ Br_n = Br_n \ (cm^{-1})$</td>
</tr>
<tr>
<td>Lor.2 (eV)</td>
<td>$\varepsilon_{n,Lorentz} = \frac{A_n E_n}{E_n^2 - E^2 - iBr_n E}$</td>
<td>$Amp_n = A_n \ (\text{dimensionless}), \ E_n = E_n \ (eV), \ Br_n = Br_n \ (eV)$</td>
</tr>
<tr>
<td>Lor.7 (cm⁻¹)</td>
<td>$\varepsilon_{n,Lorentz} = \frac{A_n E_n}{E_n^2 - E^2 - iBr_n E}$</td>
<td>$Amp_n = A_n \ (\text{dimensionless}), \ E_n = E_n \ (cm^{-1}), \ Br_n = Br_n \ (cm^{-1})$</td>
</tr>
</tbody>
</table>

![Figure 8-17. $\varepsilon_1$ and $\varepsilon_2$ for Lorentz oscillator model (Style: Lor.1, $A_n = 1, E_n = 2 \ eV, Br_n$ as indicated in Legend).](image)

5) Harmonic

This is the classic Harmonic oscillator, and is typically written in the literature as the sum of two terms in a form something like this:

$$\varepsilon_{n \text{ Harmonic}} = \frac{F_n}{E_n - E - i\Gamma_n} + \frac{F_n}{E_n + E + i\Gamma_n}$$

with oscillator strength $F_n$, center energy $E_n$, and broadening $\Gamma_n$. WVASE® uses the following equivalent form:

$$\varepsilon_{n \text{ Harmonic}} = \frac{A_n E_n}{E_n^2 - E^2 + 1/4B_{rn}^2 - iB_{rn}E}$$

where $A_n = 2F_n$, and $B_{rn} = 2\Gamma_n$. $B_{rn}$ is approximately the full-width at half-maximum value.

**Harmonic Styles:**

<table>
<thead>
<tr>
<th>Style</th>
<th>Equation</th>
<th>Fit Parameters (n = osc#)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Har.0 (eV)</td>
<td>$\varepsilon_{n \text{ Harmonic}} = \frac{A_n B_{rn} E_n}{E_n^2 - E^2 + 1/4B_{rn}^2 - iB_{rn}E}$</td>
<td>$Ampn = A_n \ (\text{dimensionless})$, $Enn = E_n \ (\text{eV})$, $B_{rn} = B_{rn} \ (\text{eV})$</td>
</tr>
<tr>
<td>Har.5 (cm⁻¹)</td>
<td>$\varepsilon_{n \text{ Harmonic}} = \frac{A_n B_{rn} E_n}{E_n^2 - E^2 + 1/4B_{rn}^2 - iB_{rn}E}$</td>
<td>$Ampn = A_n \ (\text{dimensionless})$, $Enn = E_n \ (\text{eV})$, $B_{rn} = B_{rn} \ (\text{eV})$</td>
</tr>
<tr>
<td>Har.1 (eV)</td>
<td>$\varepsilon_{n \text{ Harmonic}} = \frac{A_n E_n}{E_n^2 - E^2 + 1/4B_{rn}^2 - iB_{rn}E}$</td>
<td>$Ampn = A_n \ (\text{eV})$, $Enn = E_n \ (\text{eV})$, $B_{rn} = B_{rn} \ (\text{eV})$</td>
</tr>
<tr>
<td>Har.6 (cm⁻¹)</td>
<td>$\varepsilon_{n \text{ Harmonic}} = \frac{A_n E_n}{E_n^2 - E^2 + 1/4B_{rn}^2 - iB_{rn}E}$</td>
<td>$Ampn = A_n \ (\text{eV})$, $Enn = E_n \ (\text{eV})$, $B_{rn} = B_{rn} \ (\text{eV})$</td>
</tr>
<tr>
<td>Har.2 (eV)</td>
<td>$\varepsilon_{n \text{ Harmonic}} = \frac{A_n E_n^2}{E_n^2 - E^2 + 1/4B_{rn}^2 - iB_{rn}E}$</td>
<td>$Ampn = A_n \ (\text{dimensionless})$, $Enn = E_n \ (\text{eV})$, $B_{rn} = B_{rn} \ (\text{eV})$</td>
</tr>
<tr>
<td>Har.7 (cm⁻¹)</td>
<td>$\varepsilon_{n \text{ Harmonic}} = \frac{A_n E_n^2}{E_n^2 - E^2 + 1/4B_{rn}^2 - iB_{rn}E}$</td>
<td>$Ampn = A_n \ (\text{dimensionless})$, $Enn = E_n \ (\text{eV})$, $B_{rn} = B_{rn} \ (\text{eV})$</td>
</tr>
</tbody>
</table>

When $B_{rn} < En$, a Harmonic oscillator behaves as a Lorentz oscillator. The Harmonic and Lorentzian line shapes are compared in the figure below.

---

vi For example, see S. Adachi, *Optical properties of crystalline and amorphous semiconductors: materials and fundamental principles,* (Kluwer Academic Publishers, Norwell, MA, USA, 1999), p. 64.
6) Ionic1 & Ionic2

One of the forms of the Lorentz oscillator, Ionic is used to describe infrared-active phonon adsorptions. The form is similar the Lorentz oscillator described above, except that the numerator consists of the combinations of $E_{Tn}$ (transverse optical phonon energy) and $E_{Ln}$ (longitudinal optical phonon energy) as well as $\varepsilon_{en}$ (the contribution from electronic transitions) and $\varepsilon_{dcn}$ (the dc dielectric constant). These four quantities are related via the Lyddane-Sachs-Teller relation, $E_T/E_L = \varepsilon_{dc}/\varepsilon_{en}$. Please note that $\varepsilon_{en}$ and $\varepsilon_{dc}$ have similar effects on the high-energy value of $\varepsilon_1$. However, only $\varepsilon_{dc}$ affects the amplitude of $\varepsilon_2$ at the resonance peak centered at $E_{Tn}$, via the equations shown below. The classic Lorentz oscillator model is described in more detail in chapter 13 of the WVASE® software manual.

**Ionic1 & Ionic2 Styles:**

<table>
<thead>
<tr>
<th>Style</th>
<th>Equation</th>
<th>Fit Parameters (n = osc#)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ion1.0 (eV)</td>
<td>$\varepsilon_{Ion1_n} = \varepsilon_{en} + \frac{E_{Tn}^2 (\varepsilon_{dcn} - \varepsilon_{en})}{E_{Tn}^2 - E^2 - iBrn E}$</td>
<td>$edcn = \varepsilon_{dcn} \text{ (dimensionless)}, \varepsilon_{en} = \varepsilon_{en} \text{ (dimensionless)}, E_{Tn} = ETn (\text{eV}), Brn = Brn (\text{eV})$</td>
</tr>
<tr>
<td>Ion1.5 (cm⁻¹)</td>
<td>$\varepsilon_{Ion2_n} = \frac{E_{Tn}^2}{E_{Ln}^2} \left( 1 - \frac{E_{Tn}^2}{E_{Ln}^2} \right)$</td>
<td>$edcn = \varepsilon_{dcn} \text{ (dimensionless)}, E_{Tn} = ETn (\text{eV}), Brn = Brn (\text{eV}), E_{Ln} = ELn (\text{cm}^{-1})$</td>
</tr>
<tr>
<td>Ion2.0 (eV)</td>
<td>$\varepsilon_{Ion2_n} = \varepsilon_{dcn} \left( \frac{E_{Tn}^2}{E_{Ln}^2} \right)^\frac{1}{2} + \frac{E_{Tn}^2}{E_{Ln}^2} \left( 1 - \frac{E_{Tn}^2}{E_{Ln}^2} \right)$</td>
<td>$edcn = \varepsilon_{dcn} \text{ (dimensionless)}, E_{Tn} = ETn (\text{eV}), Brn = Brn (\text{eV}), E_{Ln} = ELn (\text{cm}^{-1})$</td>
</tr>
<tr>
<td>Ion2.5 (cm⁻¹)</td>
<td>$\varepsilon_{Ion2_n} = \varepsilon_{dcn} \left( \frac{E_{Tn}^2}{E_{Ln}^2} \right)^\frac{1}{2} + \frac{E_{Tn}^2}{E_{Ln}^2} \left( 1 - \frac{E_{Tn}^2}{E_{Ln}^2} \right)$</td>
<td>$edcn = \varepsilon_{dcn} \text{ (dimensionless)}, E_{Tn} = ETn (\text{eV}), Brn = Brn (\text{eV}), E_{Ln} = ELn (\text{cm}^{-1})$</td>
</tr>
</tbody>
</table>
7) TOLO

This factorized oscillator describes an IR-active phonon resonance with significant anharmonic coupling effects seen in multiple-phonon-mode materials. The model contains two broadening parameters, Bto and Blo, which are associated with the n<sup>th</sup> TO phonon and n<sup>th</sup> LO phonon resonance, respectively. If Bto = Blo, then the TOLO resonance assumes the classic Lorentz oscillator lineshape.

As noted in Ref vii, the dielectric function will remain physical (i.e., ε≥0) only if \[ \sum_{i} (B_{io} - B_{lo}) > 0 \], where \( i \) is the total number of TOLO oscillators. This condition must be manually enforced, since it **not** automatically enforced by the Genosc layer.

**TOLO Styles:**

<table>
<thead>
<tr>
<th>Style</th>
<th>Equation</th>
<th>Fit Parameters (n = osc#)</th>
</tr>
</thead>
<tbody>
<tr>
<td>TOLO.0 (eV)</td>
<td>( \varepsilon_{n_{TOLO}} = A_n \frac{E_{lon}^2 - E^2 - iB_{lon}E}{E_{lon}^2 - E^2 - iB_{lon}E} )</td>
<td>Ampn = An (dimensionless), Elon = E_{lon} (eV), Eto = E_{to} (eV), Blo = B_{lo} (eV)</td>
</tr>
<tr>
<td>TOLO.5 (cm&lt;sup&gt;-1&lt;/sup&gt;)</td>
<td></td>
<td>Ampn = An (dimensionless), Elon = E_{lon} (cm&lt;sup&gt;-1&lt;/sup&gt;), Eto = E_{to} (cm&lt;sup&gt;-1&lt;/sup&gt;)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Style</th>
<th>Equation</th>
<th>Fit Parameters (n = osc#)</th>
</tr>
</thead>
<tbody>
<tr>
<td>TOLO.1 (eV)</td>
<td>( \varepsilon_{n_{TOLO}} = A_n \frac{E_{lon}^2 - E^2 - iB_{lon}E}{B_{lon} E_{lon}^2 - E^2 - iB_{lon}E} )</td>
<td>Ampn = An (dimensionless), Elon = E_{lon} (eV), Eto = E_{to} (eV), Blo = B_{lo} (eV)</td>
</tr>
<tr>
<td>TOLO.6 (cm&lt;sup&gt;-1&lt;/sup&gt;)</td>
<td></td>
<td>Ampn = An (eV), Elon = E_{lon} (cm&lt;sup&gt;-1&lt;/sup&gt;), Eto = E_{to} (cm&lt;sup&gt;-1&lt;/sup&gt;)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Style</th>
<th>Equation</th>
<th>Fit Parameters (n = osc#)</th>
</tr>
</thead>
<tbody>
<tr>
<td>TOLO.2 (eV)</td>
<td>( \varepsilon_{n_{TOLO}} = A_n \frac{E_{lon}^2 - E^2 - iB_{lon}E}{B_{lon} E_{lon}^2 - E^2 - iB_{lon}E} )</td>
<td>Ampn = An (dimensionless), Elon = E_{lon} (eV), Eto = E_{to} (eV), Blo = B_{lo} (eV)</td>
</tr>
<tr>
<td>TOLO.7 (cm&lt;sup&gt;-1&lt;/sup&gt;)</td>
<td></td>
<td>Ampn = An (dimensionless), Elon = E_{lon} (cm&lt;sup&gt;-1&lt;/sup&gt;), Eto = E_{to} (cm&lt;sup&gt;-1&lt;/sup&gt;)</td>
</tr>
</tbody>
</table>

---

8) Drude, rho-tau Drude & N-mu Drude

The classic Drude oscillator describes free carrier effects on the dielectric response. Its form is a Lorentz oscillator with zero center energy (no restoring force). The $A_n$ parameter, as defined in the Drd.1 and Drd.6 styles, is related to the plasma energy $E_p$ (defined in many texts, including Wooten\textsuperscript{7}) via

$$A_n = \varepsilon_\infty E_p^2$$

(assuming $Br \ll An$). The quantity $\varepsilon_\infty$ describes the residual dielectric constant absorptions at energies greater than $E_p$. For the GenOsc layer, this residual term could include the $e1$ Offset as well as residue from other oscillator terms whose center energy is greater than $E_p$. The typical Drude dielectric function for a heavily doped Silicon sample is shown in Figure 8-22.

**Drude Styles:**

<table>
<thead>
<tr>
<th>Style</th>
<th>Equation</th>
<th>Fit Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Drd.0 (eV)</td>
<td>$\varepsilon_{n_Drd} = -\frac{A_n Br_n}{E^2 + iBr_n E}$</td>
<td>$Amp_n = A_n (eV), Bn = Br_n (eV)$</td>
</tr>
<tr>
<td>Drd.5 (cm$^{-1}$)</td>
<td></td>
<td>$Amp_n = A_n (cm^{-1}), Bn = Br_n (cm^{-1})$</td>
</tr>
<tr>
<td>Drd.1 (eV)</td>
<td>$\varepsilon_{n_Drd} = -\frac{A_n}{E^2 + iBr_n E}$</td>
<td>$Amp_n = A_n (eV^2), Bn = Br_n (eV)$</td>
</tr>
<tr>
<td>Drd.6 (cm$^{-1}$)</td>
<td></td>
<td>$Amp_n = A_n (cm^{-2}), Bn = Br_n (cm^{-1})$</td>
</tr>
</tbody>
</table>

A version of the Drude model with resistivity and mean scattering time as free parameters is described by the following\textsuperscript{viii}:

$$\varepsilon_{Drude}(E = \hbar\omega) = \varepsilon_0 \frac{-\hbar^2}{\rho (\tau \cdot E^2 + i\hbar E)}$$

where

$$\rho = \frac{m^*}{Nq^2\tau} = \frac{1}{q\mu N}$$

The adjustable Drude fit parameters are resistivity, $\rho$ (\(\Omega\)-cm) and scattering time, $\tau$ (sec). The related parameters of interest are $m^*$ (the carrier effective mass), $N$ (the carrier concentration in \(cm^{-3}\)), and $\mu$ (the carrier mobility in \(cm^2V^{-1}s^{-1}\)). The physical constants are $\hbar$ (\(\{\text{Plank's constant}\}/\pi\)), $\varepsilon_0$ (the vacuum dielectric constant), and the single electron charge $q$ (\(1.6x10^{-19}\) C).

Regardless of the chosen form, the Drude model always has only two adjustable fit parameters—the pair $A_n$ and $B_r$, is one example, another is $\rho$ and $\tau$. From the above equations, we can see that there are three related parameters—$m^*$ (the carrier effective mass), $N$ (the carrier concentration in \(cm^{-3}\)), and $\mu$ (the carrier mobility in \(cm^2V^{-1}s^{-1}\)). Provided we know one of those three, we can calculate the other two from the adjustable fit parameters. For instance, if we know effective mass, we can determine $N$ and $\mu$ from $\rho$ and $\tau$.

As shown in the following figure, when you select the Rho-tau Drude or N-mu Drude function, you will present with 5 oscillator parameter boxes labeled rho ($\rho$, \(\Omega\)-cm), tau ($\tau$, \(10^{15}\) sec), $m^*$ (\(m^*\times9.11\times10^{-31}\) kg), $N$ (\(cm^{-3}\)) and $\mu$ (\(\mu\cdot cm^2V^{-1}s^{-1}\)). However, only two quantities will be adjustable fit parameters—rho and tau for the rho-tau Drude term, and $N$ and $\mu$ for the N-mu Drude term. One can also adjust (but not fit) the effective mass, $m^*$.

Figure 8-21. Parameters Section for rho-tau Drude and N-tau Drude models showing adjustable fitting parameters, calculated parameters, and $m^*$ (adjustable non-fitting parameter).
**rho-tau Drude & N-mu Drude Styles:**

<table>
<thead>
<tr>
<th>Style</th>
<th>Equation</th>
<th>Fit Parameters (n = osc#)</th>
<th>Calculated Parameters*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rho-tau.0</td>
<td>$\varepsilon_{\text{r},0\text{Drude}} = \frac{-h^2}{\varepsilon_0 \rho_n (\tau_n \cdot E^2 + i\hbar E)}$</td>
<td>$\rho_n = \rho_n (\Omega \cdot \text{cm})$, $\tau_n = \tau_n (10^{15} \text{ sec})$</td>
<td>$N (\text{cm}^{-3})$*</td>
</tr>
<tr>
<td></td>
<td>$\rho_n = \frac{m^*}{N_n q^2 \tau_n} = \frac{1}{q \mu_n N_n}$</td>
<td>$\rho_n = \log_{10}(\rho_n) (\Omega \cdot \text{cm})$, $\tau_n = \tau_n (10^{15} \text{ sec})$</td>
<td>$\mu (\text{cm}^2 \text{V}^{-1} \text{sec})^*$</td>
</tr>
<tr>
<td>Rho-tau.5</td>
<td>$\varepsilon_{\text{r},5\text{Drude}} = \frac{-h^2}{\varepsilon_0 \rho_n (\tau_n \cdot E^2 + i\hbar E)}$</td>
<td>$\rho_n = \rho_n (\Omega \cdot \text{cm})$, $\tau_n = \tau_n (10^{15} \text{ sec})$</td>
<td>$N (\text{cm}^{-3})$*</td>
</tr>
<tr>
<td></td>
<td>$\rho_n = \frac{m^*}{N_n q^2 \tau_n} = \frac{1}{q \mu_n N_n}$</td>
<td>$\rho_n = \log_{10}(\rho_n) (\Omega \cdot \text{cm})$, $\tau_n = \tau_n (10^{15} \text{ sec})$</td>
<td>$\mu (\text{cm}^2 \text{V}^{-1} \text{sec})^*$</td>
</tr>
<tr>
<td>N-mu.0</td>
<td>$\varepsilon_{\text{n},0\text{Drude}} = \frac{-h^2}{\varepsilon_0 \rho_n (\tau_n \cdot E^2 + i\hbar E)}$</td>
<td>$\rho_n = \rho_n (\Omega \cdot \text{cm})$, $\tau_n = \tau_n (10^{15} \text{ sec})$</td>
<td>$N (\text{cm}^{-3})$*</td>
</tr>
<tr>
<td></td>
<td>$\rho_n = \frac{m^*}{N_n q^2 \tau_n} = \frac{1}{q \mu_n N_n}$</td>
<td>$\rho_n = \log_{10}(\rho_n) (\Omega \cdot \text{cm})$, $\tau_n = \tau_n (10^{15} \text{ sec})$</td>
<td>$\mu (\text{cm}^2 \text{V}^{-1} \text{sec})^*$</td>
</tr>
<tr>
<td>N-mu.5</td>
<td>$\varepsilon_{\text{n},5\text{Drude}} = \frac{-h^2}{\varepsilon_0 \rho_n (\tau_n \cdot E^2 + i\hbar E)}$</td>
<td>$\rho_n = \rho_n (\Omega \cdot \text{cm})$, $\tau_n = \tau_n (10^{15} \text{ sec})$</td>
<td>$N (\text{cm}^{-3})$*</td>
</tr>
<tr>
<td></td>
<td>$\rho_n = \frac{m^*}{N_n q^2 \tau_n} = \frac{1}{q \mu_n N_n}$</td>
<td>$\rho_n = \log_{10}(\rho_n) (\Omega \cdot \text{cm})$, $\tau_n = \tau_n (10^{15} \text{ sec})$</td>
<td>$\mu (\text{cm}^2 \text{V}^{-1} \text{sec})^*$</td>
</tr>
</tbody>
</table>

*In order for these to be calculated correctly, \( m^* \), the effective mass, must be entered.

**Figure 8.22.** \( \varepsilon_1 \) and \( \varepsilon_2 \) for a Drude oscillator + \( \varepsilon_\infty \) (Style .1). \( A_n = 0.20385 \text{ eV}^2 \), \( B_n = 0.08227 \text{ eV} \). These parameters are equivalent to a rho-tau Drude with \( \rho = 0.003 \Omega \cdot \text{cm} \), \( \tau = 8 \times 10^{15} \text{ sec} \).
9) Tauc-Lorentz & Egap Tauc-Lorentz

The Tauc-Lorentz oscillator was developed by Jellison and Modine\textsuperscript{ix}. It models the dielectric function of many amorphous materials particularly well. Close to the band edge, the absorption of the Tauc-Lorentz model follows a Tauc law formula, \( \varepsilon_2(E) \propto (E - E_g)^2/E^2 \). Multiple Tauc-Lorentz oscillators can be tied to a common bandgap energy (\( E_g \)) by specifying them as Egap Tauc-Lorentz oscillators. For these oscillators, the common \( E_g \) is entered in the up left corner of the GenOsc dialog box (below the \( e1 \) Offset term).

**Tauc-Lorentz & Egap Tauc-Lorentz Styles:**

<table>
<thead>
<tr>
<th>Style</th>
<th>Equation</th>
<th>Fit Parameters (n = osc#)</th>
</tr>
</thead>
<tbody>
<tr>
<td>T-L.0 (eV)</td>
<td>( \varepsilon_{n,T-L} = \varepsilon_{n1} + i\varepsilon_{n2} ), where</td>
<td>( An_n = A_n (eV), )</td>
</tr>
<tr>
<td>EgT-L.0 (eV)</td>
<td>( \varepsilon_{n2} = \left[ \frac{A_n E_{0n} C_n (E - E_{g n})^2}{E^2 - E_{0n}^2 + C_n^2 E^2} \right] ) ( E &gt; E_{g n} )</td>
<td>( En_n = E_{0n} (eV), )</td>
</tr>
<tr>
<td></td>
<td>( \varepsilon_{n2} = 0 ) ( E \leq E_{g n} )</td>
<td>( Cn_n = C_n (eV), )</td>
</tr>
<tr>
<td></td>
<td>( A_n = A_n (eV), ) ( En_n = E_{0n} (eV), ) ( Cn_n = C_n (eV) )</td>
<td>( Egap ) ( = E_{g n} (eV) )</td>
</tr>
</tbody>
</table>

\[ [a] \text{WVASE}\textsuperscript{®} uses the complete analytical solution to the Kramers-Kronig integral as presented in Jellison & Modine\textsuperscript{ix} (especially see the Erratum). \]

\[ [b] \text{In order to maintain } \varepsilon_2 \geq 0, \text{WVASE}\textsuperscript{®} internally constrains } E_{g_n} \text{ and } C \text{ such that } E_{g_n} < E_0, \text{ and } C < 2E_{0n}. \text{ However these values are not limited externally} \text{ – i.e., the user can enter any value. Thus, a range of external } E_{g_n} \text{ and } C \text{ values will produce the same dielectric function.} \]

Figure 8-23 shows an example of a Tauc-Lorentz dielectric function with parameter values that might be typical for amorphous silicon material.

![Figure 8-23. \( \varepsilon_1 \) and \( \varepsilon_2 \) for Tauc-Lorentz oscillator. The oscillator parameters are. \( \varepsilon_{\infty} = 1.0, \) \( An = 125, En = 3.5 \text{ eV, and } Bn = 2.5 \text{ eV, and } Eg = 1.1 \text{ eV.} \)](image)

10) Cody-Lorentz

The Cody-Lorentz oscillator, which was developed by Ferlauto, et al., is also designed for amorphous materials. It is similar to the Tauc-Lorentz in that it defines the bandgap energy, $E_g$, and a Lorentzian absorption peak (parameters $Amp$, $E_n$, and $Br$). However, the two models behave quite differently in the absorption-onset region, at photon energies slightly greater than $E_g$. In that region, the Tauc-Lorentz model follows a Tauc law formula, $\varepsilon_2(E) \propto [(E - E_g)^2/E^2]$, while Cody-Lorentz model assumes that $\varepsilon_2(E) \propto (E - E_g)^2$. The model also includes an Urbach absorption term. The $\varepsilon_2$ portion of the Cody-Lorentz oscillator model is:

$$
\varepsilon_2(E) = \begin{cases} 
\frac{E_1}{E} \exp\left(\frac{(E - E_g - E_i)}{E_u}\right), & 0 < E \leq (E_g + E_i) \\
G(E)L(E) = \left(\frac{(E - E_g)^2}{E - E_g^2} + \frac{AE_2}{E^2 + \Gamma^2E^2}\right), & E > (E_g + E_i)
\end{cases}
$$

$$
E_i = (E_g + E_i)G(E_g + E_i)L(E_g + E_i)
$$

In the equation above, $(E_g + E_i)$ is the demarcation between the Urbach tail transitions and the band-to-band transitions.

Please note that Ferlauto defines $E_i$ as an absolute energy. In contrast, WVASE® defines $E_i$ as an offset from the bandgap energy. Thus,

$$
E_{i\text{Ferlauto}} = E_{i\text{Wollam}} + E_{i\text{Wollam}}.
$$

Unlike the Cauchy model, this Urbach absorption tail is fully Kramer-Kronig consistent – that is, the exponential Urbach absorption in $\varepsilon_2(E)$ has a Kramers-Kronig transformed counterpart in $\varepsilon_2(\lambda)$ function. The internal parameter $E_i$ guarantees that the $\varepsilon_2$ function transitions smoothly at the $(E_g + E_i)$ transition point. The quantity $E_i/E$ guarantees that the Urbach exponential function exactly matches $G(E)L(E)$ at $(E_g + E_i)$. The quantity $E_i$ defines the exponential rate of decay; specifically where the Urbach absorption equal $e^{-1}$ of its maximum value of $E_i/E$.

The $G(E)$ function defines the Cody absorption behavior, while the $L(E)$ is a Lorentz oscillator function. The parameter $E_p$ allows the user to define an energy, $E_g + E_p$, where the function transitions from a Cody absorption behavior $[\varepsilon_2(E) \propto (E - E_g)^2]$ to the Lorentzian absorption. Note that $G(E) \rightarrow (E - E_g)^2/E_p^2$ when $E \approx E_g$, and $G(E) \rightarrow 1$ when $E \gg E_p$.

The log($\varepsilon_2$) curves for Lorentz, Cody-Lorentz and Tauc-Lorentz models are plotted in the next figure. The plot delineates the Lorentz, Cody, Tauc and Urbach regions for the three models. The figure also illustrates the Lorentz-Cody transition (around $E_g + E_p$) and the Cody-Urbach transition (at $E_g + E_i$).

---

Figure 8-24. Log($\varepsilon_2$) comparison of the Cody-Lorentz and Tauc-Lorentz oscillators.

A linear plot of $\varepsilon_2$ for a Cody-Lorentz oscillator model is shown the figure below, with the energy parameters labeled.

Figure 8-25. Cody-Lorentz showing details of the Et and Urbach transition regions.
**Cody-Lorentz Styles:**

Equation:
\[ \varepsilon_{n\_C-L} = \varepsilon_{n1} + i\varepsilon_{n2}, \]
where
\[ \varepsilon_2(E) = \begin{cases} 
\frac{E_i}{E} \exp \left( \frac{(E - E_{en} - E_m)}{E_{en}} \right), & 0 < E \leq (E_{en} + E_m) \\
\frac{(E - E_{en})^2}{(E - E_{en})^2 + E_{pn}^2}, & E > (E_{en} + E_m) 
\end{cases} \]

\[ G(E)L(E) = \frac{A_n E_{pn} \Gamma_n E}{(E - E_{en})^2 + E_{pn}^2} \left( \frac{(E - E_{en})^2}{(E - E_{en})^2 + \Gamma_n^2 E^2} \right). \]

\[ E_1 = (E_{en} + E_m)G(E_{en} + E_m)L(E_{en} + E_m) \]

and
\[ \varepsilon_{n1} = \frac{2}{\pi} P \int_0^\infty \frac{\xi \varepsilon_{n2}(\xi)}{\xi^2 - E^2} d\xi \]
(This is an integral in two parts\(^*\). See Ferlauto et al\(^2\)).

<table>
<thead>
<tr>
<th>Style</th>
<th>Fit Parameters (n = osc#)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C-L.0 (eV)</td>
<td>( \text{Ampn} = A_n ) (eV), ( \text{Enn} = E_{en} ) (eV), ( \text{Brn} = \Gamma_n ) (eV), ( E_{gn} = E_{en} ) (eV), ( E_{pn} = E_{en} ) (eV), ( Em = E_{en} ) (eV), ( Eun = E_{en} ) (eV)</td>
</tr>
</tbody>
</table>

\(^*\) In WVASE\(^3\), this Kramers-Kronig integration is solved analytically (as in Ferlauto\(^2\)). The integral form is presented here for the sake of brevity.

![Graph of \( \varepsilon_1 \) and \( \varepsilon_2 \) for Cody-Lorentz oscillator model](image_url)

**Figure 8.26.** \( \varepsilon_1 \) and \( \varepsilon_2 \) for Cody-Lorentz oscillator. The oscillator parameters are, \( \varepsilon_n = 1.0, \ An = 80 \text{ eV}, \ En = 3.8 \text{ eV}, \) and \( Br = 2.2 \text{ eV, Eg} = 1.6 \text{ eV, Ep} = 1.2 \text{ eV, Et} = 0.045 \text{ eV, and} \ Eun = 1.8 \text{ eV.} \)
11) Gaussian

This Oscillator type produces a Gaussian line shape in \( \varepsilon_2 \) with a Kramers-Kronig consistent line shape for \( \varepsilon_1 \) (see footnotes xi, xii for details). Figure 8-27 compares the dielectric functions of the Gaussian and the Lorentzian. Note that \( \varepsilon_2 \) of the Gaussian oscillator rapidly approaches zero beyond the FWHM positions.

**Gaussian Styles:**

\[
\varepsilon_{n,\text{Gaussian}} = \varepsilon_{n1} + i \varepsilon_{n2}, \quad \text{where}
\]

\[
\varepsilon_{n2} = A' e^{-\left(\frac{E-E_n}{\sigma}\right)^2} - A' e^{-\left(\frac{E+E_n}{\sigma}\right)^2},
\]

\[
\varepsilon_{n1} = \frac{2}{\pi} \int_0^\infty \frac{\xi}{\xi^2 + E^2} d\xi
\]

\[
\sigma = \frac{Br_n}{2\sqrt{\ln(2)}}. \quad \text{The } 1/2\sqrt{\ln(2)} \text{ factor defines } Br_n = \text{FWHM.}
\]

<table>
<thead>
<tr>
<th>Style</th>
<th>( A' ) definition</th>
<th>Fit Parameters (n = osc#)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gau.0 (eV)</td>
<td>( A' = A_n )</td>
<td>Ampn = ( A_n ) (dimensionless), ( E_{n1} = E_n ) (eV), ( Br_n = Br_n ) (eV)</td>
</tr>
<tr>
<td>Gau.5 (cm(^{-1}))</td>
<td>( A' = \frac{A_n}{Br_n} )</td>
<td>Ampn = ( A_n ) (dimensionless), ( E_{n1} = E_n ) (cm(^{-1})), ( Br_1 = Br_n ) (cm(^{-1}))</td>
</tr>
<tr>
<td>Gau.1 (eV)</td>
<td>( A' = \frac{A_n}{Br_n} )</td>
<td>Ampn = ( A_n ) (eV), ( E_{n1} = E_n ) (eV), ( Br_n = Br_n ) (eV)</td>
</tr>
<tr>
<td>Gau.6 (cm(^{-1}))</td>
<td>( A' = \frac{A_n E_n}{Br_n} )</td>
<td>Ampn = ( A_n ) (cm(^{-1})), ( E_{n1} = E_n ) (cm(^{-1})), ( Br_n = Br_n ) (cm(^{-1}))</td>
</tr>
<tr>
<td>Gau.2 (eV)</td>
<td>( A' = \frac{A_n}{Br_n} )</td>
<td>Ampn = ( A_n ) (dimensionless), ( E_{n1} = E_n ) (eV), ( Br_n = Br_n ) (eV)</td>
</tr>
<tr>
<td>Gau.7 (cm(^{-1}))</td>
<td>( A' = \frac{A_n E_n}{Br_n} )</td>
<td>Ampn = ( A_n ) (dimensionless), ( E_{n1} = E_n ) (cm(^{-1})), ( Br_n = Br_n ) (cm(^{-1}))</td>
</tr>
</tbody>
</table>

Figure 8-27. \( \varepsilon_1 \) and \( \varepsilon_2 \) comparison of two Gaussian and one Lorentz oscillator (All oscillator functions are Style 1, \( A_{n1} = I, \ E_{n1} = 2.5 \text{ eV}, Br_n \)).

12) Gauss-Lorentz

The broadening of the Gauss-Lorentz oscillator type can be varied smoothly between the Gaussian ($\sigma$) and Lorentzian ($\Gamma$) types by adjusting the parameter $B_{mix}$. The Gauss-Lorentz Oscillator type is adapted from the semiconductor dielectric function model developed by Kim and Garland\textsuperscript{xiii}, and simply replaces the joint density of states function with a delta function. The resulting $n^{th}$ Gauss-Lorentz oscillator is

$$\varepsilon_n(E) = iA_n \left[ \int_0^{\infty} e^{i(E-E_n+i\gamma_n(s))s} ds - \int_0^{\infty} e^{i(E+E_n+i\gamma_n(s))s} ds \right] / \left[ \int_0^{\infty} e^{-\gamma_n(s)} ds \right],$$

where

$$\gamma_n(s) = \Gamma_n + 2\sigma_n s^2$$

This equation is fully Kramers-Kronig consistent. The denominator integral term normalizes the equation so that $\text{Im}(\varepsilon_n(E)) \sim A_n$ as $E \rightarrow E_n$. In order to allow the broadening to vary smoothly between Lorentzian and Gaussian, WVASE\textsuperscript{®} further defines the quantities $B_{r_n}$ and $B_{mix_n}$ via the equations

$$B_{r_n}^2 = B_{\text{Lorentz}_n}^2 + B_{\text{Gaussian}_n}^2$$

$$e^{B_{mix_n}} = \frac{B_{\text{Lorentz}_n}}{B_{\text{Gaussian}_n}}$$

$$\Gamma_n = \frac{1}{2} B_{\text{Lorentz}_n}$$

$$\sigma_n = \frac{1}{4\text{Im}(\pi)} B_{\text{Gaussian}_n}$$

The intermediate calculation parameters $\Gamma_n$ and $\sigma_n$ define how much each broadening type contributes to the total broadening. By parameterizing the function in this way, the shape parameter $B_{mix_n}$ is mostly orthogonal to $A_n$, $B_{r_n}$, and $E_n$; which means that $B_{mix_n}$ can readily change without dramatically altering the peak, width, or area of the oscillator.

The broadening becomes more Gaussian as $B_{mix_n}$ becomes more negative; and it becomes more Lorentzian as $B_{mix_n}$ becomes more positive. This is shown in Figure 8-28. The function is written so that the broadening ($B_{r_n}$) is a Full-Width-Half-Maximum (FWHM) value at both the Gaussian limit ($\Gamma \rightarrow 0$, or $B_{mix} \rightarrow -10$), and Lorentzian limit ($\sigma \rightarrow 0$, or $B_{mix} \rightarrow 10$). At intermediate values of $B_{mix}$, $B_{r_n}$ is slightly larger than FWHM, as can be seen in Figure 8-28. In addition to the fit parameters $A_n$, $E_n$, $B_{r_n}$ and $B_{mix_n}$, the Gauss-Lorentz Oscillator also displays $B_{\text{Lorentz}}$ ($\Gamma_n$) and $B_{\text{Gaussian}}$ ($\sigma_n$), which are calculated from the equations above.

**Gauss-Lorentz Styles:**

\[ \varepsilon_n(E) = i\Phi_n \left[ \int_0^\infty e^{i(E-E_n+i\gamma_n s)} ds \right] \left[ \prod_{i} e^{i(E+E_i^0+i\gamma_i s)} ds \right] \left[ \int_0^\infty e^{-\gamma_n s} ds \right], \]

where \( \gamma_n(s) = \Gamma_n + 2\sigma_n^2 s \).

WVASE® also performs these intermediate calculations:

\[ B_{r\text{,}n}^2 = B_{\text{Lorentz,}n}^2 + B_{\text{Gaussian,}n}^2 \]

\[ \epsilon_{\text{mix,}n} = B_{\text{Lorentz,}n} / B_{\text{Gaussian,}n} \]

\[ \Gamma_n = \frac{1}{2} B_{\text{Lorentz,}n} \quad \text{and} \quad \sigma_n = \frac{1}{4\sqrt{\ln(4)}} B_{\text{Gaussian,}n} \]

<table>
<thead>
<tr>
<th>Style</th>
<th>Fit Parameters (n = osc#)</th>
<th>Calculated Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>G-L.0 (eV)</td>
<td>( \Phi_n = A_n ) ( A_n ) (dimensionless), ( E_n ) (eV), ( B_{\text{mix,}n} ) (dimensionless)</td>
<td>( B_{\text{Lorentz,}n} ) (eV), ( B_{\text{Gaussian,}n} ) (eV)</td>
</tr>
<tr>
<td>G-L.5 (cm(^{-1}))</td>
<td>( \Phi_n = A_n ) ( A_n ) (dimensionless), ( E_n ) (eV), ( B_{\text{mix,}n} ) (dimensionless)</td>
<td>( B_{\text{Lorentz,}n} ) (cm(^{-1})), ( B_{\text{Gaussian,}n} ) (cm(^{-1}))</td>
</tr>
<tr>
<td>G-L.1 (eV)</td>
<td>( \Phi_n = A_n ) ( A_n ) (dimensionless), ( E_n ) (eV), ( B_{\text{mix,}n} ) (dimensionless)</td>
<td>( B_{\text{Lorentz,}n} ) (eV), ( B_{\text{Gaussian,}n} ) (eV)</td>
</tr>
<tr>
<td>G-L.6 (cm(^{-1}))</td>
<td>( \Phi_n = A_n ) ( A_n ) (cm(^{-1})), ( E_n ) (cm(^{-1})), ( B_{\text{mix,}n} ) (dimensionless)</td>
<td>( B_{\text{Lorentz,}n} ) (cm(^{-1})), ( B_{\text{Gaussian,}n} ) (cm(^{-1}))</td>
</tr>
<tr>
<td>G-L.2 (eV)</td>
<td>( \Phi_n = A_n ) ( A_n ) (dimensionless), ( E_n = E_n ) (eV), ( B_{\text{mix,}n} ) (dimensionless)</td>
<td>( B_{\text{Lorentz,}n} ) (eV), ( B_{\text{Gaussian,}n} ) (eV)</td>
</tr>
<tr>
<td>G-L.7 (cm(^{-1}))</td>
<td>( \Phi_n = A_n ) ( A_n ) (cm(^{-1})), ( E_n = E_n ) (cm(^{-1})), ( B_{\text{mix,}n} ) (dimensionless)</td>
<td>( B_{\text{Lorentz,}n} ) (cm(^{-1})), ( B_{\text{Gaussian,}n} ) (cm(^{-1}))</td>
</tr>
</tbody>
</table>

*Note:* This table provides the fit parameters and calculated parameters for various Gauss-Lorentz oscillator styles. The styles include Gaussian (G), Lorentzian (L), and mixed Gauss-Lorentz (Bmix) oscillators. The table lists the general forms for the oscillator parameters and the corresponding calculated parameters for the fit. The styles are labeled with G-L.x for different values of x, indicating the specific form or parameterization.
13) GLAD

The GLAD (Gauss-Lorentz Asymmetric Doublet) oscillator is designed to fit absorbing spectral regions that have a shoulder. It consists of two Gauss-Lorentz oscillators (described in previous section) that are tied to the center energy (Eng). The broadening of the GLAD oscillator can be varied smoothly between the Gaussian and Lorentzian types by adjusting the parameter Bmix, (see previous section).

The formal definitions of the various parameters are listed in the next table. Note that the broadenings, amplitudes and center energies of the two absorption peaks are all functions of the Split parameter.

GLAD Styles part 1:

The Glad oscillator term has two absorption peaks, with center energies, amplitudes, and broadenings are defined below as follows:

Defining
Left: Lower energy peak (left on photon energy scale)
Right: Higher energy peak (right on photon energy scale)

\[
E_{\text{left}} = E_n - \frac{1}{2} \cdot \text{Split} \cdot B_{n}
\]
\[
E_{\text{right}} = E_n + \frac{1}{2} \cdot \text{Split} \cdot B_{n}
\]
\[
A_{\text{left}} = \frac{1}{2} A_n \left(1 - \text{Asym}_n \right) \left(1 + \text{Split}_n^2 \ln(2) \right)
\]
\[
A_{\text{right}} = \frac{1}{2} A_n \left(1 + \text{Asym}_n \right) \left(1 + \text{Split}_n^2 \ln(2) \right)
\]
\[
B_{\text{left:right}} = \frac{B_{n}}{1 + \text{Split}_n^2 \ln(2)}
\]

The two peaks are Gauss-Lorentz oscillators as defined in the previous section. Φ is defined in the table below.

The offset between the center energies of the two oscillators is defined as the product of the Split and the Broadening (Split x Br) as shown in the next figure.

![Image of GLAD Oscillator](image)

Figure 8.29. ε2 of a GLAD oscillator with \(A_n = 1, E_n = 3 \text{ eV}, B_{n} = 1 \text{ eV}, B_{\text{mix}} = 10, \text{Asym}_n = 0.1, \text{and Split}_n = 0.7.

\[x\]

Note that the broadenings and amplitudes of the two absorption peaks are functions of \(1 + \text{Split}^2 \ln(2)\). This keeps the overall full-width half-max (FWHM) nearly constant for the two-oscillator combination as the oscillators separate in energy, and helps to decorrelate the \(B_r\) from the \(\text{Split}\) terms. For small \(\text{Split}\) values, this primarily affects only the shape near the oscillator peak. As \(\text{Split}\) increase in value, the top becomes flatter, but the position and amplitude of FWHM remain nearly constant, until \(\text{Split}\) exceeds 0.5. This is shown in the following figure.

![Graph showing the change in FWHM for different values of \(\text{Split}\).](image)

**Figure 8-30. Comparison of \(\Phi\) for several GLAD oscillators.** \((A_n = 1, E_n = 3\ eV, Br_n = 1\ eV, B_{mix} = 10, Asym_n = 0, \text{ and Split}_n \) is as indicated in Legend).**

### GLAD Styles part 2 (\(\Phi\) defined in previous table):

<table>
<thead>
<tr>
<th>Style</th>
<th>(\Phi)</th>
<th>Fit Parameters &amp; Dimensions ((n = \text{osc#}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>GLAD.0</td>
<td>(\Phi = A_n)</td>
<td>(A_n = \text{Amp}<em>n) ((\text{dimensionless})), (E_n = E</em>{\text{Inn}}) ((\text{eV})), (B_r = Br_n) ((\text{eV})), (\text{Split}_n = \text{Split}_n), (\text{Asym}<em>n = \text{Asym}<em>n), (B</em>{mix} = B</em>{mixn}) ((\text{Split}_n, \text{Asym}<em>n, \text{ &amp; } B</em>{mixn} \text{ all dimensionless}))</td>
</tr>
<tr>
<td>GLAD.5</td>
<td>(\Phi = A_n/B_{ram})</td>
<td>(A_n = \text{Amp}<em>n) ((\text{cm}^{-1})), (E_n = E</em>{\text{Inn}}) ((\text{eV})), (Br_n = Br_{ram}) ((\text{cm}^{-1})), (\text{Split}_n = \text{Split}_n), (\text{Asym}<em>n = \text{Asym}<em>n), (B</em>{mix} = B</em>{mixn}) ((\text{Split}_n, \text{Asym}<em>n, \text{ &amp; } B</em>{mixn} \text{ all dimensionless}))</td>
</tr>
<tr>
<td>GLAD.6</td>
<td>(\Phi = A_n E_n/B_{ram})</td>
<td>(A_n = \text{Amp}<em>n) ((\text{cm}^{-1})), (E_n = E</em>{\text{Inn}}) ((\text{eV})), (Br_n = Br_{ram}) ((\text{cm}^{-1})), (\text{Split}_n = \text{Split}_n), (\text{Asym}<em>n = \text{Asym}<em>n), (B</em>{mix} = B</em>{mixn}) ((\text{Split}_n, \text{Asym}<em>n, \text{ &amp; } B</em>{mixn} \text{ all dimensionless}))</td>
</tr>
<tr>
<td>GLAD.7</td>
<td>(\Phi = A_n E_n/B_{ram})</td>
<td>(A_n = \text{Amp}<em>n) ((\text{cm}^{-1})), (E_n = E</em>{\text{Inn}}) ((\text{eV})), (Br_n = Br_{ram}) ((\text{cm}^{-1})), (\text{Split}_n = \text{Split}_n), (\text{Asym}<em>n = \text{Asym}<em>n), (B</em>{mix} = B</em>{mixn}) ((\text{Split}_n, \text{Asym}<em>n, \text{ &amp; } B</em>{mixn} \text{ all dimensionless}))</td>
</tr>
</tbody>
</table>
14) Psemi-(M0, M1, M2, M3 & Tri)

**Oscillators based on the Herzinger-Johs Psemi function**

For WVASE® versions ≥ 3.500, the genosc.mat layer contains five new Psemi oscillator types – Psemi-M0, Psemi-M1, Psemi-M2, Psemi-M3 and Psemi-Tri. All five are variations of the more general Herzinger-Johs Parameterized Semiconductor Oscillator function originally introduced in the WVASE® psemi.mat layer\(^{\text{v}}\). The Psemi oscillators combine a highly flexible functional shape with Kramers-Kronig consistent properties.

The primary purpose of the Psemi oscillators is to accurately reproduce the dielectric function of materials – especially semiconductors with complicated critical point structures in a Kramers-Kronig consistent manner. The Psemi oscillator’s primary contribution to the understanding of a material’s physical properties is the optical constants it generates, not the internal parameters that define the oscillator. The Psemi parameter values have no direct physical relationship to critical point parameters, such as energy and broadening, that one might obtain from a derivative or other type of analysis.

The Psemi-M0, M1, M2, and M3 are each shaped to approximate their respective \(\varepsilon_2\) critical point structures. The fifth oscillator, Psemi-Tri, is intended for general use. They are primarily intended to fit the dielectric functions of semiconductor and other crystalline materials. However, their flexibility means that almost any dielectric function can be modeled with one or more Psemi oscillators.

Each Psemi oscillator consists of four polynomials spline functions (labeled \(F_I, F_{II}, F_{III}\) & \(F_{IV}\) in Figure 8-31 left) connected end-to-end. These four functions are constrained such that each one connects smoothly with the adjacent function. Also, \(F_I\) and \(F_{III}\) are forced to be equal zero at the endpoints. The polynomials change shape such that the overall Psemi shape is smooth and continuous through the control points (midpoint). The overall Psemi function shape can be altered by changing the control points, endpoints, center energy and amplitude. Thus the mid-points act as control points for the overall shape. Figure 8-31 right illustrates the flexibility of these functions, showing how various combinations of left and right control point amplitudes can produce different asymmetrical \(\varepsilon_2\) curves in the Psemi-Tri oscillator. When using the default parameter values, the Psemi-Tri oscillator has a triangular shape, with the corners rounded off by the broadening parameter (see Figure 8-37).

---

\(^{\text{v}}\) The psemi.mat layer is described in detail in section 13.12 “The parametric semiconductor model,” on page 13-73.
Note that width of these oscillators is controlled by the placement of the endpoints, not the broadening parameter, B. Broadening mostly affects the region near the endpoints (and to some extent, the center energy peak region) of the $P_{semi}$.

The Genosc $P_{semi}$ oscillators allow the user to vary and fit 7 out of the 12 free parameters contained in the more general Herzinger-Johs function. The 5 other variables are fixed to pre-defined values, which gives each oscillator type its distinctive shape, as shown in Figure 8-32. $P_{semi}$ Oscillator shapes can be altered graphically by manipulating the blue boxes with the mouse, or by entering the values of the seven free variables. The five $P_{semi}$ oscillator functions in the Genosc layer are all based on the Herzinger-Johs function. The $P_{semi}$-M0, -M1, -M2, and -M3 approximate their respective $\varepsilon_2$ critical point structures. The fifth oscillator, $P_{semi}$-Tri, is a flexible function intended for general use.

![Graphs of $P_{semi}$-M0, $P_{semi}$-M1, $P_{semi}$-M2, and $P_{semi}$-M3](image)

*Figure 8-32. Genosc dielectric function display and plot of $\varepsilon_1$ and $\varepsilon_2$, showing the $P_{semi}$-M0, $P_{semi}$-M1, $P_{semi}$-M2, and $P_{semi}$-M3. All functions are using default parameter values. The $P_{semi}$-Tri oscillator is shown in Figure 8-31.*

The Genosc $P_{semi}$ oscillators allow the user to vary and fit 7 out of the 12 free parameters contained in the general Herzinger-Johs function. The 5 other variables are fixed to pre-defined values, which gives each oscillator type its distinctive shape, as shown in Figure 8-32. $P_{semi}$ Oscillator shapes can be altered graphically by manipulating the blue boxes with the mouse, or by entering the values of the seven free variables.
The function parameters are defined as follows:

- **A, E & B**: Amplitude, Center-Energy & Broadening.
- **WL & WR**: Endpoint positions relative to the center energy (E). They set the width of the oscillator on the left and right sides.
- **PL & PR**: Horizontal position of the left and right control points relative to the center energy and the endpoints. \(0 \leq PL(PR) \leq 1\), \((0 = \text{end point position})\).
- **AL & AR**: Relative magnitude of the left and right control points (compared to the Amplitude, A). \(0 \leq AL(AR) \leq 1\), \((1 = A)\).
- **O2L & O2R**: Coefficients for the 2nd order terms in the polynomials on the left and right sides of the Psemi-M0 and Psemi-M3 oscillators. Add additional flexibility to function. \(0 \leq O2L(O2R) \leq 1\).

In the following Table, check marks indicate which of the 12 parameters can be varied and fit for each of oscillator type. Also listed are pre-defined values of the fixed parameters. The discontinuity parameter (Disc) is always set to zero in the Genosc Psemi oscillators.

### Variable and fixed Parameter values for Psemi oscillator functions

(variable parameters marked with “✓”. Pre-set values of fixed variables are listed).

<table>
<thead>
<tr>
<th>psemi.mat parameters</th>
<th>Energy</th>
<th>Amp</th>
<th>Br</th>
<th>Left/Right boundaries set by E of connecting oscillators</th>
<th>Left Mid Pos</th>
<th>Mid Amp</th>
<th>Right Mid Pos</th>
<th>Mid Amp</th>
<th>Left 2nd Order</th>
<th>Right 2nd Order</th>
<th>Discontinuity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Equivalent Genosc.mat parameters</td>
<td>E</td>
<td>A</td>
<td>B</td>
<td>WL**</td>
<td>WR*</td>
<td>PL</td>
<td>AL</td>
<td>PR</td>
<td>AR</td>
<td>O2L</td>
<td>O2R</td>
</tr>
<tr>
<td>PSEMI-M0</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>0</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>0</td>
<td>✓</td>
</tr>
<tr>
<td>PSEMI-M1</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
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<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>0.75</td>
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</tr>
<tr>
<td>PSEMI-M2</td>
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<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>0.5</td>
<td>✓</td>
</tr>
<tr>
<td>PSEMI-M3</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>0</td>
<td>✓</td>
</tr>
<tr>
<td>PSEMI-TRI</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>0.5</td>
<td>✓</td>
</tr>
</tbody>
</table>

* WL: Width Left, WR: Width Right (units in eV). These values are relative to the center energy, E.

The next table lists describes the various parameters and their dimensions. Please note that only one style, .0 (eV), is available for these oscillators.
### Parameter descriptions for Psemi-M0, M1, M2, M3 & Tri

[0 (eV) only Style available]:

<table>
<thead>
<tr>
<th>Fit Parameter</th>
<th>Description</th>
<th>Dimensions (n = osc#)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_n$</td>
<td>Amplitude at oscillator center energy</td>
<td>$A_n = An$ (dimensionless)</td>
</tr>
</tbody>
</table>
| $E_{\ldots n}$ | Oscillator center energy: Labeled 
$E_{0n}$ for Psemi-E0 
$E_{1n}$ for Psemi-E1 
$E_{2n}$ for Psemi-E2 
$E_{3n}$ for Psemi-E3 
$E_{cn}$ for Psemi-Tri | $E_{0n} = E0n$ (eV) 
$E_{1n} = E1n$ (eV) 
$E_{2n} = E2n$ (eV) 
$E_{3n} = E3n$ (eV) 
$E_{cn} = Ec_n$ (eV) |
| $B_n$         | Broadening (Gaussian type) | $B_n = Bn$ (eV) |
| $WL_n$        | Width of left side absorption region 
($E_{\ldots n}$ minus lower cut-off energy) | $WL_n = WL_n$ (eV) |
| $WR_n$        | Width of Right side absorption region 
($E_{\ldots n}$ minus lower cut-off energy) | $WR_n = WR_n$ (eV) |
| $PL_n$        | Control point position for left side. 
$PL_n$ is a fraction of $WL_n$, measured from left endpoint ($E – WL_n$) | $PL_n = PL_n$ (dimensionless) |
| $PR_n$        | Control point position for right side. 
$PR_n$ is a fraction of $WR_n$, measured from right endpoint ($E + WR_n$) | $PR_n = PR_n$ (dimensionless) |
| $AL_n$        | Control point amplitude for left side 
(as a fraction of $A_n$) | $AL_n = AL_n$ (dimensionless) |
| $AR_n$        | Control point amplitude for right side 
(as a fraction of $A_n$) | $AR_n = AR_n$ (dimensionless) |
| $O2L_n$       | Second order polynomial factor for left-side polynomials $F_1$ & $F_H$. | $O2L_n = O2Ln$ (dimensionless) |
| $O2R_n$       | Second order polynomial factor for right-side polynomials $F_{III}$ & $F_{IV}$. | $O2R_n = O2Rn$ (dimensionless) |

Additional details regarding each of the 5 Psemi oscillators are discussed in the following sections.
**Psemi-M0 (PSM0)**

The **Psemi-M0 (PSM0)** models the shape of an M₀ critical point seen in direct gap semiconductors such as GaAs and InP, especially at the bandgap energy. Variable fit parameters are: $E₁$, $A$, $B$, $WR$, $WL$, $AL$, and $AR$. Fixed parameters (and their values) are: $WL=0$, $PL=AL=0.5$, and $O₂L=0$. Figure 8-33 shows the effects on the $\varepsilon₂$ line-shape for several different combinations of $AR$ and $PR$ values.

![Figure 8-33. $\varepsilon₂$ plot showing the effects on the line-shape of the Psemi-M0 oscillator for different AR and PR values.](image)

**Psemi-M1 (PSM1)**

The **Psemi-M1 (PSM1)** models the shape of an M₁ critical point. Variable fit parameters are: $E₁$, $A$, $B$, $WL$, $WR$, $AL$, and $AR$. Fixed parameters (and their values) are: $PL=0.75$, $PR=0.5$, $O₂L=1$, and $O₂R=0$.

![Figure 8-34. $\varepsilon₂$ plot showing the default line-shape of the Psemi-M1 oscillator.](image)

**Psemi-M2 (PSM2)**

The **Psemi-M2 (PSM2)** models the shape of an M₂ critical point. Variable fit parameters are: $E₂$, $A$, $B$, $WL$, $WR$, $AL$, and $AR$. Fixed parameters (and their values) are: $PL=0.5$, $PR=0.75$, $O₂L=0$, and $O₂R=1$. 
Figure 8-35. $\varepsilon_2$ plot showing the default line-shape of the Psemi-M2 oscillator.

**Psemi-M3 (PSM3)**

The Psemi-M3 (PSM3) model models the shape of an M3 critical point. Variable fit parameters are: $E_3$, $A$, $B$, $WL$, $PR$, $AR$, and $O2L$. Fixed parameters (and their values) are: $WR=0$, $PR=AR=0.5$, and $O2R=0$. Figure 8-36 shows the effects on the $\varepsilon_2$ line-shape for several different combinations of AL and PL values.

Figure 8-36. $\varepsilon_2$ plot showing the effects on the line-shape of the Psemi-E3 oscillator, for different AR and PR values.

**Psemi-Tri (PSTRI)**

The Psemi-Tri (PSTRI) is a general-use Psemi model. Variable fit parameters are: $Ec$, $A$, $B$, $WL$, $AR$, and $AL$. Fixed parameters (and their values) are: $PL=PR=0.5$, and $O2L=O2R=0$. Figure 8-37 shows the default line-shape for the Psemi-Tri model. Figure 8-31 shows the effects on the $\varepsilon_2$ line-shape for several different combinations of AL and PL values.
Examples of Psemi oscillator fits

Figure 8-37 shows the Genosc Oscillator list and Dielectric Function Display for a fit to InP.mat from the WVASE\textsuperscript{®} semiconductor material file library. The fit uses an ensemble of six Psemi oscillators to model the dielectric function of InP. One can see that all critical points in the spectra can be described accurately with these advanced oscillators. A hallmark of Psemi oscillator models is that each oscillator usually overlaps adjacent oscillators—in fact, the end point energies usually approximate the center energies of adjacent oscillators.

![Diagram showing dielectric function displays for InP fitting with Psemi oscillators](image)

Unlike a tabulated optical constants list file (such as InP.mat), a Psemi oscillator model can be altered to account for microstructural effects of strain, damage, defects or alloying. It also can be readily merged with mid-IR effects such as Drude or phonon absorption.

Two Psemi oscillators were used to fit the GaN dielectric function shown in Figure 8-39. Note how efficiently the Psemi-M0 oscillator fits the direct bandgap region. The direct bandgap shape would be difficult to do with other oscillator types. Other oscillator types could be used in place of the Psemi-M2 oscillator to describe the increasing $\varepsilon_2$ absorption at higher energy.
Because each \( P_{semi} \) oscillator is defined by seven free parameters, correlation can be a problem. Users can minimize correlation by restricting the number of fit parameters, and using no more than the minimum number of oscillators required for a good fit. Whenever possible, simpler oscillators – such as the Gaussian, which has only three free parameters – should also be used.

### 15) CPPB

The CPPB (Critical Point Parabolic Band) oscillator was developed by Aspnes\footnote{As described in D. E. Aspnes, “Modulation Spectroscopy/Electric Field Effects on the Dielectric Function of Semiconductors,” from Handbook on Semiconductors, Vol. 2, edited by M. Balkanski (North Holland, 1980), pp. 125 – 127.} to model the shape of the dielectric functions at semiconductor critical points (CP’s). The shape of each CPPB oscillator depends on five parameters: the amplitude \( A_n \), phase projection factor \( \theta_n \), threshold energy \( E_{gn} \), broadening parameter \( \Gamma_n \), and exponent \( \mu \). The exponent \( \mu \) can have three values:

\[
\mu_n = \frac{1}{2} \text{ for 1-D CP’s,}
\]

\[
\mu_n = “0” \text{ (becomes } \ln(2E_{gn} - 2E - i\Gamma) \text{) for 2-D CP’s, and}
\]

\[
\mu_n = \frac{3}{2} \text{ for 3-D CP’s.}
\]
CPPB Styles:

\[ \epsilon_n = \Phi e^{i\theta_n} \left( \frac{\Gamma_n}{2E_{gn} - 2E - i\Gamma_n} \right)^{\mu_n}, \mu_n = \pm 1/2 \]

\[ \epsilon_n = \Phi e^{i\theta_n} \ln \left( 2E_{gn} - 2E - i\Gamma_n \right), \text{ for } \mu_n = 0 \]

where \( \Phi \) is defined below.

<table>
<thead>
<tr>
<th>Style</th>
<th>( \Phi )</th>
<th>Fit Parameters (n = osc#)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPPB.0 (eV)</td>
<td>( \Phi = A_n )</td>
<td>Ampn = ( A_n ) (dimensionless), ( En_n = E_{gn} ) (eV), ( Br_n = \Gamma_n ) (eV), ( \mu_n = \pm 1/2, 0, 1/2; \text{ Phasen} = \theta_n ) (dimensionless)</td>
</tr>
<tr>
<td>CPPB.5 (cm(^{-1}))</td>
<td>( \Phi = A_n / \Gamma_n )</td>
<td>Ampn = ( A_n ) (dimensionless), ( En_n = E_{gn} ) (eV), ( Br_n = \Gamma_n ) (eV), ( \mu_n = \pm 1/2, 0, 1/2; \text{ Phasen} = \theta_n ) (dimensionless)</td>
</tr>
<tr>
<td>CPPB.1 (eV)</td>
<td>( \Phi = A_n / \Gamma_n )</td>
<td>Ampn = ( A_n ) (eV), ( En_n = E_{gn} ) (eV), ( Br_n = \Gamma_n ) (eV), ( \mu_n = \pm 1/2, 0, 1/2; \text{ Phasen} = \theta_n ) (dimensionless)</td>
</tr>
<tr>
<td>CPPB.6 (cm(^{-1}))</td>
<td>( \Phi = A_n / \Gamma_n )</td>
<td>Ampn = ( A_n ) (eV), ( En_n = E_{gn} ) (cm(^{-1})), ( Br_n = \Gamma_n ) (cm(^{-1})), ( \mu_n = \pm 1/2, 0, 1/2; \text{ Phasen} = \theta_n ) (dimensionless)</td>
</tr>
<tr>
<td>CPPB.2 (eV)</td>
<td>( \Phi = A_n / \Gamma_n )</td>
<td>Ampn = ( A_n ) (dimensionless), ( En_n = E_{gn} ) (eV), ( Br_n = \Gamma_n ) (eV), ( \mu_n = \pm 1/2, 0, 1/2; \text{ Phasen} = \theta_n ) (dimensionless)</td>
</tr>
<tr>
<td>CPPB.7 (cm(^{-1}))</td>
<td>( \Phi = A_n / \Gamma_n )</td>
<td>Ampn = ( A_n ) (dimensionless), ( En_n = E_{gn} ) (cm(^{-1})), ( Br_n = \Gamma_n ) (cm(^{-1})), ( \mu_n = \pm 1/2, 0, 1/2; \text{ Phasen} = \theta_n ) (dimensionless)</td>
</tr>
</tbody>
</table>

16) CPM0, CPM1, CPM2 & CPM3

These four oscillators were developed by Adachi\(^{xvii}\) to describe the dielectric functions at semiconductor critical points (CP’s). See Schubert, et al\(^{xviii}\) for an example of the application of these oscillators.

See Also: S. Adachi, “Optical dispersion relations for GaP, GaAs, GaSb, InP, InAs, InSb, Al\(_x\)Ga\(_{1-x}\),As, and In\(_x\)Ga\(_{1-x}\)P\(_{1-y}\),” J. of Appl. Phys. 66, 6030 (1989).
CPM0, CPM1, CPM2 & CPM3 Styles:

Defining \[ \chi'_n = \frac{(E + i\Gamma_n)}{E_n} \]

\[ \varepsilon_{CPM0} = \frac{A_n}{E_n^{1.5} \chi'_n^2} \cdot \left[ 2 - \sqrt{1 + \chi'_n} - \sqrt{1 - \chi'_n} \right] \]

\[ \varepsilon_{CPM1} = \frac{-A_n}{\chi'_n^2} \cdot \ln[1 - \chi'_n^2] \]

Defining \[ \chi''_n = \frac{(E_n - E + i\Gamma_n)}{E_n} \]

\[ \varepsilon_{CPM2} = \frac{-A_n}{\chi''_n^2} \cdot \ln[1 - \chi''_n^2] \]

\[ \varepsilon_{CPM3} = \frac{A_n}{E_n^{1.5} \chi''_n^2} \cdot \left[ 2 - \sqrt{1 + \chi''_n} - \sqrt{1 - \chi''_n} \right] \]

<table>
<thead>
<tr>
<th>Style</th>
<th>Fit Parameters (n = osc#)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPM0.0 (eV)</td>
<td>Ampn = A_n (eV^{0.5} for CPM0 &amp; CPM3)</td>
</tr>
<tr>
<td>CPM1.0 (eV)</td>
<td>Ampn = A_n (dimensionless for CPM1 &amp; CPM2)</td>
</tr>
<tr>
<td>CPM2.0 (eV)</td>
<td>Enn = E_n (eV)</td>
</tr>
<tr>
<td>CPM3.0 (eV)</td>
<td>Brn = \Gamma_n (eV)</td>
</tr>
</tbody>
</table>

17) Tguy (Tanguy model)

This expression was developed by Tanguy\textsuperscript{ix,xx} to provide an analytical expression of Wannier excitons, including bound and unbound states. The function makes no distinction between bound and unbound states. As shown below, the function depends on five parameters: amplitude \( A_n \), energy of the fundamental bound state \( E_{g_n} \) (band-gap), the unscreened binding energy\textsuperscript{xx} \( R_m \), broadening \( \sigma_n \), and \( \ln g_n \) (= \( \ln(g) \)). The parameter \( g \) is a screening factor that can vary from 0 to \( \infty \), with \( g \to \infty \) (unscreened Coulomb potential) and \( g = 0 \) (total screening).

\[ \varepsilon_{\text{Tguy},n} = A_n \sqrt{\frac{R_n}{E + i \Gamma_n}} \left\{ \tilde{g} \left( \xi \left( E + i \Gamma_n \right) \right) + \tilde{g} \left( \xi \left( E - i \Gamma_n \right) \right) - 2 \tilde{g} \left( \xi(0) \right) \right\} \]

where

\[ \tilde{g}(\xi) = -2\psi \left( \frac{e^{\ln(\xi_n)}}{\xi} \right) - \frac{\xi}{\ln(\xi_n)} - 2\psi \left( 1 - \xi \right) - \frac{1}{\xi} \]

\[ \xi(z) = \frac{2}{\left( E e^{\ln(\xi_n)} - z \right)^{1/2} + \left( E e^{\ln(\xi_n)} - z + \frac{4}{e^{\ln(\xi_n)}} \right)^{1/2}} \text{, and} \]

\[ \psi(z) = \frac{d(\ln \Gamma(z))}{dz} \text{ (digamma function)} \]

<table>
<thead>
<tr>
<th>Style</th>
<th>Fit Parameters (n = osc#)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tguy.0 (eV)</td>
<td>[ A_{pn} = A_n \text{ (eV)} ] [ E_{gn} = E_{\gamma_n} \text{ (eV)} ] [ B_{mn} = B_n \text{ (eV)} ] [ R_n = R_n \text{ (eV)} ] [ \ln g_n = \ln(g_n) \text{ (dimensionless)} ]</td>
</tr>
</tbody>
</table>

18) Lorentz-PB & Lorentz-LB

These oscillators convolve narrowly broadened Lorentz oscillators with the parabolic and linear JDOS functions. They provide a fully-Kramers-Kronig consistent method of fitting band edges. The general expression for Lorentz-based Joint Density of States JDOS model is:

\[ \varepsilon_{\text{Lorentz-JDOS}} = \frac{1}{E_{\text{band-bottom}}} \int_{E_{\text{band-bottom}}}^{E_{\text{band-top}}} \frac{\text{JDOS}_n(E')}{(E')^2 - (E + i \gamma_n)^2} dE' \]

For the **Parabolic Band model (Lorentz-PB)**, the JDOS = \( \sqrt{E' - E_{\text{band-bottom}}} \)

and the **Lorentz-PB** equation is

\[ \varepsilon_{\text{Lorentz-PB_n}} = \frac{1}{E_{\text{band-bottom}}} \int_{E_{\text{band-bottom}}}^{E_{\text{band-top}}} \sqrt{E' - E_{\text{band-bottom}}} \frac{dE'}{(E')^2 - (E + i \gamma_n)^2} \]

Similarly, for the **Linear Band model (Lorentz-LB)**, the JDOS = \( E' - E_{\text{band-bottom}} \)

and the **Lorentz-LB** equation becomes

\[ \varepsilon_{\text{Lorentz-LB_n}} = \frac{1}{E_{\text{band-bottom}}} \int_{E_{\text{band-bottom}}}^{E_{\text{band-top}}} \frac{E' - E_{\text{band-bottom}}}{(E')^2 - (E + i \gamma_n)^2} dE' \]
The table below shows the equations that result from these integrations.

### Lorentz-PB & Lorentz-LB Styles:

\[
E_{Lorentz\_PB\_n} = \frac{1.5A_n}{(E_{top\_n} - E_{bottom\_n})^2} \times f_{0PB}\left(\frac{E_{bottom\_n}}{E + i\gamma_n} + 1, \frac{E_{bottom\_n}}{E + i\gamma_n} - 1, \frac{E_{top\_n} - E_{bottom\_n}}{E + i\gamma_n}\right)
\]

where

\[
f_{0PB}(a,b,c) = e \left( a \cdot \arctan\left(\frac{c}{a}\right) - b \cdot \arctan\left(\frac{c}{b}\right) \right)
\]

\[
E_{Lorentz\_LB\_n} = A_n \left(\frac{E_{top\_n} - E_{bottom\_n}}{E_{top\_n} - E_{bottom\_n}}\right)\times f_{0LB}\left(\frac{E_{bottom\_n}}{E + i\gamma_n}, \frac{E_{top\_n}}{E + i\gamma_n}\right)
\]

where

\[
f_{0LB}(a,b,c) = a \cdot \ln\left(\frac{a - 1}{a + 1}\right) + \ln\left(\frac{b^2 - 1}{a^2 - 1}\right)
\]

<table>
<thead>
<tr>
<th>Style</th>
<th>Fit Parameters (n = osc#)</th>
</tr>
</thead>
<tbody>
<tr>
<td>LorPB.0 (eV)</td>
<td>Ampn = A_n (eV^2)</td>
</tr>
<tr>
<td>LorLB.0 (eV)</td>
<td>Etopn = Etop_n (eV)</td>
</tr>
<tr>
<td></td>
<td>Ebottm = Ebottom_n (eV), Brn = \gamma_n (eV)</td>
</tr>
</tbody>
</table>

### Using the Genosc layer

The power and flexibility Genosc layer arises not only from the its variety of oscillator types, but also its capacity to fit those oscillators directly to reference dielectric functions from within Genosc layer dialog box. This allows the user to quickly build models that accurately fit reference optical constants. Furthermore, the dielectric function display window allows the user to easily visualize the optical properties of the different oscillator combinations. After building the model, the user fits the model to ellipsometric data in the usual way. The following sections demonstrate how to build parametric models that match reference dielectric function spectra with several examples. The final example fits a genosc layer to ellipsometric data.

### Procedure for fitting reference spectra

After opening a genosc layer dialog box, use the following procedure to build a parametric model that matches a reference material.
**NOTE:** For Transparent materials, only steps 1 and 5 are necessary.

1. Load reference material file into Genosc dialog box, (making sure that the Energy range and step size is appropriate),
2. Add oscillators to approximately match the model $\epsilon_2$ to the $\epsilon_2$ reference, and
3. Fit the oscillator ensemble to $\epsilon_2$ reference spectra only.
4. repeat steps 2 – 3 as necessary. When model adequately fits $\epsilon_2$ reference, proceed to step 5.
5. Fit Poles & $\epsilon_1$ Offset to $\epsilon_1$ reference spectra.

### Reference Spectra Fit Procedure Flow Chart

![Reference Spectra Fit Procedure Flow Chart](image)

**Examples of Reference Spectra Fitting:**

**Amorphous Si$_3$N$_4$ & the Tauc-Lorentz oscillator**

1. Load reference material.

To load a reference material, select the Reference Material button in the Genosc layer dialog box. Any WVASE® material file can be used as a reference spectrum – whether it is tabulated, genosc, parametric, EMA, alloy temperature, or any other WVASE®-compatible material file. In this example, we are going to load a tabulated material file called `sinnx.mat`, which is found in the Genosc_examples directory. After `sinnx.mat` is loaded, the Genosc layer dialog box should look something like the figure below.

![Genosc layer dialog box after loading sinnx.mat as the Reference material](image)
NOTE: the range should not exceed the valid energy range of the reference material file.

For material files with tabulated optical constants, WVASE® automatically sets the range and step size to that found in the tabulated list. When the Reference Material is a parameterized model, the user must set the range and step size manually.

2. Create Oscillator ensemble and fit to reference material.

The Oscillator ensemble is created by adding one or more oscillators to the Oscillator List. Generally, the oscillator parameter values are set so that the model \( \varepsilon_2 \) roughly matches that of the reference material. The procedure for adding an oscillator is described earlier in “Description of Dialog Box” section (subsections 8 and 9). **Remember that the most frequently used oscillator types can be added graphically** by moving the cursor to the desired location, then holding down the shift key while clicking the left mouse button (see subsection 9).

For this model, add a Tauc-Lorentz oscillator with an \( En \approx 8 \) and \( An \approx 690 \). The resulting Genosc layer dialog box should look something like Figure 8.42.

![Figure 8-42. Genosc layer dialog box after adding a Tauc-Lorentz to the Oscillator List.](image)

Before fitting the model to the \( \varepsilon_2 \) spectrum, it is generally a good idea to adjust model parameters until the model \( \varepsilon_2 \) is a reasonably good close fit the reference \( \varepsilon_2 \) spectrum. In this example, \( Amp \approx 68, En \approx 8, C \approx 5 \) and \( Eg \approx 3 \). **NOTE:** the broadening can be adjusted by dragging the small blue boxes on the side of the selected oscillator (see previous figure and next figure). In anticipation of the next step, the four parameters of Osc #1: T-LO have been selected for fitting by selecting the adjacent check box. The Genosc layer dialog box should look something like the next figure.
3. **Fit the oscillator ensemble to \( \varepsilon_2 \) reference spectra only.**

The next step is to select which parameters are varied in the fit (via the check boxes next to the parameter values – see figure above), and selecting the Fit to Ref. button. After a few moments, you should see a WVASE® Message box similar to the next figure. This box contains information regarding the fit, including MSE and correlation matrices.

![Post-“Fit to Reference” Message box.](image)

When the user makes the Message box disappear by selecting “OK”, the Genosc layer dialog box should look something like the figure below.

![Genosc layer dialog box after Tauc-Lorentz (Osc #1: T-LO) has been Fit to Reference \( \varepsilon_2 \) spectrum sinx.mat.](image)
4. Repeat steps 2 – 3 as necessary.
   The model is a very good fit to \( \varepsilon_2 \) reference, so we can proceed to step 5.

5. Fit Poles & \( \varepsilon_1 \) Offset to \( \varepsilon_1 \) reference spectra.

   The next step is to fit the model to the \( \varepsilon_1 \) spectrum. First, select either the **Fit Both** or **Fit \( \varepsilon_1 \) only** button – the choice is up to the user. (In cases where the \( \varepsilon_2 \) fit is not very good, or the reference spectra is not precisely Kramers-Kronig consistent; it might be useful to fit \( \varepsilon_1 \) spectra separately). The GenOsc dialog box should now look similar to the figure below.

   ![Figure 8-46. Genosc layer dialog box prior to fit of \( \varepsilon_1 \) Offset to the sinx.mat reference spectra.](image1)

   For this Reference spectrum, the only change in \( \varepsilon_1 \) is a slight adjustment of the \( \varepsilon_1 \) Offset parameter. Select the \( \varepsilon_1 \) Offset check box and then select the **Fit Osc. to Ref.** button. After fitting, the Genosc dialog box should look similar to the figure below.

   ![Figure 8-47. Genosc layer dialog box after fit of \( \varepsilon_1 \) Offset to the sinx.mat reference spectra.](image2)

   Once you are satisfied with the model’s fit to the reference spectra, you can close the Genosc dialog box and fit the model to ellipsometric data using normal WVASE® fitting procedures.
Examples of Reference Spectra Fit:
Other Amorphous materials (Tauc-Lorentz oscillator)

In a similar fashion, we can fit other amorphous materials. The user can practice fitting similar materials such as a-ge.mat, a-si.mat, a-si_asp.mat, and As2S3_vitreous.mat, which are found in the Genosc_examples directory. Another material file, SiON_pbp.mat, provides an opportunity to fit a reference spectrum using multiple oscillators and is discussed in more detail.

The reference spectra for a-ge.mat, a-si.mat, a-si_asp.mat, and As2S3_vitreous.mat can all be modeled with a single Tauc-Lorentz oscillator layer. Applying a procedure similar to the one described above, the user should get results similar to those shown in the next figure.

Figure 8-48a). Genosc fit for a-ge.mat.
Figure 8-48b). Genosc fit for a-si.mat.
Figure 8-48c). Genosc fit for a-si_asp.mat.
Figure 8-48d). Genosc fit for As2S3_vitreous.mat.

Figure 8-48. Genosc layer dialog boxes after Osc #1: T-LO and 'e1 Offset' have been Fit to \( \varepsilon_1 \) and \( \varepsilon_2 \) reference spectra from four different amorphous materials.

Another amorphous material reference spectrum, SiON_pbp.mat, requires multiple oscillators in the model. We will fit this reference spectrum first with two Tauc-Lorentz oscillators, using a total of eight parameters. We then fit the same reference with two Gaussian oscillators, using a total of six parameters.

Load the SiON_pbp.mat reference material into Genosc Layer dialog box. Unlike the previous amorphous examples, the \( \varepsilon_2 \) reference spectrum only contains the absorption tail, not the central peak, which exists at some higher energy.
To fit this spectrum, we use two Tauc-Lorentz oscillators—one with a center energy near the maximum energy (8.7 eV) and an $E_g$ of about 7 eV, the other with a center energy of about 7 eV and an $E_g$ of about 6 eV. The figures below show the Genosc layer dialog box before and after fitting. As the figures shows, the resulting fit is very good. However, this model requires a total of 8 parameters to fit the $\varepsilon_2$ spectrum alone.

This same reference spectrum can be fit using two Gaussian oscillators. The $\varepsilon_2$ absorption of the Gaussian effectively equals zero at (approximately) $\pm B\varepsilon$ from the center energy. Under certain circumstances, this allows the user to use a Gaussian to create an effective band edge similar to a Tauc-Lorentz. Since the Gaussian has only three fit parameters compared to four for the Tauc-Lorentz, this effectively reduces the number of free parameters.

Before creating this Gaussian model, we must be sure to delete the two Tauc-Lorentz oscillators by highlighting them, then selecting the Delete Oscillator(s) button.

We then added two Gaussian oscillators using the same approximate center energies as the Tauc-Lorentz oscillators (8.7 and 7.3 eV). The figures below show the Genosc layer dialog box before and after fitting. The resulting fit is just as good as the Tauc-Lorentz, but only required a total of six parameters to fit the $\varepsilon_2$ spectrum.
Figure 8-51a). Before Fit to Reference.  

Figure 8-51b). After Fit to Reference.

Figure 8-51. Genosc layer dialog box with two Gaussian oscillators before and after Fit to Reference of SiON_pbp.mat $\varepsilon_2$ spectrum.

Next, we will try to fit the $\varepsilon_1$ spectrum of SiON_pbp.mat using $e1$ Offset.  First, fit both $\varepsilon_1$ and $\varepsilon_2$ simultaneously by selecting the Fit Both button.  Then select $e1$ Offset as a fit parameter, and perform a Fit to reference.  Notice that this attempt to correctly fit the $\varepsilon_1$ reference spectra severely degraded the Gaussian oscillators fit to $\varepsilon_2$ (see figure below).  This is one example where the user should “Fit $e1$ only” instead of “Fit both” $e1$ and $e2$ simultaneously.  Be sure to select ‘Reset’ before moving to the next step.

Figure 8-52. Genosc layer dialog box with two Gaussian oscillators and $e1$ Offset after simultaneous fit to both the $\varepsilon_1$ and $\varepsilon_2$ spectra of SiON_pbp.mat.

After using Reset to return the Gaussian oscillator model to its original $\varepsilon_2$ fit, we now select Fit e1 only, and fit $e1$ Offset again.  The resulting fit is shown in the next figure.  As one would expect, the $\varepsilon_2$ fit remains excellent.  It is also clear that the $e1$ Offset term alone cannot fit the $\varepsilon_1$ reference spectrum.
Examples of Reference Spectra Fit: Fitting transparent spectra

When fitting transparent reference spectra, the model only needs to fit the $\varepsilon_1$ spectrum, since $\varepsilon_2 = 0$. Therefore, after the user immediately selects **Fit $\varepsilon_1$ only** after loading the reference spectrum. Why use the Genosc layer instead of, for example, the Cauchy layer? The reference material may require a Sellmeier model, or the user may be anticipating the need for a model requiring other oscillator terms to model absorption when the spectral range is extended to accommodate the actual experimental data spectral range.

In the following example, we will fit the reference spectrum of *sio2_jaw.mat* to two Pole terms, using one to match upward dispersion at higher
energies (resulting from electronic absorptions in the VUV) and another to match downward dispersion at lower energies (resulting from vibrational absorptions in the mid-IR). After loading sio2_jaw.mat (found in the Default Materials directory) and selecting the Fit e1 only button, the user’s screen should look similar to the next figure.

![Figure 8-55. Genosc layer dialog box after loading the sio2_jaw.mat.](image)

The upward dispersion in $\varepsilon_1$ at higher energies is obvious. What is less obvious is the subtle downward dispersion at the lowest energy regions. We are going to fit the high-energy dispersion first. To accomplish this, we adjust the Position and Magnitude of Pole#1 until we have a good starting value for a fit (Position=9 and Magnitude=80 will work). We then select them as fit parameters, and perform a Fit to Ref. After the fit, the Genosc dialog box should look something like the following figure.

![Figure 8-56. Genosc layer dialog box after fitting the high-energy dispersion of sio2_jaw.mat $\varepsilon_1$ reference spectrum.](image)

Note that the reference still has a small amount of downward dispersion at lower energies. This can be fit using the Position and Magnitude of Pole#2. After the fit, the Genosc dialog box should look something like the following figure.
The fit to reference is finished, and the layer is ready for integration into a optical model. The user should be aware that some correlation might exist between the Position and Magnitude of the Poles.
Chapter 9 The Generated Data Window

9.1 Generated Data window overview

The Generated Data window is used to store and manipulate data calculated from the optical model in the Model window.

The Generated Data window contains, in tabular form, simulated data which has been calculated from the associated Model window. This simulated data is calculated (1) when you manually command WVASE® to generate the data using the Gen_Data|Generate_Data command, and (2) when you perform a fit from the Fit window. As with the Experimental Data window, the displayed data is not restricted to one type and can contain any combination of ellipsometric, reflection, and transmission data. Data can also be loaded from a file into the Generated Data window for comparison with data in the Experimental Data window.

Features displayed in the Generated Data window

![Generated Data window example]

Figure 9-1. A general Generated Data window with non time-dependent (static) data.

Title bar

Under most circumstances, the title bar will display the words “Generated Data:”. However, if the generated data has been read from or saved to a disk, the title bar gives the name of the file loaded or saved most recently.

Comment line

Each data file has an optional comment line which appears above the tabulated data. This is typically used to indicate the sample name and other important measurement considerations. This comment line is only associated with data sets that have been saved to a disk file.

Scroll bar

This is used to change which of the data rows are displayed.
Type column

This column contains the code for what type of data is in that particular row (see Experimental Data Window Overview). Multiple data types can be mixed in the Generated Data window. In the above examples, only normal ellipsometric data “E” is shown.

Wavelength column

This column contains the wavelength applied to this data row. The heading of this column is the current units for wavelength as set by the |Global|Defaults command. Data files saved to disk can be in any of the recognized wavelength units, but in Generated Data windows the current global setting is used. Wavelengths, regardless of units, are rounded to 3 significant digits right of the decimal point. When the generated data is based on the experimental data wavelengths and angles, the generated data will show the same wavelengths and angles even if the actual angle of the calculation is different or the wavelength shift option is in effect (see Model|Options).

Angle column

This column contains the angle of incidence that was assumed when the data was acquired. When the generated data is based on the experimental data wavelengths and angles, the generated data will show the same wavelengths and angles even if the actual angle of the calculation is different or the wavelength shift option is in effect (see Model|Options).

Data columns

For each row, two data values can be present. Error bars (standard deviations) are not displayed in the Generated Data window. The meaning of these columns is dependent on the Type Column.

Time column

This is the time, in minutes, associated with measured data. Only dynamic data has a time column which is shown to the right of the data column.

The Generated Data window menubar

As shown below, there are five items on the main menubar plus the |Window and |Global menus.

![Figure 9-2. Menu bar when the Generated Data window is active.](image)

The general functions of these menus is given in the following table. The specific action will be described in succeeding sections.
Calculations performed for the different data types

Simulated data calculations revolve around determining which reflected or transmitted beams are collected by the detector. This section describes how WVASE® performs calculations of the various data types. A more detailed discussion of back surface corrections can be found in B. Johs et al, “Optical Analysis of Complex Multilayer Structures Using Multiple Data Types”, SPIE Vol. 2253, pp. 1098, 1994.

A general representation of the possible beams is shown below.

\[
\begin{align*}
\text{Input Light Beam} & \quad \text{Reflected Beams} \\
\text{Multilayer Film Stack} \quad \text{(coherent propagation)} & \\
\text{Transparent Substrate} \quad \text{(incoherent propagation)} & \\
R_f & = \text{ambient/film stack reflection} \\
T_f & = \text{film stack/substrate transmission} \\
R_b & = \text{substrate/ambient reflection} \\
T_b & = \text{substrate/ambient transmission} \\
R_{fr} & = \text{substrate/film stack reflection} \\
T_{fr} & = \text{film stack/ambient transmission} \\
\end{align*}
\]

Figure 9-3. Sample schematic showing possible reflected/transmitted beams.

Each of outgoing beams is considered to be incoherent with respect to all of the other outgoing beams. Within each beam however, there are p- and s-polarized
components which are considered to be internally coherent. These two polarizations are treated separately and the Fresnel coefficient definitions given above are evaluated appropriately.

Each of the depicted beams can have its own unique elliptical polarization, but these elliptical polarizations are added incoherently at the detector. However, when a real sample measurement is performed, only a single $\psi$ and $\Delta$ pair is evaluated from the detector signal. For a standard ellipsometric reflection measurement on a sample with an absorbing substrate, the measured ellipsometric parameters are defined simply by

$$\tan \psi = \frac{|\tilde{R}_p|^2}{|\tilde{R}_s|^2},$$  \hspace{1cm} (9.1)

$$\cos \Delta = \frac{\text{Re}(\tilde{R}_p \cdot \tilde{R}_s^*)}{\sqrt{|\tilde{R}_p|^2 \cdot |\tilde{R}_s|^2}}.$$

When modeling the collection of multiple incoherent beams, the effective $\psi$ and $\Delta$ values are calculated using the following formulas where the summations are performed over the collected beams.

$$\tan \psi_{\text{eff}} = \frac{\sum |\tilde{R}_p|^2}{\sum |\tilde{R}_s|^2},$$  \hspace{1cm} (9.3)

$$\cos \Delta_{\text{eff}} = \frac{\sum \text{Re}(\tilde{R}_p \cdot \tilde{R}_s^*)}{\sqrt{\sum |\tilde{R}_p|^2 \cdot \sum |\tilde{R}_s|^2}}.$$

The number of collected reflected beams is set using the Model|Options command. This number can also be fractional, and in that case the last beam is weighted with a lower fraction. When simulating transmission measurements, the transmitted beam coefficients are used in place of the reflection coefficients.

$E, \text{AnE}, \text{Aps}, \text{Asp}, \text{pR}, \text{sR}, \text{uR}, \text{ARpp}, \text{ARss}, \text{ARps}, \text{ARuu}, \text{ARux}, \text{ARxx}, \text{ARxu}, \text{qJ}, \text{E0}, \text{E}_{+45}, \text{E}_{-45}, \text{E}_{90}, \text{dpolE}, \text{and m11 … m43}$: These data types are calculated using only the primary reflected beam.

$E_b, \text{AnEb}, \text{Apsb}, \text{Aspb}, \text{pRb}, \text{sRb}, \text{uRb}, \text{ARppb}, \text{ARssb}, \text{ARpsb}, \text{ARuub}, \text{ARuxb}, \text{ARxxb}, \text{AXub}, \text{qJb}, \text{E0b}, \text{E}_{+45b}, \text{E}_{-45b}, \text{E}_{90b}, \text{dpolEb}, \text{and m11b … m43b}$: These data type are calculated using the set of beams defined by the Model|Options command. The anisotropic calculations can be performed only when the substrate is isotropic.

$E_r, \text{AnEr}, \text{Apsr}, \text{Aspr}, \text{pRr}, \text{sRr}, \text{uRr}, \text{ARppr}, \text{ARssr}, \text{ARpsr}, \text{ARuur}, \text{ARuxr}, \text{AXxr}, \text{AXur}, \text{qJr}, \text{E0r}, \text{E}_{+45r}, \text{E}_{-45r}, \text{E}_{90r}, \text{dpolEr}, \text{and m11b … m43b}$: This data type is calculated in the same way as “Eb” except that the probe beam is considered incident on the backside.
Et, AnEt, Apst, Aspt, pT, sT, uT, ATpp, ATss, ATps, ATsp, ATuu, ATux, ATxx, ATxu, qJt, E0t, E+45t, E-45t, E90t, dpolEt, and m11t … m43t: These data type are calculated using all of the transmitted beams. The set of beams defined by the Model|Options command are not used for this data type.

Simulated data

Any simulated data displayed in the Generated Data window can also be used as “synthetic” experimental data in the Experimental Data window. When working to characterize a new kind of sample, you may find it useful to try different data fitting approaches on data where you already know the correct result.

As an example, you could perform a test to determine how much a fitted thickness would change if slightly incorrect optical constants were used. Working with simulated data sets is very useful when developing external monitoring/control programs using real-time acquisition with an M-XX ellipsometer. In this case, you can simulate the data coming from the process (including random noise, see |Gen_Data|Range) and test your controlling software many times without ever actually taking “real” data. (Program development with “synthetic” data can not account for all real-world effects, but it can greatly reduce the amount of time needed in the real measurement environment.)

Simulated data standard deviations

To make “synthetic” data sets closer to real data, simulated standard deviations (error bars) are also calculated. These simulated deviations are also applied when opening an experimental data file that does not contain standard deviation information. The purpose of including calculated deviations is to approximate the relative noise levels of data acquired with different $\psi$ and $\Delta$ combinations.

For ellipsometric data, these standard deviations are calculated assuming a rotating analyzer type of ellipsometer. The standard deviation formulas for $\psi$ and $\Delta$ are derived by assuming the random noise in the measured normalized Fourier coefficients $\alpha$ and $\beta$ is constant. The Fourier coefficient standard deviations are then converted to deviations in $\psi$ and $\Delta$ by taking the necessary partial differentials with respect to $\alpha$ and $\beta$ in equations 8.5 and 8.6. Assuming a constant noise level in the Fourier coefficients means that noise effects associated with the intensity of the probe beam and with averaging time at acquisition are not simulated. Only the dependence on $\psi$ and $\Delta$ is simulated.

\[
\alpha = \frac{\tan^2(\psi) - \tan^2(P)}{\tan^2(\psi) + \tan^2(P)}, \quad (9.5)
\]

\[
\beta = 2 \frac{\tan(\psi) \tan(P) \cos(\Delta)}{\tan^2(\psi) + \tan^2(P)}, \quad (9.6)
\]

\[
\sigma_{\psi} = dVASE \times \frac{1}{1 + \tan^2(\psi)} \times \frac{\tan(P)}{(1 - \alpha) \sqrt{1 - \alpha^2}}, \quad (9.7)
\]
The polarizer angle $P$ is assumed to be equal to $\psi$, except when $\psi$ is less than 10° ($P = 10^\circ$) and $\psi$ is greater than 80° ($P = 80^\circ$). Defining the polarizer angle in this way assumes that the data was taken with a polarizer tracking ellipsometer, which is the standard acquisition method with a VASE® instrument. (If the data was not acquired in this mode, it should not significantly affect fits using the simulated standard deviations.)

Simulated standard deviations on intensity reflection (R) and intensity transmission data (T) are also calculated. The formulas for these standard deviations are considerably simpler.

$$\sigma_T = dTrans \times T,$$  \hspace{1cm} (9.9)  

$$\sigma_R = dRefl \times R,$$  \hspace{1cm} (9.10)  

The values $dVASE$, $dTrans$, and $dRefl$ are specified in the WVASE® configuration file, wvase.cnf. See Appendix C for details on how to change these values in the configuration file.

---

9.2 Gen_Data|File menu

This option is used to load a previously saved data file into the Generated Data window. The loaded data will replace any existing data in the Generated Data window. Loading a data file in to this window is done only for comparison with the experimental data. Data loaded from a file will be replaced the next time a fit is started or the Gen_Data|Generate_Data command is used. The file loading and naming conventions are same as for the Exp_Data|File|Open_Exp_File command.

This option is used to add another data file to the end of the data that already exists in the Generated Data window. Loading a data file in to this window is done only for comparison with the experimental data. The Generated Data window’s Title Bar and Comment Line will reflect the most recently added file. There is no corresponding merge command as there is with the Exp_Data|File menu.
**Gen_Data|File|Save_Gen_Data item**

This option is used to save data from the Generated Data window to a file. Multiple data types can be saved together in a single file. A standard Windows™ dialog box is used to select the filename. The file will automatically receive the .dat extension. You are also permitted to input/change the experimental data comment line when you save the file. If a file with the same name already exists, you will be asked for confirmation that you do indeed want to overwrite it. When data is saved from the Generated Data window to a file, simulated data standard deviations will be added. These simulated standard deviations are described earlier in this chapter.

**Gen_Data|File|Comment_Data item**

This allows you to manually input the text for the generated data comment line. You are also given the option of commenting the data when you save it.

**Gen_Data|File|Information item**

This item brings up a message box containing the information string attached to the data. If the data is simulated data then the information pertains to how the data was generated. If this is a previously acquired experimental data file then this string contains the software version and information on the acquisition parameters used to acquire the data.

**Gen_Data|File|Copy_to_Clipboard item**

This item allows you to copy the generated data onto the Windows™ Clipboard. From there it can be pasted into other Windows™ based applications such Microsoft Word™. The data is stored on the Clipboard as a <tab> delimited text table. All the data displayed in the Generated Data window is copied to the clipboard except the comment lines and column headers.

### 9.3 Gen_Data|Range item

![VASE for Windows](image)

**Figure 9-6.** The Range option from the Generated Data window.

The Gen_Data|Range option is used to select the type and range of data which will be generated from the optical model in the Model window.

**The generation range dialog box**

When you perform a manual data generation, the data type, wavelength range, and angle of incidence range used is taken from the settings specified in the Generation Range dialog box.
Range setting

This range selection applies only when manually generating data using the Gen_Data|Generate_Data command. When fitting, the data displayed in the Generated Data window was calculated in direct correspondence to the experimental data. This selection box has two options for defining the data points that will be calculated. If the Experimental Range is selected, then the data calculations will be performed for the data types and at the wavelengths and angles as specified in the Experimental Data window. Only selected experimental data points will be correspondingly simulated. If the Specified Range is selected, then the data calculations will be performed on a grid of angles and wavelengths for the data type defined in this dialog box. The Experimental Range selection is only available if experimental data exists in the Experimental Data window.

Angle range

These editable boxes specify the minimum, maximum, and step size for the grid of incident angles to be simulated when the Specified Range mode is in effect (see Range: above).

Wavelength range

These editable boxes specify the minimum, maximum, and step size for the grid of wavelengths to be simulated when the Specified Range mode is in effect (see Range: above). The currently selected wavelength units (see |Global|Defaults) are labeled to the right of these boxes.

Data type

This single item selection box specifies the type of data to be simulated when the Specified Range mode is in effect (see Range: above). For more information on how the different data types are simulated see the earlier section in this chapter on ‘How calculations are performed for different data types’.
**Dynamic in-situ data**

This check box is used to manually generate dynamic growth data for the model. When generating dynamic data, only the first angle of incidence defined by the Angle Boxes is used.

**Time increment box**

This editable box is used to define the step size between successive time slices. At each time, a spectroscopic array of data points is generated for the wavelengths specified in the Wavelength Boxes.

**Dynamic VASE data**

This check box is used to manually generate dynamic VASE data. When generating dynamic VASE data, only the first angle of incidence defined by the Angle boxes is used.

**Duration**

This edit box is used to define the duration of the simulated dynamic VASE data. The Dynamic VASE Data checkbox must be checked for this parameter to have an effect.

**Increment**

This edit box is used to define the time required for one pass through all of the wavelengths set in the wavelength range section.

**Random noise box**

This editable box defines how much random noise is added to the data. The amount of random noise added is defined as a percentage of the simulated standard deviations describe earlier in this chapter. In most cases, you will not want to add random noise and you will leave this value at zero. However, if you are trying the simulate data to test a new fitting procedure it can be added with this feature.

**Generation mode setting**

There are three possible settings: “Normal”, “Sensitivity”, and “Vary Parameter”. Of these, “Normal” is the most commonly used because it simply simulates the measured data values in the active data range. The “Sensitivity” mode is used to investigate what angle and wavelength regime is best when trying to characterize a single model parameter. The “Vary Parameter” mode is used to investigate how simulated data changes for different values of a single parameter. Use of the “Sensitivity” and “Vary Parameter” modes is detailed in the section describing the Gen_Data|Generate_Data command.

**Description of Data types**

WVASE® supports many types of optical data. WVASE® can simulate many different types of data. The primary data types are standard ellipsometry (reflection & transmission modes), reflection intensity, and transmission intensity. These data types can be acquired by J.A. Woollam Co., Inc. VASE® and M-XX systems. Data from other optical measurement instruments can also be analyzed. The proper file formats for experimental (and generated) data files are described in Appendix B of the WVASE manual.
The data type also includes information on how the measurement was performed, so that the proper calculation is performed when model generated data is calculated. The different data types are explained briefly in the following sections. The complete list of currently supported data types is presented, however, the vast majority of sample characterizations will use only three types: (1) Standard Ellipsometry “E”, (2) Backside Corrected Ellipsometry “Eb”, and (3) Intensity Transmission “pT”.

Ellipsometric data types

Users may need to change the data type after data acquisition, prior to modeling and analysis.

At the time of acquisition, the ellipsometer hardware is unable to distinguish among some of the multiple ellipsometric data types and by default will store the data as standard ellipsometric data, type “E” (i.e. Backside Corrected Ellipsometry “Eb” will be stored as Standard Ellipsometry “E”). However, for analysis purposes you may need to change the data type so that the model calculation will simulate the actual measurement process.

The parameters named $\psi$ and $\Delta$ are always used to define the measured complex ratio as:

$$\tilde{\rho} = \tan(\psi)e^{i\Delta}. \quad (9.11)$$

In the case of standard reflection ellipsometry, this ratio is $\tilde{R}_p/\tilde{R}_s$. For other data types, the ratio is used as described in the preceding section on samples with transparent substrates.

Standard Ellipsometry – types E, Eb Er, Et

The Standard Ellipsometry types are:

<table>
<thead>
<tr>
<th>Type</th>
<th>Mode</th>
<th>Data acquired from sample:</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$</td>
<td>Reflection</td>
<td>Top side</td>
</tr>
<tr>
<td>$\tilde{\rho} = \frac{\tilde{R}_p}{\tilde{R}_s}$</td>
<td>No substrate backside effects will be included in the model calculations. If a layer with anisotropic optical constants is present, the optical axis for that layer will be assumed to be perpendicular to the surface of the sample.</td>
<td></td>
</tr>
<tr>
<td>$Eb$</td>
<td>Reflection</td>
<td>Top side</td>
</tr>
<tr>
<td>$\tilde{\rho} = \frac{\tilde{R}_p}{\tilde{R}_s}$</td>
<td>Substrate effects associated with a transparent substrate will be included in the model calculations. If a layer with anisotropic optical constants is present in the model, the optical axis for that layer will be assumed to be perpendicular to the surface of the sample. The calculation is not performed correctly if the substrate is anisotropic.</td>
<td></td>
</tr>
<tr>
<td>$Er$</td>
<td>Reflection</td>
<td>Back side</td>
</tr>
<tr>
<td>$\tilde{\rho} = \frac{\tilde{R}_p}{\tilde{R}_s}$</td>
<td>Only required when combined with data acquired from the top side of the same sample. Substrate effects will be included in the model calculations. If a layer with anisotropic optical constants is present, the optical axis for that layer will be assumed to be perpendicular to the surface of the sample. The calculation is not performed correctly if the substrate is anisotropic.</td>
<td></td>
</tr>
<tr>
<td>$Et$</td>
<td>Transmission</td>
<td>Top side</td>
</tr>
<tr>
<td>$\tilde{\rho} = \frac{\tilde{T}_p}{\tilde{T}_s}$</td>
<td>As with all transmission-type experiments, substrate effects will be included in the model calculations. If a layer with anisotropic optical constants is present, the optical axis for that layer will be assumed to be perpendicular to the surface of the sample. The calculation is not performed correctly if the substrate is anisotropic.</td>
<td></td>
</tr>
</tbody>
</table>
%Depolarization: depolE, depolEb, depolEr, depolEt

These data types quantify the %Depolarization of the sample, and are acquired during a “Ellipsometric + Depolarization” measurement. They are only acquired with the standard ellipsometric data types (E, Eb, Er or Et). The various Depolarization data types can be fit using the model non-idealities such as backsurface reflections, non-uniform films, non-zero bandwidth effects, angular spread and patterning.

<table>
<thead>
<tr>
<th>Type</th>
<th>Mode</th>
<th>Data acquired from sample:</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>depolE</td>
<td>Reflection</td>
<td>Top side</td>
<td>No substrate backside effects will be included in the model calculations.</td>
</tr>
<tr>
<td>depolEb</td>
<td>Reflection</td>
<td>Top side</td>
<td>Substrate effects associated with a transparent substrate will be included in the model calculations.</td>
</tr>
<tr>
<td>depolEr</td>
<td>Reflection</td>
<td>Back side</td>
<td>Only required when combined with data acquired from the top side of the same sample. Substrate effects will be included in the model calculations.</td>
</tr>
<tr>
<td>depolEt</td>
<td>Transmission</td>
<td>Top side</td>
<td>As with all transmission-type experiments, substrate effects will be included in the model calculations.</td>
</tr>
</tbody>
</table>

Generalized Ellipsometry – types AnE, Aps, Asp including types ...b, ...t and ...r

These Generalized Ellipsometry data types correspond to three related complex ratios, and are acquired simultaneously using anisotropic measurement options. The Generalized Ellipsometry types calculate ratios from all four of the sample Jones matrix, normalized to \( \tilde{R}_{ss} \):

\[
J_{\text{sample}} = \begin{bmatrix} \tilde{R}_{pp} & \tilde{R}_{sp} \\ \tilde{R}_{ps} & \tilde{R}_{ss} \end{bmatrix} = \tilde{R}_{ss} \begin{bmatrix} \text{AnE} & \text{Asp} \\ \text{Aps} \cdot \text{AnE} & 1 \end{bmatrix}
\]

\[
\text{AnE} = \frac{\tilde{R}_{pp}}{\tilde{R}_{ss}} = \tan(\Psi_{\text{AnE}}) e^{i \Delta_{\text{AnE}}}
\]

\[
\text{Asp} = \frac{\tilde{R}_{sp}}{\tilde{R}_{ps}} = \tan(\Psi_{\text{Asp}}) e^{i \Delta_{\text{Asp}}}
\]

\[
\text{Aps} = \frac{\tilde{R}_{pp}}{\tilde{R}_{pp}} = \tan(\Psi_{\text{pToE}}) e^{i \Delta_{\text{pToE}}}
\]

For transmission types \( \tilde{R} \) is replaced with \( \tilde{T} \) in the above equations. All three ratios are complex, so relative phase information is included. AnE is the “normal” ratio, and is equivalent to the standard ellipsometric measurement values for all isotropic and many anisotropic samples. The “p into s” ratio, Aps, is indicative of how p-light is converted into s-light relative to how p-light is reflected as p-light. The “s into p” ratio, Asp, is indicative of how s-light is converted into p-light relative to how s-light is reflected as s-light. The generalized ellipsometry types are:
<table>
<thead>
<tr>
<th>Type</th>
<th>Mode</th>
<th>Data acquired from sample:</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>AnE</td>
<td>Reflection</td>
<td>Top side</td>
<td>The “normal” ellipsometric ratio using the generalized anisotropic measurement mode.</td>
</tr>
<tr>
<td>Aps</td>
<td>Reflection</td>
<td>Top side</td>
<td>The “p into s” ellipsometric ratio using the generalized anisotropic measurement mode.</td>
</tr>
<tr>
<td>Asp</td>
<td>Reflection</td>
<td>Top side</td>
<td>The “s into p” ellipsometric ratio using the generalized anisotropic measurement mode.</td>
</tr>
<tr>
<td>AnEb</td>
<td>Reflection</td>
<td>Top side</td>
<td>The backside-corrected, “normal” ellipsometric ratio using the generalized anisotropic measurement mode.</td>
</tr>
<tr>
<td>Apsb</td>
<td>Reflection</td>
<td>Top side</td>
<td>The backside-corrected, “p into s” ellipsometric ratio using the generalized anisotropic measurement mode.</td>
</tr>
<tr>
<td>Aspb</td>
<td>Reflection</td>
<td>Top side</td>
<td>The backside-corrected, “s into p” ellipsometric ratio using the generalized anisotropic measurement mode.</td>
</tr>
<tr>
<td>AnEr</td>
<td>Reflection</td>
<td>Back side</td>
<td>The reverse-side, “normal” ellipsometric ratio using the generalized anisotropic measurement mode. Only required when combined with top side ellipsometric measurements on the same sample. Substrate effects will be included in the model calculations.</td>
</tr>
<tr>
<td>Apsr</td>
<td>Reflection</td>
<td>Back side</td>
<td>The reverse-side “p into s” ellipsometric ratio using the generalized anisotropic measurement mode. Only required when combined with top side ellipsometric measurements on the same sample. Substrate effects will be included in the model calculations.</td>
</tr>
<tr>
<td>Aspr</td>
<td>Reflection</td>
<td>Back side</td>
<td>The reverse-side, “s into p” backside-corrected ellipsometric ratio using the generalized anisotropic measurement mode. Only required when combined with data acquired from the top side of the same sample. Substrate effects will be included in the model calculations.</td>
</tr>
<tr>
<td>AnEt</td>
<td>Transmission</td>
<td>Top side</td>
<td>The “normal” transmission-ellipsometric ratio using the generalized anisotropic measurement mode. As with all transmission-type experiments, substrate effects will be included in the model calculations.</td>
</tr>
<tr>
<td>Apst</td>
<td>Transmission</td>
<td>Top side</td>
<td>The “p into s” transmission-ellipsometric ratio using the generalized anisotropic measurement mode. As with all transmission-type experiments, substrate effects will be included in the model calculations.</td>
</tr>
<tr>
<td>Aspt</td>
<td>Transmission</td>
<td>Top side</td>
<td>The “s into p” transmission-ellipsometric ratio using the generalized anisotropic measurement mode. As with all transmission-type experiments, substrate effects will be included in the model calculations.</td>
</tr>
</tbody>
</table>

**Mueller-Matrix Ellipsometry – types mm11, etc. including types …b, …r and …t**

These Mueller Matrix Ellipsometry data types corresponding to the Mueller Matrix elements, and are acquired simultaneously using the Mueller matrix measurement options. The Mueller matrix data types are all real-valued quantities.
that describe how the sample transforms the Stokes vector of the incident light-beam. The Mueller matrix is:

$$M_{\text{sample}} = \begin{bmatrix}
m_{11} & m_{12} & m_{13} & m_{14} \\
m_{21} & m_{22} & m_{23} & m_{24} \\
m_{31} & m_{32} & m_{33} & m_{34} \\
m_{41} & m_{42} & m_{43} & m_{44}
\end{bmatrix}.$$  

(9.13)

The $m_{11}$ element represents the total intensity reflection or transmission of the sample. WVASE records other 15 Mueller matrix quantities "$m_{jk}$" normalized to $m_{11}$, so they always range between -1 and +1:

$$m_{jk} = \frac{m_{jk}}{m_{11}}, \quad j, k = 1, 2, 3, 4.$$  

(9.14)

WVASE reports $m_{12}, m_{13}, \ldots m_{14}$, and they are correctly plotted when the Type|Psi or Type|Delta are selected. The $m_{11}$ element is only directly recorded during an M-2000® R.T scan, and is plotted using the Intensity Reflection or Transmission Type. See the “Reflected intensity data types” and Transmitted intensity data types” section for further details.

<table>
<thead>
<tr>
<th>Type</th>
<th>Mode</th>
<th>Data acquired from sample:</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m_{11}$ … $m_{44}$</td>
<td>Reflection</td>
<td>Top side</td>
<td>$m_{12}, m_{13}, \ldots m_{14}$ are all normalized to $m_{11}$.</td>
</tr>
<tr>
<td>$m_{11b}$ … $m_{44b}$</td>
<td>Reflection</td>
<td>Top side</td>
<td>Backside-corrected MM data. $m_{12b}, m_{13b}, \ldots m_{14b}$ are all normalized to $m_{11b}$. Substrate effects will be included in the model calculations.</td>
</tr>
<tr>
<td>$m_{11r}$ … $m_{44r}$</td>
<td>Reflection</td>
<td>Back side</td>
<td>Reverse-side MM data acquired from reverse side of sample. $m_{12r}, m_{13r}, \ldots m_{14r}$ are all normalized to $m_{11r}$. Only required when combined with data acquired from the top side of the sample. Substrate effects will be included in the model calculations.</td>
</tr>
<tr>
<td>$m_{11t}$ … $m_{44t}$</td>
<td>Transmission</td>
<td>Top side</td>
<td>Transmission MM data. $m_{12t}, m_{13t}, \ldots m_{14t}$ are all normalized to $m_{11t}$. As with all transmission-type experiments, substrate effects will be included in the model calculations.</td>
</tr>
</tbody>
</table>

**Jones Quality factor: $qJ$, $qJb$, $qJr$, $qJt$**

The $qJ$ or "Jones quality factor" data types are always acquired whenever general Mueller Matrix data are acquired. The $qJ$ data type is a quantitative measure of how closely experimental Mueller matrix data can be described by a Jones matrix. The $qJ$ value is calculated by finding the Jones matrix which has a Mueller matrix representation closest to the measured Mueller matrix values. The Jones quality factor is the "average" difference (root-mean-square) between the measured Mueller matrix values and the Mueller matrix values for the "closest" Jones matrix representation.

Mathematically all Jones matrices have a particular Mueller matrix representation, but the reverse is not true. For experimental values with measurement noise included, measured Mueller matrix values will not exactly correspond to any particular Jones matrix, even if the sample is essentially describable as a Jones matrix. If a sample is non-depolarizing, it can be described by a Jones matrix.
(isotropic or anisotropic). If a sample produces depolarized light upon reflection or transmission, then a Jones matrix will not completely describe the sample.

- For depolarizing ISOTROPIC samples, WVASE® uses a $\Psi$, $\Delta$, %Depol representation which is similar to the standard non-depolarizing $\Psi$-$\Delta$ representation.
- For ANISOTROPIC samples that depolarize upon reflection or transmission, a general Mueller matrix measurement is probably needed. However, with anisotropic samples there is no simple way to handle depolarization with a single %Depol value as can be done for isotropic samples. This fact also makes it hard to know whether a particular situation only requires anisotropic AnE, Aps measurements, or anisotropic + depolarization – i.e., Mueller Matrix measurements.

If the measured Mueller matrix exactly corresponds to a Jones matrix, then theoretically the $qJ = 0$. With noise included, $qJ$ values are typically similar in magnitude to the noise of the measured Mueller matrix elements. $qJ$ data acquired during a Mueller Matrix measurement of ~25nm thermal oxide on silicon sample suggests that typical instrument errors for $qJ \leq \pm 0.001$. Also, since Mueller matrix elements are effectively bounded by ±1, the maximum $qJ$ value is effectively bounded to something less than 1.

$qJ$ data are not used during the fit process.

The $qJ$ data are NOT used for fitting like the Depol data can be because the calculation speed for $qJ$ data is somewhat slow. The final generation of a fit will place $qJ$ data in the generated window if $qJ$ data exists in the experimental window, but the misfit between generated and experimental $qJ$ data does not affect the MSE value.

It is generally recommended that if anisotropic data are required for analysis, that general Mueller matrix measurements are used, at least during the initial data acquisition process for a given sample set. Since the general Mueller matrix measurement also reports the Jones matrix values of AnE, Aps and Asp, one gets both sets of data in about the same amount of time. And since the $qJ$ data are included, the user can make a more objective determination about whether the Mueller matrix data is required or whether the Jones matrix data is sufficient.

Please note that if depolarization is required to model the sample, the Jones matrix data (AnE,Aps,and Asp) should NOT be included in the fit because the Jones matrix data measurement assumed (wrongly) that the sample was non-depolarizing.

**Unregressed Anisotropic Ellipsometric data types E+45, E-45, E0, and E90**

The Unregressed Anisotropic measurement mode was implemented early in the development of generalized ellipsometry. This type can be used if light reaching the detector from the anisotropic sample is an incoherent mixture of light beams.

However, it is recommended that you use one of the Mueller-Matrix measurement modes for samples that generate incoherent mixtures of light.

---

2 The detected light beam can be a mixture of incoherent “sources” when, for example: (a) light is reflected from both the back and front sample surfaces, (b) thickness non-uniformity exists on one or more layers on the sample (especially for “thick” films >1μm), (c) the instrument spectrometer bandwidth is sufficiently wide that there are significant range of $\Psi$-$\Delta$ values across the band at each wavelength “step”, (d) beam focusing cause sufficient wide angle-of-incidence variation as to produce significant variations in $\Psi$-$\Delta$, and (e) the sample has patterning.
The Unregressed Anisotropic mode is a robust anisotropic measurement mode, but it does not allow the Auto-Retarder to be used and the measured \( \psi \) and \( \Delta \) values do not have a direct Jones matrix representation. This anisotropic measurement mode acquires data with the polarizer set at +45°, -45°, 0° and 90° and then stores data of types \( E_{+45}, E_{-45}, E_0, \) and \( E_{90} \). These stored data are simply direct conversions of the measured \( \alpha \) and \( \beta \) values to \( \psi \) and \( \Delta \) with the polarizer set to the 4 values listed above. (For an explanation of \( \alpha \) and \( \beta \) and their relationship to \( \psi \) and \( \Delta \), see Eqs. (2-27) and (2-28) in the “Jones matrix analysis of the rotating analyzer ellipsometer” section of Chapter 2.) These \( E_{+45}, E_{-45}, E_0, \) and \( E_{90} \) data types can be modeled, but they do not have a direct physical significance.

WVASE reports \( \Psi_{pol} \) and \( \Delta_{pol} \) for each polarizer angle (pol) of 0°, +45°, -45° and 90°. \( \Psi_{pol} \) and \( \Delta_{pol} \) are defined by the equation:

\[
\tan(\Psi_{pol}) e^{i\Delta_{pol}} = \tan\left(\frac{E_{pol}}{E_{pol}}\right) e^{i\left(\Delta_{pol} - \Delta_{pol}\right)}, \quad \text{where} \quad (9.15)
\]

\[
\begin{bmatrix}
E_p \\
E_s
\end{bmatrix} = \begin{bmatrix}
\tilde{R}_{pp} & \tilde{R}_{sp} \\
\tilde{R}_{ps} & \tilde{R}_{ss}
\end{bmatrix} \begin{bmatrix}
\cos P \\
\sin P
\end{bmatrix} = \begin{bmatrix}
\tilde{R}_{pp} \cos P + \tilde{R}_{sp} \sin P \\
\tilde{R}_{ps} \cos P + \tilde{R}_{ss} \sin P
\end{bmatrix}
\]

<table>
<thead>
<tr>
<th>Type</th>
<th>Mode</th>
<th>Data acquired from sample:</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>( E_{0}, E_{\pm45}, E_{90} )</td>
<td>Reflection</td>
<td>Top side</td>
<td>Measurements assuming no backsurface or reverse-side effects .</td>
</tr>
<tr>
<td>( E_{0b}, E_{\pm45b}, E_{90b} )</td>
<td>Reflection</td>
<td>Top side</td>
<td>Backside-corrected MM data. ( m12b, m13b, ... m14b ) are all normalized to ( m11b ). Substrate effects will be included in the model calculations.</td>
</tr>
<tr>
<td>( E_{0r}, E_{\pm45r}, E_{90r} )</td>
<td>Reflection</td>
<td>Back side</td>
<td>Reverse-side Unregressed Anisotropic Ellipsometric data. Only required when combined with data acquired from the top side of the same sample. Substrate effects will be included in the model calculations.</td>
</tr>
<tr>
<td>( E_{0t}, E_{\pm45t}, E_{90t} )</td>
<td>Transmission</td>
<td>Top side</td>
<td>Transmission Unregressed Anisotropic Ellipsometric data. As with all transmission-type experiments, substrate effects will be included in the model calculations.</td>
</tr>
</tbody>
</table>

**Reflected intensity data types**

Reflected intensity (“reflectance”) measurements acquired with M-2000® and VASE® instruments generally use a “straight through no sample” intensity scan (full probe beam) as the baseline. Therefore, when WVASE® calculates intensity reflection values for the model, it works with absolute reflection values from 0 to 1. Other reflection measurement systems may report reflectance relative to another material. For WVASE® to correctly model such data, it must first be converted to absolute reflection data.

It must be remembered that the ellipsometer always acquires polarized reflected-intensity data. That is, the incident beam always has a single, known polarization state\(^{iii}\) – s, p, or a user-specified. The ellipsometer then detects the

\(^{iii}\) For an M-2000®, the incident polarization state is a (known) continuously-varying function of the compensator’s fast axis azimuth as it rotates with time. This means that the sample is illuminated with known values of both p- and s-
intensities for the p, s, or user-specified polarization components of the reflected beam. The detected intensities can be reported as separate quantities, or added all together and reported as the total reflected-intensity.

Reflectance: polarized-incident, total reflected intensity

The table below lists all the data types where the all the polarization components of the reflected beam are added together and reported as total reflected-intensity for a specific input polarization. For example, “pR” means “p-polarized incident, all reflected polarizations added together”. The m11 data type, which can only be recorded by M-2000® ellipsometersiv, represents the total unpolarized reflected-intensity (sum of all reflected polarizations for an unpolarized incident beam).

Also listed are the backside-corrected and reverse-side data types. At the time of acquisition, the ellipsometer hardware is unable to distinguish between “standard” reflected intensity measurement and a backside-corrected or reverse-side data measurement. Therefore, by default WVASE stores the data at the standard data type – “pR”, for example. For analysis purposes you may need to change the data type so that the model calculation will simulate the actual measurement process – “pR” would become “pRb” or “pRr”, for example.

<table>
<thead>
<tr>
<th>Data Types</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Std</td>
<td>Backside corrected</td>
</tr>
<tr>
<td>pR</td>
<td>pRb</td>
</tr>
<tr>
<td>sR</td>
<td>sRb</td>
</tr>
<tr>
<td>uR</td>
<td>uRb</td>
</tr>
<tr>
<td>xR</td>
<td>xRb</td>
</tr>
<tr>
<td>m11iv</td>
<td>m11biv</td>
</tr>
</tbody>
</table>

a u = User-defined polarizer azimuth.  
b x = u + 90°, u = user-defined polarizer angle.

Reflectance: polarized-incident, polarized reflected intensity

The next table lists the data types where the individual output polarization components are reported. For instance “ARpp” means “p-polarized incident, p-polarized reflected only”. Some of these data types record the reflected intensities of light that has been converted from one polarization type to another. For example, “ARps” quantifies the conversion of p-polarized incident light into s-polarized light upon reflection.

polarized light during the course of one compensator rotation, and p- and s-incidence reflectance, values such as pR and sR, can be determined.

iv Because the M-2000® illuminates the sample with both p- and s-polarized light during the course of one compensator rotation, it can record the Mueller Matrix m11 value, which is the “unpolarized” reflectance/transmittance.
Data Types

<table>
<thead>
<tr>
<th>std</th>
<th>Backside corrected</th>
<th>Reverse side</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>ARpp</td>
<td>ARppb</td>
<td>ARppr</td>
<td>Electric field of incident beam is linearly polarized (p, s, u or θ). The ellipsometer records only one polarization component (p, s, u or θ) of the reflected light.</td>
</tr>
<tr>
<td>ARps</td>
<td>ARpsb</td>
<td>ARpsr</td>
<td>The ‘b’ postscript indicates backside-corrected data. Substrate effects will be included in the model calculations.</td>
</tr>
<tr>
<td>ARss</td>
<td>ARssb</td>
<td>ARssr</td>
<td></td>
</tr>
<tr>
<td>ARsp</td>
<td>ARspb</td>
<td>ARspr</td>
<td></td>
</tr>
<tr>
<td>ARuu</td>
<td>ARuub</td>
<td>ARuur</td>
<td>The ‘r’ postscript indicates reverse-side data. This is only required when combined with data acquired from the front side of the same sample. Substrate effects will be included in the model calculations.</td>
</tr>
<tr>
<td>ARux</td>
<td>ARuxb</td>
<td>ARuux</td>
<td></td>
</tr>
<tr>
<td>ARxx</td>
<td>ARxxb</td>
<td>ARxxr</td>
<td></td>
</tr>
<tr>
<td>ARxu</td>
<td>ARxub</td>
<td>ARxur</td>
<td></td>
</tr>
</tbody>
</table>


Normal-incidence reflected intensity

Normal incidence measurements (incident angle of zero) on isotropic samples and for uniaxial-anisotropic samples with the optic axis oriented normal to the surface reflect the same way regardless of incident polarization. That is, all total reflected intensity and same-polarization reflected intensity measurements (pR, sR, uR, m1, ARpp, ARss, ARuu, ARxx, ARsp, ARux, ARxu) are equal, since the p- and s-directions are indistinguishable. Furthermore, all cross-conversion reflected intensities (ARps, ARsp, ARux, ARxu) equal zero.

For anisotropic samples with an optic axis not oriented normal to the surface, normal-incidence reflected intensity are polarization dependent, and the cross-conversion reflected intensities do not always equal zero.

Transmission intensity data types

Transmission intensity ("transmittance") measurements acquired with M-2000® and VASE® instruments generally use a “straight through no sample” intensity scan (full probe beam) as the baseline. Therefore, when WVASE® calculates intensity transmission values for the model, it works with absolute transmission values from 0 to 1. Other transmission measurement systems may report transmittance relative to another material. For WVASE® to correctly model such data, it must first be converted to absolute transmittance data.

Just like reflectance measurements, the ellipsometer always acquires polarized transmission intensity data. That is, the incident beam always has a single, known polarization state (p, s, u) or a user-specified. The ellipsometer then detects the intensities for the p, s, or user-specified polarization components of the transmitted beam. The detected intensities can be reported as separate quantities, or added all together and reported as the total transmission-intensity.

Transmittance: polarized-incident, total transmitted intensity

The table below lists all the data types where the all the polarization components of the reflected beam are added together and reported as total transmitted-intensity for a specific input polarization. For example, “pT” means “p-polarized incident, all transmitted polarizations added together”. The m1I data type, which can only be recorded by M-2000® ellipsometers, represents the total...
unpolarized transmitted-intensity (sum of all transmitted polarizations for an unpolarized incident beam).

<table>
<thead>
<tr>
<th>Data Types</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>pT</td>
<td>Electric field of incident beam is linearly polarized (p, s, u(^a) or x(^b)). The ellipsometer records the sum of all polarization components of the transmitted light.</td>
</tr>
<tr>
<td>sT</td>
<td>m11 can only be measured using M-2000(^b) R(\mid T) scans(^a), and is plotted using the Intensity Reflection or Transmission Type.</td>
</tr>
<tr>
<td>uT</td>
<td>As with all transmission-type experiments, substrate effects will be included in the model calculations.</td>
</tr>
<tr>
<td>xT</td>
<td></td>
</tr>
<tr>
<td>m11(^{(iv)})</td>
<td></td>
</tr>
</tbody>
</table>

\(^a\) u = User-defined polarizer azimuth.  
\(^b\) x = u + 90\(^\circ\), u = user-defined polarizer angle.

**Transmittance: polarized-incident, polarized transmitted intensity**

The next table lists the data types where the individual output polarization components are reported. For instance “ATpp” means “p-polarized incident, p-polarized transmitted only”. Some of these data types record the transmitted intensities of light that has been converted from one polarization type to another. For example, “ATps” quantifies the conversion of p-polarized incident light into s-polarized transmitted light.

<table>
<thead>
<tr>
<th>Data Types</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>ATpp</td>
<td>Incident beam is linearly polarized (p, s, u(^a) or x(^b)).</td>
</tr>
<tr>
<td>ATps</td>
<td>The ellipsometer records only one polarization component (p, s, u(^a) or x(^b)) of the transmitted light.</td>
</tr>
<tr>
<td>ATss</td>
<td>As with all transmission-type experiments, substrate effects will be included in the model calculations.</td>
</tr>
<tr>
<td>ATsp</td>
<td></td>
</tr>
<tr>
<td>ATuu</td>
<td></td>
</tr>
<tr>
<td>ATux</td>
<td></td>
</tr>
<tr>
<td>ATxx</td>
<td></td>
</tr>
<tr>
<td>ATxu</td>
<td></td>
</tr>
</tbody>
</table>

\(^a\) User-defined polarizer azimuth taken from the ‘Polarizer Angle’ box described below.  
\(^b\) x = u + 90\(^\circ\), u = user-defined polarizer angle.

**Normal-incidence transmitted intensity**

Normal incidence measurements (incident angle of zero) on isotropic samples and for uniaxial-anisotropic samples with the optic axis oriented normal to the surface transmit the same way regardless of incident polarization. That is, all total transmitted intensity and same-polarization transmitted intensity measurements (p\(T\), s\(T\), u\(T\), m11, ATpp, ATss, ATuu, ATxx) are equal, since the p- and s-directions are indistinguishable. Furthermore, all cross-conversion transmitted intensities (ATps, ATsp, ATux, ATxu) equal zero.

For anisotropic samples with an optic axis not oriented normal to the surface, normal-incidence transmitted intensities are polarization dependent, and the cross-conversion reflected intensities do not always equal zero.
Other data types recognized by **WVASE®**

Advanced. These data types were implemented to meet the needs of specific customers, however, they have been made available to all users. These data types cannot be acquired using J.A. Woollam Co., Inc. hardware. These data types are included for analysis and simulation purposes only.

**N - Neutron reflection**

Data acquired in a neutron reflection experiment can also be modeled using **WVASE®**. This data type cannot be acquired using **WVASE®**. This feature was added for a particular customer working with neutron reflection data on polymers. For modeling, the *neutron.mat* layer is used (not described in this manual). If you wish to use this data type for analyzing your neutron reflection data, please contact the J.A. Woollam Co., Inc. directly for more details.

**Tph - Transmitted phase**

This data type represents the total phase difference of light transmitted through a layer stack relative to transmission through air of the same distance. This data type cannot be acquired using **WVASE®**. This type of data is usually associated with phase-shifted photomasks. For model calculations, **WVASE®** calculates the phase difference from only the layers on top of the substrate. The phase difference does not include propagation through the substrate. If acquired on another measurement instrument, data of this type can be used in the fitting process. Alternatively, **WVASE®** can be used to simulate this data type for a given model, and the model used may be the result of fitting to other ellipsometric and transmission data.

**Complex Fresnel Reflectance coefficients**

The complex Fresnel reflection (or transmission) coefficients cannot be measured directly at optical frequencies (which is one reason that we use ellipsometry!). However, they can be generated for simulations. Please note that these quantities are automatically generated by **WVASE®** during data generation for the other data types.

*Do not confuse the generated Fresnel coefficient plots with the ellipsometric $\Psi$ and $\Delta$ quantities!*

The generated complex quantities are plotted magnitude and phase form, with the magnitude axis labeled as “$\Psi$”, and the phase axis labeled as “$\Delta$” – do not confuse the plots with the ellipsometric $\Psi$ and $\Delta$ quantities! The figure below shows a plot of $R_{pp}$ and $R_{ss}$ for a silicon sample with native oxide.

---

**Figure 9-8. Generated Fresnel coefficient plots.**

"$\Psi$" = complex magnitude, "$\Delta$" = complex phase.
Fresnel Data Types

<table>
<thead>
<tr>
<th>std</th>
<th>Backside corrected</th>
<th>Reverse side</th>
</tr>
</thead>
</table>
| cRpp | cRppb | cRppr | Complex Fresnel coefficients (for simulation only – these quantities cannot be directly measured at optical frequencies).
| cRps | cRpsb | cRpsr | The ‘b’ postscript indicates backside-corrected data. Substrate effects will be included in the model calculations.
| cRss | cRssb | cRssr | The ‘r’ postscript indicates reverse-side data. Substrate effects will be included in the model calculations.
| cRsp | cRspb | cRspc | The transmission data types always include backside correction and substrate effects.
| cTpp | cTppb | cTppr | For simulation purposes only. These data types cannot be measured at optical frequencies.
| cTps | cTpsb | cTpsr |
| cTss | cTssb |
| cTsp | cTspb |

Other specialized data types

There are other highly-specialized data types included in Generate Range list, such as Ri, Ret, Rot, OD, PDev, Kerr, and Faru. Contact the Woollam Co. for details (Contact information is located at beginning of this manual).

9.4 Gen_Data|Generate_Data command

Figure 9-9. The Generate Data option from the Generated Data window.

This command causes a manual generation of data using the associated model. The data type, wavelength, and angle for each model calculation is determined by the Range setting (experimental or user specified) as defined by the Gen_Data|Range command. The Generation Mode is also defined by the Gen_Data|Range command. In the “Normal” generation mode the values are calculated directly from the model as displayed in the Model window. In the “Sensitivity” mode, two calculations are performed with one model parameter varied slightly, and the difference between the calculations is stored in the Generated Data window. In the “Vary Parameter” mode, one model parameter is varied through a range of values and a model calculation is performed at each value. The full set of generated data for each parameter value is then stored in the Generated Data window. The following simple model is used to illustrate the different generation modes.

![Model](image)

Figure 9-10. SiO₂ on Silicon model used to illustrate the different generation modes.
Normal generation mode

For this example the wavelength range has been set for 300 to 1000 nm and the incident angle range has been set for 75° only. Standard ellipsometric data, type “E”, is being generated.

![Figure 9-11. Generated ψ values using the “Normal” generation mode.](image)

![Figure 9-12. Generated Δ values using the “Normal” generation mode.](image)

The ellipsometric parameters ψ and Δ are calculated from the model in the Model window over the defined wavelength range.

Sensitivity generation mode

To use the “Sensitivity” mode exactly one model parameter must be selected for fitting. (Any parameter that can be varied can be used.) If the number of selected parameters is anything but exactly one, you will receive a reminder message box. When the sensitivity generation is started, you will need to complete a dialog box to specify the following.

![Figure 9-13. Dialog box used for “Sensitivity” generations.](image)
**Parameter name**

This identifies which parameter has been selected for testing.

**Increment value box**

This is the value by which the parameter will be varied during the test.

The sensitivity calculation at each wavelength and angle combination is performed in the following manner. First the data is calculated using the original parameter value plus the incremental value in the model. Next the data is calculated using just the original parameter value. The second data calculation is subtracted from the first, and the result is stored in the Generated Data window. If standard ellipsometry data is being modeled, the data stored in the ψ column is now the change in ψ due to the incremental change in the model parameter.

This procedure can be used to find wavelength and angle ranges where there is maximum sensitivity to the parameter of interest. In the following figure, the ψ sensitivity to a 10Å change in an oxide thickness of 300Å is shown. The model in Fig. 8.8 was used, with the SiO₂ thickness defined as the only fit parameter.

![Figure 9-14](image)

*Figure 9-14. Change in ψ due to a 10Å change in oxide thickness as a function of wavelength and angle of incidence. Sensitivity generations map very well into 3-D graphs.*

Note that the maximum sensitivity is seen for a wavelength around 500 nm and an incident angle around 75°. In this example, ψ would change about 0.55° for a 10Å change in thickness. The graph also indicates that if data were taken near 1000 nm at 60°, there would be much less sensitivity to the thickness.

**Vary parameter generation mode**

To use the “Vary Parameter” mode exactly one model parameter must be selected for fitting. (Any parameter that can be varied can be used.) If the number of selected parameters is anything but exactly one, you will receive a reminder message box. When the vary parameter generation is started, you will need to complete a dialog box similar to the following.

![Figure 9-15](image)

*Figure 9-15. Dialog box used for “Vary Parameter” generations.*
**Parameter name**

This identifies which parameter has been selected for testing.

**Start box**

This is first parameter value that will be used for generations.

**End box**

This is the maximum parameter value that will be used for generations.

**Incr box**

This is the value by which the parameter will be stepped between the Start and End values.

The vary parameter calculation is performed for each parameter value over the full range of wavelengths and angles. This command is nothing more than series of “Normal” generations with the one parameter being varied from the Start value to the End value. Each of these generations is then appended together in the Generated Data window. When graphed, the generated data is displayed as a series of curves like those below.

![Graph showing vary parameter modes](image)

**Figure 9-16. Generated \( \psi \) values using the “Vary Parameter” generation mode. Data curves for oxide thicknesses of 200, 300, 400, and 500 Å are displayed.**

![Graph showing vary parameter modes](image)

**Figure 9-17. Generated \( \Delta \) values using the “Vary Parameter” generation mode. Data curves for oxide thicknesses of 200, 300, 400, and 500 Å are displayed.**

You should be aware that the individual curves are not automatically labeled in the legend. In the above example, the \( \psi \) curves from bottom to top (\( \Delta \) curves from top to bottom) are for an oxide a thicknesses of 200 to 500 Å. Because there are multiple values at each wavelength and angle combination, this kind of data does not map well into a 3-D graph like the sensitivity data does.

### 9.5 Gen_Data| Copy_to_Exp command
Figure 9-18. The Copy_to_Exp option from the Generated Data window.

This menubar item is used to copy the data displayed in the Generated Data window to the Experimental Data window. This allows you to create “synthetic” data sets. Synthetic data sets can be used just like any other data set containing measured experimental data. Synthetic data sets can also be created by directly saving the generated data to file (Gen_Data|File|Save_Gen_Data) and then loading it into the Experimental Data window.

When you copy data to the Experimental Data window, you will be presented with a dialog box like the following if data already exists in that window.

Figure 9-19. A message box appears when you copy data from the Generated Data window to the Experimental Data window if data already exists in the Experimental Data window.

Selecting the ‘Cancel’ button will abort the copy command before any data is moved. Selecting the ‘Yes’ button will cause the data in the Generated Data window to be appended to the data already present in the Experimental Data window. Selecting the ‘No’ button will cause the data in the Generated Data window to overwrite the data already present in the Experimental Data window.

When data is moved from the Generated Data window to the Experimental Data window, simulated data standard deviations will be added. These simulated standard deviations are described earlier in this chapter.

9.6 Gen_Data|Delete_Data command

Figure 9-20. The Delete_Data option from the Generated Data window.

This menubar item is used to delete the currently displayed generated data from memory. Data files already saved to disk will be unaffected. Only the generated data associated with the currently selected model will be deleted. A caution dialog box is used to confirm your choice of this action.
Chapter 10 The Graph Window

10.1 Graph window overview

The Graph window is used to display experimental and calculated data, or fit results.

The Graph window is used to display experimental data, generated data, optical constants, and calibration data. The data can be displayed in 2-D and 3-D formats. A movable legend is automatically updated as the displayed data changes. The title and axis labels are editable. The axes are manually scalable. The graphs can be copied to the Windows™ Clipboard and pasted into other applications like a word processor. The Graph window is quite flexible but its primary use is to display data within WVASE®, and as such it is not a completely general graphing utility. If you need to make very sophisticated graphs that WVASE® cannot, the numeric data currently being displayed in the Graph window can be copied to another Windows™ application.

Features of a 2-D graph

The elements of a standard 2-D graph are listed below.

Title

This is an editable title that appears above the graph box. The title is edited using the Graph|Edit|Titles menu item.

X-axis

This is the numeric scale for the displayed X values. Only one X-axis, labeled at the bottom, is labeled. The scale and tick marks can be changed using the Graph|Edit|Scale menu item.

Figure 10-1. A general 2-D graph copied from WVASE®.
**X-axis label**

This is an editable label that appears on the bottom of the graph box. This label is edited using the Graph|Edit|Titles menu item.

**Y1 axis**

This is the numeric scale for values displayed against the left side Y axis. For double Y axis plots, the Y2 Axis appears on the right side. The scale and tick marks can be changed using the Graph|Edit|Scale menu item.

**Y1-axis label**

This is an editable label that appears on the left side Y axis. This label is edited using the Graph|Edit|Titles menu item. For some graphs a Y2-axis Label will be displayed on the right side.

**Legend**

This is a series of labels for the displayed curves. These labels are editable using the Graph|Edit|Legend menu item. The legend can be moved by clicking on it and dragging it to a new location.

**Data curves**

In the above examples two data curves are shown. The line/symbol combination used to display the data can be changed using the Graph|Edit|Legend menu item.

**Features of a 3-D graph**

The elements of a standard 3-D graph are listed below.

![3-D Graph](image)

*Figure 10-2. A general 3-D graph copied from WVASE®.*

**Title**

This is an editable title that appears above the graph box. The title is edited using the Graph|Edit|Titles menu item.
**X axis**

This is the numeric scale for the X values displayed on the lower left of the graph box. The scale and tick marks can be changed using the Graph|Edit|Scale menu item.

**X-axis label**

This is an editable label that appears on the lower left of the graph box. This label is edited using the Graph|Edit|Titles menu item.

**Y axis**

This is the numeric scale for values displayed on the lower right of the graph box. The scale and tick marks can be changed using the Graph|Edit|Scale menu item. The boxes associated with the ‘Y2’ axis pertain to the Y axis in 3-D graphs.

**Y-axis label**

This is an editable label that appears on the lower left of the graph box. This label is edited using the Graph|Edit|Titles menu item. The boxes associated with the ‘Y2’ axis pertain to the Y axis in 3-D graphs.

**Z axis**

This is the numeric scale for values displayed vertically on the left side of the graph box. The scale and tick marks can be changed using the Graph|Edit|Scale menu item. The boxes associated with the ‘Y1’ axis pertain to the Z axis in 3-D graphs.

**Z-axis label**

This is an editable label that appears on the left side on the graph box. This label is edited using the Graph|Edit|Title menu item. The boxes associated with the ‘Y1’ axis pertain to the Z axis in 3-D graphs.

**The Graph window menubar**

There are five menus on the main menubar plus the |Window and |Global menu.

![Graph Window Menubar](image)

*Figure 10-3. Menubar when the Graph window is active.*

The general functions of these menus are given in the following table. The specific action will be described in the succeeding sections.

<table>
<thead>
<tr>
<th>Menu</th>
<th>Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Graph</td>
<td>File</td>
</tr>
<tr>
<td>Graph</td>
<td>Edit</td>
</tr>
<tr>
<td>Graph</td>
<td>Data</td>
</tr>
</tbody>
</table>
Preparing formatted graphs

*WVASE* supports a number of graph formatting options for graph titles, axis labels, axis scales, line style, and the legend. However, because the *WVASE* Graph window is tightly integrated to the rest of the main windows, these formatting options are reset to default values after many operations. Graph formats can be saved and later reapplied to all or part of the format settings. Using graph formats is explained in the ‘Graph|Edit menu’ section of this chapter. To produce final graphs for reports or papers without using graph formats, the following ordered procedure is suggested.

1) Get the appropriate data displayed in the Graph window. Use the Graph|Data menu to select the data class. Use the Graph|Type menu as needed for generated and/or experimental data. Use the Exp_Data|Range_Select command to set the data range for display. Then make the Graph window the active window.

2) Set the fonts for the titles and axis labels using the Graph|Edit|Font menu item.

3) If you need to manually rescale the axes or change the numeric display precision, then use the Graph|Edit|Scale menu item.

4) Use the Graph|Edit|Legend command to set the legend text and line styles for the curves. You can drag the legend within the Graph window to place it where you want it.

5) Use the Graph|Edit|Titles command to set the text for the graph title and axis titles.

6) To export the graph, use the Graph|File|Copy_Graph_to_Clipping command to place the graph on the Windows™ Clipboard. Then paste the graph into another Windows™ application such as a word processor. To print the graph directly from *WVASE®,* use the Graph|File|Print command.

During this sequence of steps, it is important that you do not switch between the *WVASE®* windows as this may reset some of your formatting options to default values. Also, changing the data class or data type may also reset some of your formatting options.

Another feature of the *WVASE®* graph is that special embedded character sequences can be used to control formatting of font (normal and Symbol), typeface (bold, italics, and underline), and position (subscript and superscript). The text in the title, axis labels, and legends can all use the formatting controls. The backslash “\” character is used to change a formatting option or to include some specific content. See the “Graph|Edit menu” section below for lists of the different format controls and content types available as well as a conversions between Arial (normal) and Symbol fonts.
If you do not feel WVASE<sup>®</sup> will generate a graph as sophisticated as you want, then you can export the actual data in ASCII format to another graphing application. This is done using options on the Graph|File menu.

### 10.2 Graph|File menu

![Graph Window](image)

**Figure 10-4. The File menu from the Graph window.**

#### Graph|File|Print item

This option is used to print the graph currently displayed in the Graph window. The Default Windows™ printer is used. The options for this printer are set using the Windows™ Control Panel. (Refer to the Windows™ reference manual for help on installing and setting up printers). WVASE<sup>®</sup> will center the graph on the page, using the orientation defined in the printer setup.

#### Graph|File|Copy_Graph_to_Clipboard item

This option allows you to copy the graph to other Windows™ applications using the Windows™ Clipboard. The data are transferred in the Windows™ metafile format. From the clipboard, the graph can then be pasted into any other application that can utilize the metafile format. When using this command you are asked to set the desired width of the graph in a dialog box like Figure 10.5. This sets the preferred size of the graph in the metafile.

![Dialog Prompt](image)

**Figure 10-5. Dialog prompt for the size of the graph to be copied to Windows™ Clipboard.**

After pasting the graph into another application, you can resize and relocate the graph within that application. Some applications may also allow you to edit the graph to add additional features. However, not all applications interpret metafiles in the same way, and editing the graph in another application may change its appearance unpredictably. This is especially true for the rotated Y axis labels.

#### Graph|File|Copy_Data_Points_to_Clipboard item

This option allows you to copy the Windows™ Clipboard, in ASCII format, the data points currently displayed in the Graph window. The data can be copied using one of six different formats. The specific format is chosen using the extended menu item list as shown in Figure 10.6. The table below describes each of the data formats.
**Graph data ASCII formats**

<table>
<thead>
<tr>
<th>Format</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sequential Curves, Data Only</td>
<td>The data for the x and y axes are placed one after another, vertically. If the Graph window displays a double Y axis plot, the third column is the second Y axis value.</td>
</tr>
<tr>
<td>Curves in Columns, Single X-Columns, Data Only</td>
<td>The first column will contain the x axis values and then each column after that will contain the data for one of the curves (y-axis values). If the Graph window displays a double Y axis plot, the second Y axis value is placed in the column next to the first Y axis value.</td>
</tr>
<tr>
<td>Curves in Columns, Multiple X-Columns, Data Only</td>
<td>The first column will contain the x axis values and the second column will contain the data for one of the curves (y-axis values). This is repeated for each of the curves. If the Graph window displays a double Y axis plot, the second Y axis value is placed in the column next to the first Y axis value.</td>
</tr>
<tr>
<td>Sequential Curves, With Headers</td>
<td>The data for the x and y axes are placed one after another, vertically. The legend for each curve appears in the third column where that curve’s data starts. If the Graph window displays a double Y axis plot, the third column is the second Y axis value.</td>
</tr>
<tr>
<td>Curves in Columns, Single X-Columns, With Headers</td>
<td>The first column will contain the x axis values and then each column after that will contain the data for one of the curves (y-axis values). The legend and axis text for each curve appears above the column which contains the curve’s data. If the Graph window displays a double Y axis plot, the second Y axis value is placed in the column next to the first Y axis value.</td>
</tr>
<tr>
<td>Curves in Columns, Multiple X-Columns, With Headers</td>
<td>The first column will contain the x axis values and the second column will contain the data for one of the curves (y-axis values). This is repeated for each of the curves. The legend and axis text for each curve appears above the column which contains the curve’s data. If the Graph window displays a double Y axis plot, the second Y axis value is placed in the column next to the first Y axis value.</td>
</tr>
</tbody>
</table>
Graph|File|Output_Data_Points_to_Text_File item

This option exports the data points into a text file (.txt) using data formats as described for the Graph|File|Copy_Data_Points_to_Clipboard command. You will be asked for the name of the file in which to store the data. If not otherwise specified, the “.txt” extension will be added to the file. Files saved using this command cannot be read in by WVASE®. This command is solely for exporting data to other applications. Do not save experimental data using this command if you want to later use it in WVASE®; instead, use the Exp_Data|File|Save_Exp_Data command.

10.3Graph|Edit menu

Figure 10-7. The Edit menu from the Graph window.

The items on this menu are used to format the appearance of the plot displayed in the Graph window. Many of these formatting options are reset to default values when performing non-Graph window related operations. The ‘Save Graph Setup’ and ‘Apply Graph Setup’ menu items can be used to save and restore specific graph options. The Graph window is tightly integrated with the other WVASE® windows to keep the display current.

Character formatting for Graph|Edit|Titles & Legends

Special embedded character sequences can now be used to control formatting of font (normal and Greek), typeface (bold, italics, and underline), and position (subscript and superscript). The text in the title, axis labels, and legend entries can all use the new embedded formatting controls. The backslash “\" character is used to change a formatting option or to include some specific content.

**Formatting Controls**

<table>
<thead>
<tr>
<th>Format controls</th>
<th>Content shortcuts</th>
</tr>
</thead>
<tbody>
<tr>
<td>\s</td>
<td>symbol</td>
</tr>
<tr>
<td>\n</td>
<td>normal</td>
</tr>
<tr>
<td>^</td>
<td>superscript</td>
</tr>
<tr>
<td>\v</td>
<td>subscript</td>
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<td>b</td>
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<td>i</td>
<td>italics</td>
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</tr>
<tr>
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<td>experimental file name</td>
</tr>
<tr>
<td>c</td>
<td>comment for exp file</td>
</tr>
<tr>
<td>m</td>
<td>model file name</td>
</tr>
<tr>
<td>\</td>
<td>backslash</td>
</tr>
</tbody>
</table>

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Examples:
\[ \psi \text{ and } \Delta \text{ in degrees} \]
\[ \textbf{Bold} \ \textit{Italics} \ \underline{Underline} \]
\[ \textit{Al}_x\text{Ga}_{1-x}\text{As} \ \textbf{c} \ e^{-\alpha} \]

**Arial-Symbol Conversion**

<table>
<thead>
<tr>
<th>a</th>
<th>α</th>
<th>n</th>
<th>ν</th>
<th>A</th>
<th>A</th>
<th>N</th>
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<tbody>
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<td>b</td>
<td>β</td>
<td>o</td>
<td>o</td>
<td>B</td>
<td>B</td>
<td>O</td>
<td>O</td>
</tr>
<tr>
<td>c</td>
<td>χ</td>
<td>π</td>
<td>C</td>
<td>X</td>
<td>P</td>
<td>Π</td>
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<td>d</td>
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<td>q</td>
<td>θ</td>
<td>D</td>
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<td>Σ</td>
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<td>τ</td>
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<td>Y</td>
</tr>
<tr>
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<td>ζ</td>
<td>M</td>
<td>M</td>
<td>Z</td>
<td>Z</td>
</tr>
</tbody>
</table>

**Graph|Edit|Titles item**

This option is used to edit the main title for the plot and the descriptive labels for the X and Y axes. The text for these items change in response to many WVASE\(^6\) actions, so it is advisable not to set these items until you ready to print or export the graph. This option uses a dialog box like that shown in Figure 10.8.

![Graph Titles dialog box](image)

*Figure 10-8. Dialog box presented by the Graph|Edit|Titles command.*

**Title**

This text will be displayed on the graph centered over the plot box. Special characters, including Greek and other symbols, can be used (see Character Formatting section above).
X axis

For 2-D graphs, this text will be displayed on the graph centered under the plot box. For 3-D graphs, this text will be displayed on the left side of the base grid.

Y1-axis

For 2-D graphs, this text will be displayed along the left side Y axis. For 3-D graphs, this text will be displayed along the left side vertical Z axis.

Y2-axis

For double Y axis 2-D graphs, this text will be displayed along the right side Y axis. For 3-D graphs, this text will be displayed on the right side of the base grid.

Scale

The relative scale of these text items can be adjusted using the Scale boxes on the right. Once set, this value will not be automatically reset by other WVASE® actions.

Graph|Edit|Legends item

This option allows you define the legend text, line color, and line style for each plotted curve. Many of these items change in response to many WVASE® actions, so it is advisable not to set these items until you ready to print or export the graph. The desired formats are applied using the Edit Legends dialog box.

Legend

This box list all the curves currently displayed. The legend text and an example of the line style are shown together. This is a multiple selection list box for the purposes of setting the line color and style. This is a single selection list box for the purpose of editing the Legend Text.
Legend text

The text for the highlighted legend row is displayed and can be edited in this text box. Items marked <blank> have no text associated with them, and these items will not be included in the displayed graph legend. The curves themselves will be plotted in the displayed line color and style. Special characters, including Greek and other symbols, can be used (see Character Formatting section above).

Color

The color for the highlighted curve (or curves) is set using this pull down menu of color options.

Style

The line style (dashes and symbols) for the highlighted curve (or curves) is set using this pull down menu of style options.

Scale

This box is used to alter the size of legend text displayed in the graph. Once set, this value will not be automatically reset by other WVASE® actions.

Black default legends

This check box allows you to change the default display of the legend. The standard mode of operation (checked) is assumed throughout this manual. When this box is unchecked, different text and line styles are used as the default values. Once set, this value will not be automatically reset by other WVASE® actions.

Suppress legend display

This check box allows you to prevent the legend text and line style from being drawn on the graph. In some cases, the legend may become very large or it may always be covering some region of interest, so it is useful to suppress it. Once set, this value will not be automatically reset by other WVASE® actions.

Graph|Edit|Font item

This option is used to select the font used to draw titles, legends, and numbers in the Graph window. Under most circumstances, a True Type™ font such as “Arial” is preferred. However, if the final output device is a plotter, you might choose a more compatible vector-based font such as “Modern.” The font is chosen from the list of all available fonts using the Graphics Font dialog box. You can use the Windows™ Control Panel to find out which fonts are True Type™.

Figure 10-10. Font selection dialog box used by the Graph|Edit|Font menu item.
Graph|Edit|Scale item

This menu item is used to modify axis scaling and numeric displays of plots in the Graph window. These items are set in the dialog box displayed in Figure 10.11.

![Graph Scale dialog box](image)

Figure 10-11. Graph Scale dialog box used by the Graph|Edit|Scale command.

**X column**

The items associated with this column are used for the horizontal axis on 2-D plots and the lower left axis on 3-D plots.

**Y1 column**

The items associated with this column are used for the left vertical axis on 2-D plots and the vertical axis on 3-D plots.

**Y2 column**

The items associated with this column are used for the right vertical axis on 2-D plots and the lower right axis on 3-D plots.

**Automatic**

When this option is selected for a given axis, the scaling of the axis is done automatically.

**Manual**

When this option is selected for a given axis, manual values can be entered for the plot. When new data is generated by the Gen_Data|Generate_Data command or as the result of a fit, the manual setting is temporarily overridden and new autoscaled values are placed in the edit boxes. If you change the displayed data using the Graph|Data or Graph|Type menus, the manual range settings may become confused. Typically it is best to use manual scaling only when you are preparing a final graph for printing or exporting.

**Reset**

This button sets all the axes back to automatic scaling mode, returns the check boxes to their default values, and dismisses the dialog box.
**Minimum**

This is value at the left end (X axis) or at the bottom end (Y axis) of the corresponding axis.

**Maximum**

This is value at the right end (X axis) or at the top end (Y axis) of the corresponding axis.

**# of divisions**

This is the number of segments that will be separated by major tick marks along the corresponding axis.

**Precision box**

This box allows you to define how many digits will be displayed right of the decimal point for the numeric labels. A numeric label will be placed next to each major tick mark. To display only integer values use “0.f”. To display 3 digits to the right of the decimal point use “3.f”

**Scale box**

This box is used to alter the size of the numeric labels placed next to the major tick marks. Once set, this value will not be automatically reset by other WVASE® actions.

**Grid lines vertical**

When this box is checked the graph will include vertical grid lines for the major tick marks on the X axis. Once set, this check box will not be automatically reset by other WVASE® actions.

**Grid lines horizontal**

When this box is checked the graph will include horizontal grid lines for the tick marks on the left side Y axis. Once set, this check box will not be automatically reset by other WVASE® actions.

**Tick marks**

These check boxes allow you to turn the display of tick marks on and off for the corresponding axis. Once set, these check boxes will not be automatically reset by other WVASE® actions.

**Log scale on Y-axis OR Log scale on X-axis**

This check box allows you to plot log₁₀(Y) and/or log₁₀(X) values instead of the normal Y and X values. This option may not function properly if some of the displayed Y values are zero or negative.

**Graph|Edit|Save_Graph_Setup**

This menu item is used for saving different formatting options that define the graph. The dialog that appears is shown in Figure 10.12. By splitting the options into groups, one can create templates which can be applied to different data sets. For instance, by using only the first three options, one could create a setup file to set the wavelength units (Global|Defaults menu), switch to Experimental Only data...
(Graph|Data menu) presented in <e1>-<e2> form (Graph|Type menu), make the graph have two y-axes (Graph|Options|2D menu option). The remaining options (Graph|Edit|Titles, Graph|Edit|Scaling, and Graph|Edit|Legends menu options) would be set as defaults. If one was trying to create a “final” graph with custom titles, scaling, and legends, then all 6 groups could be selected to get the exact same graph back assuming the same data was selected.

![Graph Save Setup dialog](image)

*Figure 10.12. The Graph Save Setup dialog.*

**Graph|Edit|Apply_Graph_Setup item**

This menu item is used for applying a previously saved graph format to the currently displayed graph. When a graph setup file is applied to a graph, essentially the same dialog box shown in Figure 10.12 is used to define which of the graph formatting options will be applied. Even if an entire graph format was defined when saved, it is possible to apply only those sections desired.

### 10.4 Graph|Data menu

![Data menu](image)

*Figure 10-13. The Data menu from the Graph window.*

This menu is used to select the class of data to display. These classes include measurement data, optical constants, fit parameters, and calibration data. The currently selected menu item has a check mark next to it on the menu.

**Generated and/or experimental data types**

The first four items on the Graph|Data menu are used to display one of the measurable data types (ellipsometric, transmission, reflection). The data for these graphs come from the Experimental Data and/or Generated Data windows. The
specific type of data displayed comes from the selected item on the Graph|Type menu.

**Generated and experimental**

This option will graph data from the Experimental Data window and the Generated Data window. The specific type of the data is set using the Graph|Type menu.

**Difference between gen. and exp.**

This option will graph the difference between data stored in the Generated Data window and the Experimental Data window (Gen. minus Exp.). The specific type of data is set using the Graph|Type menu. If the data wavelengths and angles in the Generated Data window do not exactly match those in the Experimental Data window, then it is possible nothing will be displayed. If the Generated Data window has been filled using the Gen_Data|Generate_Data command or by a fit procedure, the wavelengths and angles will automatically be matched. If the Generated Data window was filled by opening a file (Generated Data|File) then that file should match exactly the experimental list of wavelengths and angles of incidence.

**Generated only**

This option will graph data from the Generated Data window only. The specific type of the data is set using the Graph|Type menu.

**Experimental only**

This option will graph data from the Experimental Data window only. The specific type of the data is set using the Graph|Type menu.

**Optical constant data types**

The next four items on the Graph|Data menu allow you to display optical constants in the Graph window. The data for these graphs come from the layers displayed in the Model window. The wavelengths used for graphing the optical constants come from the combined set of wavelengths of all selected data points (Exp_Data|Range_Select) in all of the models which will be included in the data fitting process (Model|Select).

**Current layer (opt. const.)**

This option will graph optical constants for the current layer in the Model window. This layer is indicated by the > symbol on the left side of the Model window (see Model Window Overview).

For anisotropic layers, the exact configuration of the plots depend upon the Tensor Display Mode configuration (see Tensor Display Mode).

**All layers (opt. const.)**

This option will graph optical constants for all layers in the current model. This is a useful way to compare the optical constants of different materials.

**Depth profile (opt. const.)**

This option will graph optical constants as a function of position relative to the substrate at a single wavelength. This menu option brings up a dialog box for
you to set the desired wavelength. For examples of depth profiles see Model|AddLayer, Composite Layers, Graded Layer.

The optical constants will either be parts of the complex dielectric function, \( \tilde{\varepsilon} = \varepsilon_1 + i\varepsilon_2 \), or parts of the complex refractive index, \( \tilde{n} = \sqrt{\varepsilon} = n + ik \). The display setting is established using the [Global]Defaults command. Selecting this option causes the following dialog box to be displayed.

![Optical Constants Graph](image)

Figure 10-14. Dialog box used to select the optical constants to be displayed.

In this dialog box ‘n’ refers to the real part of the optical constant (\( n \) or \( \varepsilon_1 \)) and ‘k’ refers to the imaginary part of the optical constant (\( k \) or \( \varepsilon_2 \)). The absorption coefficient will cause the intensity absorption coefficient to be displayed. The intensity absorption coefficient is defined as \( 2\pi \times \text{extinction coefficient} / \text{wavelength} \), and has units of cm\(^{-1}\). If the layer has anisotropic optical constants, the extraordinary optical constants can be displayed by checking the Graph Anisotropic box.

The ‘Depth Profile’ feature also correctly plots the behavior of the intermix and graded intermix layers (intermix2.mat). The figures below show a model and its index profile at 500nm. Note that the horizontal lines indicate the thickness of the 15nm plymid_c.mat and 20nm ito.mat, while the sloping line shows the 5nm grading of the interface.

![Depth Profile of Optical Constants at 500nm](image)

Figure 10-15. Dialog box used to select the optical constants to be displayed.

**Tensor Display Mode**

This option is applicable to models with one or more anisotropic layers. It specifies which elements optical constants tensors are plotted for the Current layer (Opt. Const.), All layer (Opt. Const.) and Depth Profile.

In its most general form, a layer’s electromagnetic properties can be described in terms of the \( E, H, D & B \) fields, as described by these constitutive relations

\[
D = \varepsilon_0 E + c^{-1} \gamma H \\
B = c^{-1} \zeta E + \mu \mu_0 H
\]  

(10.1)
For most materials at optical frequencies $\mu = 1$, & $B = \mu_0 H$. Therefore, we only describe the electric field parts, $D$ & $E$. The cross coupling term $\gamma$ (Gamma) couples the magnetic field $H$ to the electric-displacement field $D$, and $\zeta$ (Zeta) couples the electric field $E$ to the Magnetic flux field $B$.

In their most general forms, $\varepsilon$, $\mu$, $\gamma$ and $\zeta$ are anisotropic, so they become tensor quantities:

$$
\tilde{D} = \varepsilon_0 \begin{bmatrix} 
    \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\
    \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\
    \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} 
\end{bmatrix} \tilde{E} + \frac{1}{c} \begin{bmatrix} 
    \gamma_{xx} & \gamma_{xy} & \gamma_{xz} \\
    \gamma_{yx} & \gamma_{yy} & \gamma_{yz} \\
    \gamma_{zx} & \gamma_{zy} & \gamma_{zz} 
\end{bmatrix} \tilde{H}
$$

(10.2)

$$
\tilde{B} = \frac{1}{c} \begin{bmatrix} 
    \zeta_{xx} & \zeta_{xy} & \zeta_{xz} \\
    \zeta_{yx} & \zeta_{yy} & \zeta_{yz} \\
    \zeta_{zx} & \zeta_{zy} & \zeta_{zz} 
\end{bmatrix} \tilde{E} + \begin{bmatrix} 
    \mu_{xx} & \mu_{xy} & \mu_{xz} \\
    \mu_{yx} & \mu_{yy} & \mu_{yz} \\
    \mu_{zx} & \mu_{zy} & \mu_{zz} 
\end{bmatrix} \tilde{H}
$$

In a more compact form:

$$
\begin{bmatrix} 
    \tilde{D} \\
    \tilde{B} 
\end{bmatrix} = \begin{bmatrix} 
    \varepsilon_0 \varepsilon & \gamma / c \\
    \zeta / c & \mu_0 \mu 
\end{bmatrix} \begin{bmatrix} 
    \tilde{E} \\
    \tilde{H} 
\end{bmatrix} = \tilde{\epsilon}_{eff} \begin{bmatrix} 
    \tilde{E} \\
    \tilde{H} 
\end{bmatrix}
$$

(10.3)

- **Full Rotate Tensor**: When selected, all nine elements of the specified tensor for the anisotropic layer will be plotted. When not selected, only the three elements of the diagonalized tensor are plotted. This selection does not affect the display of isotropic layer optical constants.

- **Dielectric Tensor Show**: $\varepsilon_0$ ($\tilde{\varepsilon}$), is the familiar 3x3 dielectric tensor, multiplied by $\varepsilon_0$. $\varepsilon = \varepsilon_1 - i\varepsilon_2$

- **Magnetic Tensor Show**: $\mu_0$ ($\tilde{\mu}$), 3x3 magnetic susceptibility tensor multiplied by $\mu_0$. $\mu = \mu_1 - i\mu_2$

- **Gyrotopic Gamma Tensor Show**: $\gamma$ ($\tilde{\gamma}$), 3x3 gyrotopic tensor multiplied by $1/c$. $\gamma = \gamma_1 - i\gamma_2$

- **Gyrotopic Zeta Tensor Show**: $\zeta$ ($\tilde{\zeta}$), 3x3 gyrotopic tensor multiplied by $1/c$. $\zeta = \zeta_1 - i\zeta_2$

**Point by point fit parameters data type**

This option will cause the fit parameters from the most recent point-by-point fit to be displayed. You can also graph the fit confidence limits for the selected fit parameter. There are three typical applications for this data class: (1) displaying wavelength-by-wavelength fit parameter confidence limits for optical constants, (2) displaying time-by-time fit parameters and confidence limits from fits to dynamic data, and (3) displaying channel-by-channel calibration parameters and confidence limits after calibrating an $M$-$XX$ system.
Calibration data type

This option will display the acquired and modeled data from the most recent calibration. The data displayed using this option will be graphed as a function of input polarizer setting.

10.5 Graph|Type menu

The ‘Type’ menu is used to select the form in which the experimental and/or generated data will be plotted. Recall that ellipsometric data may be equivalently specified in a number of different ways (psi and delta, rho, pseudo-optical constants). WVASE® allows you to view the data in many different ways by selecting the desired data type from this menu.

![Figure 10-16. The Type menu from the Graph window.](image)

When generated and/or experimental data is displayed (see Graph|Data), this menu is used to select which of the data type(s) will be displayed. The currently selected type has a check mark next to it. For more information on the definition of the ellipsometric parameters see chapter 2 - “A Short Course in Ellipsometry.”

Displayable data types

There are a number of different data types to which the experimental and generated data may be converted to for display.
**Psi**
Displays the ellipsometric parameter $\psi$.

**Delta**
Displays the ellipsometric parameter $\Delta$.

**Tan(Psi)**
Displays the quantity $\tan(\psi)$.

**Cos(Delta)**
Displays the quantity $\cos(\Delta)$.

**<e1>**
Displays the real part of the pseudodielectric function calculated from the data in the Experimental data window.

**<e2>**
Displays the imaginary part of the pseudodielectric function calculated from the data in the Experimental data window.

**<n>**
Displays the real part of the pseudo refractive index calculated from the data in the Experimental data window.

**<k>**
Displays the imaginary part of the pseudo refractive index calculated from the data in the Experimental data window.

**Re(rho)**
Displays real part of ellipsometric parameter $\rho$. $\text{Re}(\rho)=\tan(\psi)\cos(\Delta)$.

**Im(rho)**
Displays imaginary part of ellipsometric parameter $\rho$. $\text{Im}(\rho)=\tan(\psi)\sin(\Delta)$.

**cos(2*Psi)**
Displays $\cos(2\psi)$, which is equivalent to ‘N’ in NCS notation.

**sin(2*Psi)cos(Delta)**
Displays $\sin(2\psi)\cos(\Delta)$, which is equivalent to ‘C’ in NCS notation, and $C = \frac{2\text{Re}(\rho)}{1+|\rho|^2}$.

**sin(2*Psi)sin(Delta)**
Displays $\sin(2\psi)\sin(\Delta)$, which is equivalent to ‘S’ in NCS notation, and $S = \frac{2\text{Im}(\rho)}{1+|\rho|^2}$.

**Transmission**
Displays intensity transmission data.

**Reflection**
Displays intensity reflection data.

**Absorption**
Displays absorption values which are derived from reflection and transmission data. Both reflection and transmission data must be present at the same wavelength, angle of incidence, and polarization to calculate absorption.

**Transmitted phase**
Displays the transmitted sample phase. See chapter 6 - “The Experimental Data Window” for details on this data type.

**Depolarization**
Displays %depolarization data if it was acquired. A VASE with an Auto-Retarder or an M-2000 instrument is necessary to acquire the data. See the Hardware chapter for information on acquiring %depolarization data.

**Jones Matrix Quality**
Displays the ‘$q_j$’ data type, which is a quantitative measure of how closely experimental Mueller matrix data can be described by a Jones matrix. Only available for Mueller Matrix measurement data types. Contact the Woollam Co. for details.

**Neutron reflectivity**
Displays the neutron reflection data type. See chapter 6 - “The Experimental Data Window” for details on this data type.

**R*^k^4**
This data type is calculated from the neutron reflectivity data as the reflectivity multiplied by the neutron momentum raised to the fourth power. See chapter 6 - “The Experimental Data Window” for details on this data type.
10.6 Graph|Style menu

This option opens a dialog box as shown in Figure 10.17.

**Double Y-axis**

This check box allows WVASE® to display two Y axes when displaying experimental and/or generated data. The double Y axis display works with the following data type pairs: \((\psi \text{ and } \Delta)\), \((\tan \psi \text{ and } \cos \Delta)\), \((<\varepsilon_1> \text{ and } <\varepsilon_2>)\), \((<n> \text{ and } <k>)\), \((\text{Re}(\rho) \text{ and } \text{Im}(\rho))\), and \((\text{Trans. and Refl.})\). If the first data type of one of these pairs is the currently displayed data type and the Double Y-axis box is checked, then both data types will be displayed. (One potentially confusing behavior involving intensity transmission data is known. If transmission data is selected but there is no corresponding reflectivity data to display, the transmission data will not be displayed because the Y2 axis cannot be scaled.) The following graph (Figure 10.18) illustrates a double Y axis graph showing \(\psi\) and \(\Delta\) data.

**Graph as a function of angle**

Check this box if you want to display data as a function of the angle of incidence. Normally data is only displayed as function of wavelength or time.
**Trajectory plot**

This plotting option is only used with dynamic data. This plotting option produces a time dependent parametric curve which plots one data type versus another. The data pairs described in the Double Y-axis section are plotted against one another. The trajectory graph in Figure 10.19 was produced from a time dependent data file at 546 nm with $\psi$ as the selected data type. Multiple wavelength trajectories can be plotted on the graph.

![Generated and Experimental Data](image)

*Figure 10-20. Example of a trajectory plot of $\psi$ and $\Delta$ at wavelength of 546 nm.*

**Plot derivatives**

Checking this box causes a modeled derivative of the selected data to be plotted instead of the usual data. The derivative order is selected from ‘Order’ pull down box. (An Order of 0 can be used to smooth the displayed data.) The derivative is calculated by locally fitting a polynomial to the normal data centered about the point of interest. The number of data points used to display the data is set by the ‘# of Points’ box. The degree of the fitting polynomial is set by the ‘Polynomial Degree’ box. The # of Points box should always be at least as large as the Polynomial Degree, which in turn should be at least as large the derivative Order. The fitting polynomial uses only data that would normally be displayed in the graph, and therefore edge effects can occur where the best fit polynomial can no longer be centered about the data point.

**Graph|Style|3D item**

This option opens a dialog box as shown Figure 10.20.

*Figure 10-21. Dialog box of 3-D graphing options.*

The following items are present in this dialog box.

**Elevation**

This is used to set the viewing perspective with respect to the base X-Y plane. A larger value puts the viewing point higher above the base plane.
Reverse axis

The X check box will cause the numeric values of the X axis to be displayed in a reversed order. Likewise, the Y check box will cause the numeric values of the Y axis to be reversed. There is no option for interchanging the X and Y axes.

Contours on Surface

If this box is checked then contours will be displayed on the graph mesh in either color or gray scale depending on whether Colors or Grays is selected (see below).

Colors OR Grays

If Colors is selected the 3-D graph will be displayed using a black grid mesh with color inside the mesh section. The color indicates the height in a fashion similar to a contour plot. If Grays is selected, the display will be a simple black grid with shades of gray inside the mesh section. Contours on Surface must be check in order for this to have an effect.
Chapter 11 The Fit Window

11.1 Fit window overview

The Fit window is used to fit the optical model to the experimental data.

When the Fit window is active, you have access to the various menubar items that perform and control the data fitting process. The Fit window itself displays the fit parameter values from the last fit procedures. The results of calibration fit procedures are also displayed in this window.

The concepts involved with fitting the data to obtain the parameters of interest is discussed in chapter 2 - “A Short Course in Ellipsometry”. This section covers the specific WVASE® actions used to perform the fit and examine the fit results. Without going into great detail in this section, the following items are assumed to exist:

- A set of selected experimental data which is to be fit. (see Exp_Data|Range_Select)
- A model (or models) which is used to generate data for comparison with the experimental data.
- A set of model fit parameters which can be varied by the fitting algorithm to change the generated data.
- A value called the MSE which in some way measures how close the experimental and generated values are.

The data fitting is performed using the iterative Marquardt-Levenberg fitting algorithm. This algorithm is designed to minimize the MSE by varying the model fit parameters. When a fit is completed, the fit parameters from the iteration that achieved the best (lowest) MSE are displayed in the Fit window and stored in the model.

Features displayed in the Fit window

![Figure 11-1. A Fit window after a normal fit.](image)

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**Title bar**

For the Fit window, the title bar always contains “Fit”.

**Final**

This word above the numbers indicates that these are the final results of the last fitting process.

**MSE**

This is the parameter which is being minimized during the fitting process. When fitting ellipsometric data this value is defined as

\[
MSE = \sqrt{\frac{1}{2N-M} \sum_{i=1}^{N} \left[ \left( \frac{\psi_{i} \text{mod} - \psi_{i} \text{exp}}{\sigma_{\psi_{i}}} \right)^{2} + \left( \frac{\Delta \text{mod} - \Delta \text{exp}}{\sigma_{\Delta_{i}}} \right)^{2} \right]}.
\]

The number of measured \( \psi \) and \( \Delta \) pairs is \( N \), and the total number of real valued fit parameters is \( M \).

**Parameter names and values**

In Figure 10.1, only one parameter “Thick.1” was fitted and its final value was 319.29Å. The estimated error bar on Thick.1 was 0.16Å. Then the fit process was completed, this fit value was transferred to model layer #1.

**Init**

This word above the numbers (Figure 10.2) indicates that these are the starting values for the current normal fitting process.

**Iter**

The fitting process is iterative and this column displays the results for the most recent fit iteration. The goal of the fitting process is reduce the MSE, however, not all iterations produce a better result (lower MSE) than the previous iteration. When the fit process ends, the results of the iteration that achieved the lowest MSE will be inserted as the final results.

**<Esc> exits**

This tells you that the current fit process can be interrupted by pressing the <Esc> key. The interrupt will occur after the next iteration is finished. For some large scale fits, it make take some time for the next iteration to be completed.

**The Fit window menubar**

As shown below, there are eight items on the main menubar plus the Window and Global menus.
The general functions of these menubar items is given in the following table. The specific actions which result when these items are selected will be described in the succeeding sections.

<table>
<thead>
<tr>
<th>Menu</th>
<th>Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fit</td>
<td>File</td>
</tr>
<tr>
<td>Fit</td>
<td>Normal_Fit</td>
</tr>
<tr>
<td>Fit</td>
<td>Pt_by_Pt</td>
</tr>
<tr>
<td>Fit</td>
<td>Reset</td>
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<tr>
<td>Fit</td>
<td>Edit_Parms</td>
</tr>
<tr>
<td>Fit</td>
<td>Studies</td>
</tr>
</tbody>
</table>

**Fit parameter naming conventions**

Every parameter that appears in the Fit window has its own name. This name allows you to distinguish the various parameters during and after the fit process. There are many different parameters, but the names are usually similar to the description of the fit box that was used to select it. Since most fit parameters are associated with a particular layer in a particular model, most fit parameters will end in “.N” or “.N.M” where N is the layer number and M is the model number. If the parameter is from model #1, the “.1” indicating the model is not included. If the fit parameter is accessed from the Model Options dialog (Model|Options), then the fit parameter will end with a “-M” where M is again the model number. The following illustrates the naming conventions for some of the standard fit parameters.

**Thickness**

In the Fit window, a thickness from model #1 is designated “Thick.N” where N is the layer number. A thickness from one of the other models is designated “Thick.N.M”, where N is layer number and M is the model number. For example “Thick.2” represents the thickness of layer #2 in model #1 and “Thick.-1.3” represents the thickness of layer #1 in model #3.

**Angle**

Angles are an exception to the standard parameter naming convention. Since angles are associated with a model, as opposed to an individual layer, their
notation does not specify a layer number (there is no period). Further more, 
WVASE® only keeps track of one set of angles for all of the models. For example, if 
the data for model #1 was acquired at 65° and 75° and the data for model #2 was 
acquired at the same angles, then only one set of angles appears in the “Experimental 
Angles of Incidence” dialog (Model|Angles or Exp_Data|Angles). Setting the 65° 
angle as a fitting parameter will cause the 65° in both models to be fit. In the Fit 
window, an angle is designated “AngleX” where X is an integer which represents the 
position of the angle in the “Experimental Angles of Incidence” dialog. If the data 
were acquired at two angles then the angles are labeled “Angle0” and “Angle1”.

**Optical constants**

In the Fit window, optical constants are designated according to the type of 
optical constants as set using the [Global|Defaults] command. If the complex 
refractive index mode is selected (n & k), the real and imaginary parts of the optical 
constants are designated as “n.Wvl.N” and “k.Wvl.N”, where N is the layer number 
and Wvl is the wavelength. The wavelength is expressed in the current wavelength 
units (see [Global|Defaults]). If the optical constant is for a layer in a model other 
than #1, then an additional “.M” extension is used where M is the model number. If 
the complex dielectric constant mode is selected (ε1 & ε2), the real and imaginary 
parts of the optical constants are designated in a similar way as “ε1.Wvl.N” and 
“ε2.Wvl.N”. For example the real part of the refractive index at a wavelength of 
5000Å for layer #2 of model #1 would be designated as “n.5000.2”, and the 
imaginary part of the dielectric constant at a photon energy of 4.4eV for layer #0 of 
model #3 would be designated as “ε2.4.4.0.3”.

**Cauchy parameters**

The Cauchy optical constants layer is commonly used to model transparent 
materials. The parameters describing the index dispersion are labeled “An”, “Bn”, 
and “Cn” in the layer edit dialog box. As might be expected, the corresponding 
descriptions in the Fit window begin with “An”, “Bn”, “Cn”. The parameters 
describing the exponential absorption tail are labeled “Amplitude” and “Exponent” 
in the layer edit dialog box. The corresponding descriptions in the Fit window are 
“Ak” and “Bk”. Note the only difference is the “n” versus the “k” indicating the 
difference between the real and imaginary parts of the Cauchy layer model.

**EMA layer fraction**

When the component fraction of material #2 in an EMA layer is set as fit a 
parameter, the name that appears in the Fit window is “EMA%2” with the 
appropriate “.N” and “.M” attached.

**Fitting optical constants at every wavelength**

WVASE® determines at which wavelengths optical constants are needed by 
examining all selected experimental data points in all Experimental Data windows 
which are active in the current fit. When multiple experimental data sets are being 
analyzed, it may be important that the component files use exactly the same 
wavelengths when spectral ranges overlap. For instance, if you are combining 
transmission data with ellipsometric data for the purpose of determining optical 
constants, then it is very important that the wavelengths match identically. Such 
problems may occur when combining data from different measurement tools, or 
when combining a file acquired as a function of wavelength with a file acquired as a 
function of photon energy.
Consider two problem cases: 1) transmission data exists but ellipsometric data does not exist for a given wavelength, or 2) transmission data does not exist for one wavelength but does exist for wavelengths on either side. For case 1, WVASE® will try and fit real and imaginary parts of the optical constants at a wavelength where it has only one measured transmission data point. In this case there would be two fit parameters, one measured value, and the fitted values would not be meaningful. For case 2, the middle wavelength which has only ellipsometric data, may fit to optical constants which are out of line with respect to other wavelengths which have additional transmission data. This may create “noise” in the resulting optical constants which is only due to the lack of transmission data at some wavelengths.

To overcome difficulties associated with different experimental files having slightly different wavelength values, there are several different approaches that can be used:

- Replace one or more of the experimental files with newly acquired data using a compatible set of wavelengths.
- Edit one of the data files to remove the conflicting or unmatched data points.
- Interpolate between the data points in one file onto a new grid of compatible wavelengths.
- Use functional optical constant models like the Cauchy, Lorentz, or User layers which do not require optical constants to be fit at every wavelength.

Remember, if you are fitting only optical constants, then at different wavelengths those optical constant fit parameters are totally independent.

### 11.2 Fit|File menu

**Figure 11-4. The File menu from the Fit window.**

**Fit|File|Copy_to_Clipboard item**

This option copies the final fit parameters and confidence limits to the Windows™ Clipboard as text. From there the information can be pasted into other applications. The exported text contains the fit confidence limits as well as the parameter values.
11.3 Fit|Normal_Fit menu

![Figure 11-5. The Normal Fit option from the Fit window.]

**Fit|Normal_Fits|Normal_Fit item**

This menu item starts the iterative Marquardt-Levenberg fitting algorithm. The normal fit is distinguished from a pt-by-pt fit in that a normal fit works with all the selected data simultaneously. A pt-by-pt fit, on the other hand, works the selected data on a wavelength-by-wavelength (spectroscopic data) or on a time-by-time (dynamic data) basis.

The fit parameters and MSE for each iteration will be displayed in the Fit window. The Graph window will also be updated with the new generated data unless that option is disabled. A normal stop to the fit process will occur when one of the following three criteria is met.

- The maximum allowed number of iterations has been exceeded.
- The MSE has become lower than some absolute lower limit.
- The last improvement in the MSE was lower than some relative limit.

These limits are set using the Fit|Defaults menubar item. If the maximum number of iterations is exceeded, WVASE® will simply stop the fit and set the final values to the results from the best iteration. If the fit stops due to one of the other two limits the following message box will be displayed.

![Figure 11-6. Message box when an MSE limit has been exceeded during a fit.]

You can also intervene and stop the fitting process early pressing the <Esc> during a fit.

There are two error conditions which may occur and stop a fit prematurely, a singular matrix error and a floating point error. A singular matrix error almost always means that there is no sensitivity to one or more of the fit parameters. If changing one of the fit parameters does not change any of the generated data values, there is no sensitivity to that parameter. This may be an obvious statement, but you can not fit for the value of parameter when the data has no sensitivity to that parameter. If you are convinced that the fit should be sensitive to all of the selected fit parameters, you might try increasing the derivative increment value using the Fit|Defaults menu item. The default value generally works very well, so change this value only as a last resort. If the derivative increment has at sometime been set to zero then every fit attempt should produce a singular matrix error.
A floating point error usually means that WVASE® has attempted to divide by zero or that it has attempted to take the square root of a negative number. There are no very common ways of producing this error. If you are trying to track down the source of this error, you might look for very thick absorbing layers or for a model where all the layers have a refractive index of approximately \( n=1 \).

**Fit|Normal_Fits|Defaults item**

The Fit|Defaults command is used to select the weighting for the experimental data and to set the control limits for ending the fit process.

**The fit defaults dialog box**

The Fit|Defaults command will bring up the Fit Defaults dialog box.

![Fit Defaults dialog box](image)

*Figure 11-7. The Fit Defaults dialog box.*

The following items are visible in this dialog box.

**Fit weighting**

This is the weighting type used when calculating the MSE for ellipsometric data. Exactly, one item on this list will always be selected (highlighted). The exact weighting scheme is described in detail later in this section.

**R&T weighting**

For experimental transmission and reflection, this is the weighting used relative to that used for ellipsometric data. Setting these values greater than 100% will increases the importance of reflection/transmission data in a fit relative to ellipsometric data. Setting these values less than 100% will reduce the importance of reflection/transmission data. Do not set these values to 0%, because that is likely to produce a floating point error. The exact weighting scheme is described in detail later in this section.

**Maximum iterations**

This box sets the maximum number of fit iterations that will be attempted for a normal fit or for a single point of a point-by-point fit.
**Minimum MSE**

This box sets an absolute minimum for the MSE. If the MSE for a fit iteration falls below this value, the fit process will end.

**Change in MSE**

This box sets a relative limit for improvements of the MSE. If the MSE improves and the fractional improvement is less than the value in this box, the fit process will end.

**Derivative increment**

This is a control setting used to calculate numerical derivatives of modeled data with respect to the fit parameters. The default value of 0.001 works very well for most situations. If you are receiving many singular matrix errors messages that you cannot trace to improperly-defined fit parameters then you might try increasing this value to 0.01. Do not set this value to 0, as that will guarantee a singular matrix error.

**Singular Matrix Handling**

This box selects the method of handling singular matrix errors when they occur during a data fit. The default, “End Fit”, is to stop the fit, reporting the error. Another option, “End Fit, Find Problem”, stops the fit when a singular matrix is encountered and then performs a subsequent analysis to determine which parameter(s) is causing the problem. The third option, “Continue, Alternate Mode”, allows the fit to continue using a more rugged but slower matrix handling algorithm.

**Parameter Formatting (Significant Figures)**

Selecting the ‘Parm Formatting>>’ button in the Fit Defaults dialog box allows the user to independently select different significant figures for the general fit parameters (non-thickness parameters), FOM (error-bars), and thickness. Note that the Thickness Decimal Pts are always set in Angstrom (Å) units.

![Fit Parameter Formatting dialog box.](image)

In the fit window shown below, the Thick.2 units are nm. The Thickness Decimal Pts = -1 (Å), which is 0 decimal places for nm units. Therefore, Thick.2 is reported as “23 nm”. The significant figures for the non-thickness parameter Angle0 (angle of incidence) is 5, while the significant figures for the FOM (error bars) is 1.
Weighting of ellipsometric data

The user can choose any of the various fit-weighting schemes by selecting the Fit|Normal_Fit|Defaults to open the Fit Defaults dialog box (see figure below). For all these schemes, the $MSE$ describes how closely the generated data matches the experimental data.

\[ \text{MSE} = \frac{1}{N-M} \sum (\phi - \phi_0)^2 \]

where $N$ is the number of measured pairs of $\phi$ and $\Delta$. In most cases, $N$ equals the number of measured wavelengths times the number of measured incident angles.

$MSE_0$ is calculated from the same equations as $MSE$, except that $M = 0$ when $MSE_0$ is calculated.

In the equations below, the $MSE$ is always normalized with respect to the number of free parameters; that is, the number of measured values ($N$ or $2N$) minus number of fit parameters ($M$). $N$ is the number of measured $\phi$-$\Delta$ pairs. In most cases, $N$ equals the number of measured wavelengths times the number of measured incident angles.

The Fit|Fit_Studies|MSE and Fit|Fit_Studies|Uniqueness_Fit commands return the $MSE$ and the $MSE_0$ values. $MSE_0$ is calculated from the same weighting equations as $MSE$; except that $M$ – the number of fit parameters – is set equal to 0 for the $MSE_0$ calculation. For example, the normalization prefactor in Eq. (1) below would be $(2N)^{-1}$ instead of $(2N-M)^{-1}$.

For a given model, $MSE$ and $MSE_0$ are independent of which parameters are currently fit parameters.

Experimental & Standard Deviation

This is the WVASE® default mode, and it calculates the $MSE$ by weighting the ellipsometric data with the standard deviations displayed in the Experimental Data window.
The MSE is calculated using

$$\sqrt{\frac{1}{2N-M} \sum_{j=1}^{N} \left[ \frac{(\psi_{j}^{\text{mod}} - \psi_{j}^{\exp})^2}{\sigma_{\psi_{j}}^2} + \left(\Delta_{j}^{\text{mod}} - \Delta_{j}^{\exp}\right)^2 \right]}.$$  \hspace{1cm} (11.2)$$

If the ellipsometric data was acquired using a VASE®, IR-VASE® or M-2000® system, the standard deviations were calculated from the known error bars on the calibration parameters and the fluctuations of the measured data over the averaged cycles of the rotating analyzer. If the ellipsometric data file contained no standard deviations, then WVASE® used the default standard deviation model. In the above equation, \(N\) is the number of measured \(\psi - \Delta\) pairs being included in the fit and \(M\) is the number of fit parameters. This equation has \(2N\) in the prefactor because there are two measured values included in the calculation for each \(\psi - \Delta\) pair.

The statistical significance of measuring and using accurate standard deviations is described at length in chapter 2 - "A Short Course in Ellipsometry". However, for the purposes of this section, you only need to understand that the standard deviations will be larger when the experimental data is noisier, which usually occurs in spectral regions where the arc lamp exhibits low output or the sample exhibits very low reflectance. Thus, noisier regions will contribute less to the MSE because the larger standard deviation appears in the denominator.

WVASE® supports other weighting schemes for ellipsometric data that have other uses. The MSE is still calculated from the experimental data, but the exact weighting depends on the Fit Weighting selected.

**Psi and delta**

The MSE is calculated using \(\psi\) and \(\Delta\) values, but the standard deviation is assumed to 1 for all measured values. Compared to the Experimental Standard Deviations mode, this mode tends to weight \(\Delta\) values more heavily relative to the \(\psi\) values, and the measured values are uniformly weighted across the measured spectral range.

$$\sqrt{\frac{1}{2N-M} \sum_{j=1}^{N} \left[ \frac{(\psi_{j}^{\text{mod}} - \psi_{j}^{\exp})^2}{1} + \left(\Delta_{j}^{\text{mod}} - \Delta_{j}^{\exp}\right)^2 \right]}.$$  \hspace{1cm} (11.3)$$

**Tan(Psi) and cos(Delta)**

The MSE is calculated with respect tan(\(\psi\)) and cos(\(\Delta\)). This may be done to compare fit results from WVASE® with results from other published fits.

$$\sqrt{\frac{1}{2N-M} \sum_{j=1}^{N} \left[ \left(\tan\psi_{j}^{\text{mod}} - \tan\psi_{j}^{\exp}\right)^2 + \left(\cos\Delta_{j}^{\text{mod}} - \cos\Delta_{j}^{\exp}\right)^2 \right]}.$$  \hspace{1cm} (11.4)$$

**Psi only**

In this mode, the MSE is calculated using only the \(\psi\) values.

$$\sqrt{\frac{1}{N-M} \sum_{j=1}^{N} \left(\psi_{j}^{\text{mod}} - \psi_{j}^{\exp}\right)^2}.$$  \hspace{1cm} (11.5)$$
Cos(Delta) only

In this mode, the MSE is calculated using only cos(Δ) values.

\[ MSE = \sqrt{\frac{1}{N-M} \sum_{j=1}^{N} \left( \cos(\Delta_j^{\text{mod}}) - \cos(\Delta_j^{\text{exp}}) \right)^2}. \] (11.6)

<ε₁> and <ε₂>

In this mode, the MSE is calculated using the derived pseudo dielectric values, which are

\[ \langle \tilde{\varepsilon} \rangle = \langle \varepsilon_1 \rangle - i \langle \varepsilon_2 \rangle = \sin^2 \phi \left[ 1 + \tan^2 \phi \frac{\varepsilon_2}{\varepsilon_1} \right], \] (11.7)

where \( \tilde{\rho} = \tan(\psi)e^{i\delta} \) and \( \phi \) is the angle of incidence.

\[ MSE = \sqrt{\frac{1}{N-M} \sum_{j=1}^{N} \left( \langle \varepsilon_1 \rangle_j^{\text{mod}} - \langle \varepsilon_1 \rangle_j^{\text{exp}} \right)^2 + \left( \langle \varepsilon_2 \rangle_j^{\text{mod}} - \langle \varepsilon_2 \rangle_j^{\text{exp}} \right)^2}. \] (11.8)

<ε₁> only

In this mode, the MSE is calculated using the real part of the derived pseudo dielectric values.

\[ MSE = \sqrt{\frac{1}{N-M} \sum_{j=1}^{N} \left( \langle \varepsilon_1 \rangle_j^{\text{mod}} - \langle \varepsilon_1 \rangle_j^{\text{exp}} \right)^2}. \] (11.9)

<ε₂> only

In this mode, the MSE is calculated using the imaginary part of the derived pseudo dielectric values.

\[ MSE = \sqrt{\frac{1}{N-M} \sum_{j=1}^{N} \left( \langle \varepsilon_2 \rangle_j^{\text{mod}} - \langle \varepsilon_2 \rangle_j^{\text{exp}} \right)^2}. \] (11.10)

Rho (complex reflectance ratio)

In this mode, the MSE is calculated using the real and imaginary parts of the complex reflectance ratio, \( \rho = \rho_r + i\rho_i \).

\[ MSE = \sqrt{\frac{1}{2N-M} \sum_{j=1}^{N} \left( \rho_j^{\text{mod}} - \rho_j^{\text{exp}} \right)^2 + \left( \rho_j^{\text{mod}} - \rho_j^{\text{exp}} \right)^2}. \] (11.11)
Re\{\text{Rho} \}\ only

In this mode, the MSE is calculated using the real part $\rho_r$ of the complex reflectance ratio, $\rho = \rho_r + i\rho_i$.

$$MSE = \sqrt{\frac{1}{N-M} \sum_{j=1}^{N} \left( \rho_{r,j}^{\text{mod}} - \rho_{r,j}^{\exp} \right)^2}.$$  \hfill (11.12)

Im\{\text{Rho} \}\ only

In this mode, the MSE is calculated using the imaginary part $\rho_i$ of the complex reflectance ratio, $\rho = \rho_r + i\rho_i$.

$$MSE = \sqrt{\frac{1}{N-M} \sum_{j=1}^{N} \left( \rho_{i,j}^{\text{mod}} - \rho_{i,j}^{\exp} \right)^2}.$$  \hfill (11.13)

Delta only

In this mode, the MSE is calculated using only the $\Delta$ values.

$$MSE = \sqrt{\frac{1}{N-M} \sum_{j=1}^{N} \left( \Delta_{r,j}^{\text{mod}} - \Delta_{r,j}^{\exp} \right)^2}.$$  \hfill (11.14)

Renormalized Exp Standard Deviation

In this mode, the MSE is calculated using the Renormalized Experimental Standard Deviations. Compared to the other Fit Weightings (like "Psi and Delta"), this MSE definition maintains the relative weighting of the data points based on the experimental error bars. At the same time, the RMS “average” error bars are factored out of the MSE, which should give more consistent MSE values when analyzing data sets with differing signal/noise.

$$MSE = \sqrt{\frac{1}{2N-M} \sum_{j=1}^{n} \left( \frac{\Psi_{j}^{\text{mod}} - \Psi_{j}^{\exp}}{\sigma_{j}^{\Psi}} \right)^2 + \left( \frac{\Delta_{j}^{\text{mod}} - \Delta_{j}^{\exp}}{\sigma_{j}^{\Delta}} \right)^2} \right) \hfill (11.15)$$

$\cos^2 \Psi$, $\sin^2 \Psi \cos \Delta$

In this mode, the MSE is calculated using the two quantities $\cos^2 \Psi$ and $\sin^2 \Psi \cos \Delta$, which are calculated from $\Psi$ and $\Delta$.

$$MSE = \sqrt{\frac{1}{2N-M} \sum_{j=1}^{N} \left( \cos 2\Psi_{j}^{\text{mod}} - \cos 2\Psi_{j}^{\exp} \right)^2 + \left( \sin 2\Psi_{j}^{\text{mod}} \cos \Delta_{j}^{\text{mod}} - \sin 2\Psi_{j}^{\exp} \cos \Delta_{j}^{\exp} \right)^2}.$$  \hfill (11.16)
In this mode, the MSE is calculated using the two quantities \( \cos^2 \psi \) and \( \sin^2 \psi \sin \Delta \), which are calculated from \( \psi \) and \( \Delta \).

\[
MSE = \sqrt{\frac{1}{2N-M} \sum_{j=1}^{N} \left( \cos^2 \psi_j^{\text{mod}} - \cos^2 \psi_j^{\text{exp}} \right)^2 + \left( \sin^2 \psi_j^{\text{mod}} \sin \Delta_j^{\text{mod}} - \sin^2 \psi_j^{\text{exp}} \sin \Delta_j^{\text{exp}} \right)^2}
\]  
\[\text{Equation (11.17)}\]

**cos2\( \psi \) only**

In this mode, the MSE is calculated using \( \cos^2 \psi \), which is calculated from \( \psi \).

\[
MSE = \sqrt{\frac{1}{N-M} \sum_{j=1}^{N} \left( \cos^2 \psi_j^{\text{mod}} - \cos^2 \psi_j^{\text{exp}} \right)^2}
\]  
\[\text{Equation (11.18)}\]

**sin2\( \psi \cos \Delta \) only**

In this mode, the MSE is calculated using the quantity \( \sin^2 \psi \cos \Delta \), which is calculated from \( \psi \) and \( \Delta \).

\[
MSE = \sqrt{\frac{1}{N-M} \sum_{j=1}^{N} \left( \sin^2 \psi_j^{\text{mod}} \cos \Delta_j^{\text{mod}} - \sin^2 \psi_j^{\text{exp}} \cos \Delta_j^{\text{exp}} \right)^2}
\]  
\[\text{Equation (11.19)}\]

**sin2\( \psi \sin \Delta \) only**

In this mode, the MSE is calculated using the quantity \( \sin^2 \psi \sin \Delta \), which is calculated from \( \psi \) and \( \Delta \).

\[
MSE = \sqrt{\frac{1}{N-M} \sum_{j=1}^{N} \left( \sin^2 \psi_j^{\text{mod}} \sin \Delta_j^{\text{mod}} - \sin^2 \psi_j^{\text{exp}} \sin \Delta_j^{\text{exp}} \right)^2}
\]  
\[\text{Equation (11.20)}\]

**cos2\( \psi \), sin2\( \psi \) cos\( \Delta \), sin2\( \psi \) sin\( \Delta \)**

In this mode, the MSE is calculated using the three quantities \( \cos^2 \psi \), \( \sin^2 \psi \cos \Delta \), and \( \sin^2 \psi \sin \Delta \), which are calculated from \( \psi \) and \( \Delta \).

\[
MSE = \sqrt{\frac{1}{N-M} \sum_{j=1}^{N} \left( \cos^2 \psi_j^{\text{mod}} - \cos^2 \psi_j^{\text{exp}} \right)^2 + \left( \sin^2 \psi_j^{\text{mod}} \cos \Delta_j^{\text{mod}} - \sin^2 \psi_j^{\text{exp}} \cos \Delta_j^{\text{exp}} \right)^2 + \left( \sin^2 \psi_j^{\text{mod}} \sin \Delta_j^{\text{mod}} - \sin^2 \psi_j^{\text{exp}} \sin \Delta_j^{\text{exp}} \right)^2}
\]  
\[\text{Equation (11.21)}\]

**Weighting of reflection / transmission data**

The contribution to the total MSE from intensity reflection/transmission data is included in a root mean square (RMS) manner.

\[
MSE_{\text{total}} = \sqrt{MSE_{\text{ellipsometric}}^2 + MSE_{\text{reflection}}^2 + MSE_{\text{transmission}}^2}
\]  
\[\text{Equation (11.22)}\]
The ellipsometric contribution was described in the previous section. The reflection contribution is defined as

\[ MSE_{\text{reflection}}^2 = \frac{1}{N_R - M} \sum_{j=1}^{N_R} \left( \frac{R_j^{\text{mod}} - R_j^{\text{exp}}}{w_R \sigma_{R,j}^2} \right)^2, \]  

(11.23)

where \( N_R \) is the number of experimental intensity reflectance measurements and the reflection data weighting ratio, \( w_R \), is defined as \( w_R = 100/R \), where \( R \) is the weighting value defined in the ‘R&T Weighting’ section of the Fit Defaults dialog box (see figure above). Thus, compared to a 100% weighting value, a larger weighting factor yields a larger contribution to the MSE.

The transmission contribution is defined in an equivalent way as

\[ MSE_{\text{transmission}}^2 = \frac{1}{N_T - M} \sum_{j=1}^{N_T} \left( \frac{t_j^{\text{mod}} - t_j^{\text{exp}}}{w_T \sigma_{T,j}^2} \right)^2, \]  

(11.24)

The weighting ratio is defined as \( w_T = 100/T \), where \( T \) is the weighting value defined in the ‘R&T Weighting’ section of the Fit Defaults dialog box (see figure above).

Fit|Normal_Fits|Stats item

This option displays the fit parameter results, the fit parameter confidence limits, and the fit parameter correlation matrix. Confidence limits and correlation values are described more fully in chapter 2 - “A Short Course in Ellipsometry” and chapter 13 - “VASE® Data Analysis.” This option is only enabled after a fit has been performed.

Once the final parameter values have been determined the resulting parameters need to be evaluated for sensitivity and for possible correlations. The sensitivity is expressed in terms of a confidence limit and describes “how much” information is available about a given parameter. The correlation is expressed in terms of a set of two-parameter correlation coefficients and describes “how independent” the fit parameters are.

Both of these pieces of information come form an important element of the fitting procedure, the curvature matrix \( \alpha \):

\[ \alpha_{kl} = \sum_{i=1}^{N} \frac{1}{\sigma_{y,i}^2} \left[ \frac{\partial y_{kr}^{\text{mod}}}{\partial x_{ki}} \frac{\partial y_{kr}^{\text{mod}}}{\partial x_{lj}} + \frac{\partial y_{kr}^{\text{mod}}}{\partial x_{ij}} \frac{\partial y_{kr}^{\text{mod}}}{\partial x_{kl}} \right], \]  

(11.25)
The covariance matrix of the fit parameters \( \{C\} \) may be obtained from the inverse of the curvature matrix, as \( \mathbf{C} = \alpha^{-1} \). The figure of merit (FOM) we have adopted to describe confidence in the \( i \)th fit parameter is given by

\[
FOM_i = 1.65 \times MSE \times \sqrt{C_{ii}}. \tag{11.26}
\]

\( C_{ii} \) is the \( i \)th diagonal element of the covariance matrix. When \( \text{WVASE}^\circledR \) returns the “error bars” on a fit parameter the FOM is used. \( \text{WVASE}^\circledR \) treats the terms “confidence limit” and “confidence FOM” as the same quantity. The displayed format is Fit Value±FOM. The assumptions required to accurately determine confidence limits and methods of interpreting confidence limits are discussed in chapter 2 - “A Short Course in Ellipsometry” and chapter 13 - “\text{VASE}^\circledR Data Analysis.”

The two-parameter correlation coefficient is given by

\[
S_{jk} = \frac{C_{jk}}{\sqrt{C_{jj} \sqrt{C_{kk}}}}. \tag{11.27}
\]

An absolute value of \( S_{jk} \) near 1 indicates significant correlation between the \( j \)th and \( k \)th fit parameters. The two-parameter correlation coefficients are given in matrix form in the Fit|Stats dialog box.

**The fit statistics dialog box**

After a normal fit, the Fit|Stats dialog might look like the following.

**Confidence limits**

This gives the final fit value and the confidence FOM for each fit parameter.

**Correlation matrix**

This is the matrix of two-parameter correlation coefficients calculated from the covariance matrix.
Fit|Normal_Fits|Reset menu item

Same Fit|Reset command that is described in a section below.

Fit|Normal_Fits|Pt_by_Pt menu item

A pt-by-pt fit works with the selected data on a wavelength-by-wavelength (spectroscopic) or on a time-by-time (dynamic data) basis. The normal fit is distinguished from a pt-by-pt fit in that a normal fit works with all the selected data simultaneously.

A pt-by-pt fit can be thought of as a series of normal fits with the selected data ranges grouped by wavelength or time. At each wavelength, the same conditions which will end a normal fit will cause a pt-by-pt fit to move on to the next wavelength or time. The results of pt-by-pt fit are usually graphed using the Graph|Data|Point_by_Point_Fit_Parms option. This graphing option allows you to view a fit parameter and its fit confidence limit for each wavelength or each time. Wavelength-by-wavelength fitting of spectroscopic and time-by-time fitting of dynamic data are described in the following sections.

**Point by point fitting of static spectroscopic data**

When spectroscopic data that is not time dependent is selected, a pt-by-pt fit will work with all the available data at a given wavelength, one wavelength at a time. This is most commonly done when fitting optical constants with all layer thicknesses and other parameters held fixed. With all other parameters held fixed, the optical constants at different wavelengths are totally independent for the purposes of fitting.

For the following example, the optical constants of the substrate are being fit wavelength-by-wavelength. The spectroscopic data (not shown) extends over the wavelength range from 2500 to 10000 Å. When the fit is started using the Fit|Pt_by_Pt command, a startup dialog box like that shown below is presented.

![Figure 11-14. Dialog box used to start a wavelength-by-wavelength fit.](image)

**Starting position**

You can choose to start the wavelength-by-wavelength fit at either the longest wavelength or the shortest wavelength of the selected experimental data. In this example, the longest wavelength ($\lambda = 10000$ Å) is chosen starting point.
# pts to Ave. for next guess

This box allows you to have some control over what starting parameter values will be used at the succeeding wavelength. If this edit box value is less than two, then the fit parameters from the last wavelength analyzed will be used as the starting values for the next wavelength to be analyzed. If this value is two or more, then that many previously analyzed wavelengths will be used to extrapolate what would be likely results for the next wavelength. Most parameters you would fit for on a wavelength-by-wavelength basis will tend to be smooth functions of wavelength, and this averaging feature can help a pt-by-pt fit stay on the correct track.

Show iterations

If this box is checked, then the results of all fit iterations at each wavelength will be displayed in the Fit window. If this box is unchecked, only the final results at each wavelength will appear in the Fit window. If many iterations are being performed at each wavelength, turning this option off may speed up the fit process.

Fit parameter boxes

This series of editable boxes shows the starting values for the fit process. Up to 6 parameters can be fitted on a wavelength-by-wavelength basis. In this example only the real and imaginary parts of the complex refractive index are being fitted. The parameter name is shown to the left of these boxes. In this example, the starting wavelength is 10000 Å and the parameter names are “n.10000.0” and “k.10000.0”.

Cancel

This button cancels the request for a pt-by-pt fit.

Ok

This button initiates the pt-by-pt fit at the starting wavelength.

After the OK button is used in the above dialog box, the data for the first wavelength is analyzed. The fit parameters are then displayed in the Fit window and a second message box like the following appears.

Figure 11-15. Message box displayed after the first wavelength has been analyzed.

This message box allows you to continue the fit, restart the fit, or cancel the fit. Selecting ‘No’ (the default option) will continue the point-by-point fit using the values determined at the first wavelength as initial values for the next wavelength. Selecting ‘Yes’ will allow you to restart the fit using different initial values for the fit parameters. This option will return you to a dialog box like that shown in figure 10.8. Selecting the ‘Cancel’ button will abort the point-by-point fit.
After the fit is completed, the fit parameters and confidence limits can be examined using the Graph|Data menu to select pt-by-pt data.

![Figure 11-16. Graph example of pt-by-pt fit optical constants and the associated parameter confidence limit.](image)

**Point by point fitting of dynamic data**

When dynamic data is being analyzed and the data is displayed as a function of time, a pt-by-pt fit will work with the selected spectroscopic data at a given time, one time slice at a time. This is commonly done when fitting the time dependent thickness of a layer which was deposited (or removed, etched). (If the dynamic data is being displayed in spectroscopic mode, you should only perform normal fits.)

For the following example, a simulated growth of $\text{Al}_{0.2}\text{Ga}_{0.8}\text{As}$ on a GaAs substrate is analyzed. The thickness of the growing AlGaAs layer is fitted as a function of time using a pt-by-pt fit. The experimental $\psi$ values for this example are shown below.

![Generated and Experimental Data](image)

*Figure 11-17. Simulated ellipsometric data for $\text{Al}_{0.2}\text{Ga}_{0.8}\text{As}$ growing on GaAs.*

Note the growth begins at time = 1 min. and ends at time = 4 min. These times are identifiable in the data, because the $\psi$ values change with time only when the layer is growing. The dialog box which comes up after starting the pt-by-pt fit (Fit|Pt_by_Pt) is shown in Figure 10.12.
This dialog box is similar to the dialog box for a wavelength-by-wavelength fit except that the Show Iterations and Starting Position sections are not present. When pt-by-pt fitting dynamic data, *WVASE* always assumes you want to start with the earliest experimentally selected time.

**# pts to ave.**

This box allows you to have some control over what starting parameter values will be used at the succeeding time. If this edit box value is less than two, then the fit parameters from the last time analyzed will be used as the starting values for the next time to be analyzed. If this value is two or more, then that many previously analyzed wavelengths will be used to extrapolate what would be likely results for the next time. Most parameters you fit for on a time-by-time basis will tend to be smooth function of time, and this averaging feature can help a pt-by-pt fit stay on the correct track.

**Fit parameter boxes**

This series of editable boxes shows the starting values for the fit process. Up to 6 parameters can be fitted on a time-by-time basis. In this example only the thickness of the growing AlGaAs layer is being fit. the parameter name is shown to the left of these boxes. In this example, the parameter is “Thick.1”.

After the Ok button is used in the above dialog box, the data for the first time is analyzed. The fit parameters are then displayed in the Fit window and a second message box like the following appears.

![Dynamic Fit: Starting Parameter Values](image)

*Figure 11-18. Dialog box used to start a time-by-time fit. The starting parameter value has been changed to 0 before starting the fit.*

This message box allows the user to continue the fit, restart the fit, or cancel the fit. Selecting the ‘No’ option (the default option) will continue the point-by-point fit using the values determined for the initial time as starting values for the next time. Selecting ‘Yes’ will restart the fit using different initial values for the fit parameters by returning you to the dialog box shown in figure 10.12. Selecting ‘Cancel’ will abort the point-by-point fit.

![WV by WV Fit](image)

*Figure 11-19. Message box displayed after the first time has been analyzed, and the Fit window from the same screen display.*
After the fit is completed, the fit parameters and fit confidence limits can be examined using the Graph|Data menu to select pt-by-pt data.

![Graph Example](image.png)

*Figure 11-20. Graph example of a pt-by-pt fit of the thickness of growing AlGaAs layer and the associated parameter confidence limit.*

### Fit|Normal_Fits|Grid_Global menu item

Grid Global fit functions the same as the ‘Global Fit’ option in the ‘Edit Fit Parameters’ dialog box. That is, the fit global fit starts from one edge of the parameter space and methodically tests the adjacent point until all points have been tested.

### Fit|Normal_Fits|Random_Global menu item

Random Global Fit randomly tests different points in parameter space, until all points are tested, or the user stops the process by selecting the “Cancel” button at top of window, or by pushing the “Esc” key.

### 11.4 Fit|Reset command

![V.A.S. for Windows](image.png)

*Figure 11-21. The Reset option from the Fit window.*

The reset option is not available if an error occurred during the last fit!

When selected, this menu bar item will reset all selected fit parameters to the values they had before the most recent fit process (normal or pt-by-pt) was performed. Sometimes the fitting algorithm will get “lost” and find a local minimum in the MSE which is very far from the absolute minimum. In this case, it may be advantageous to reset all the parameter values to their previous values and try the fit again after changing or removing a few parameters.

This option can be very useful when fitting for optical constants and thicknesses together. If the thickness starts too far away from the true value, the optical constants may become very unphysical. If left in that unphysical state, the fitting algorithm may have trouble getting the model back into a physically reasonable state. Without this option you would either have to replace the layer with a new set of starting optical constants or manually edit the optical constants.

If the fit process is terminated by an error condition, the Fit|Reset option may not be available and the previous starting values are lost.
11.5 Fit|EditParms item

Figure 11-22. The EditParms option from the fit window.

This option is used for two primary reasons: 1) to place allowed ranges on fit parameters, and 2) to couple fit parameters together when fitting. This command can be used with static spectroscopic data or dynamic data which is being displayed as a function of time. When dynamic data is being displayed in the spectroscopic mode, do not use this command. In that display mode, parameter ranging and coupling is accomplished using the Model|Select command.

The edit fit parameters dialog box

Using the Fit|Edit_Parms command opens the Edit Fit Parameters dialog box (Figure 10.18). In this example two thickness, “Thick.1 and Thick.2”, two Cauchy parameters, “An.1” and “Bn.1”, for layer #1, and the optical constants for the substrate “n.0” and “k.0” are the current fit parameters.

Figure 11-23. Dialog box displayed by the Fit|Edit_Parms command. Default parameter ranges are shown.

Parameter list

All currently active fit parameters appear in the list on the left side of this box. Each parameter is numbered, has its current value displayed, has its allowed fit range defined, and has a number of guesses indicated for use when doing a global fit (all of the parameters in Figure 10.18 have a guess value of 1). This list is where parameters are selected so that their status can be altered using the ‘Change Parm Coupling’ button. Note that the substrate optical constants appear only as “n.0” and “k.0”, and that they have no current value. For the purposes of this box, the optical constants at every experimental wavelength for a layer are grouped together. When the fitting process starts the individual fit parameters at each wavelength will be used and will be displayed in the Fit window.
‘Change Value’ button and parameter value box

This button is either used to change the currently-selected parameter in the parameter list to the value found in the box located above the button, upper-right corner of the dialog box (the box is labeled “Thick.1” in the figure above).

Users can also change the values by placing the mouse cursor over the parameter value box and then rotating the mouse scroll wheel. As the scroll wheel changes the parameter, WVASE also automatically recalculates the generated data and updates the graph window. The selected-value’s rate-of-change is increased by holding the ‘Shift’ or ‘Ctrl’ key down while rotating the scroll wheel. The rate-of-change will be even greater if both the ‘Shift’+‘Ctrl’ keys are held down simultaneously.

‘Change Parm Coupling’ button

This button is either used to change the upper and lower bounds on the fit parameters or to couple one parameter to another. The values specified in the corresponding sections below this button will be applied to the currently selected parameter or parameters.

Minimum and Maximum boxes

The Minimum and Maximum boxes are used in conjunction with the ‘Change Parm Coupling’ button to set new upper and/or lower bounds on the fit parameters. When the “Uncoupled Parameter” bubble is selected, the current values of the Minimum and Maximum edit boxes can be applied to the selected parameter or parameters. An example of this operation is described in a later section. You must use the ‘Change Parm Coupling’ button to change parameter limits; using the OK button will not change the parameter information.

# of Global Guesses

This box is used in conjunction with the ‘Change Parm Coupling’ button to set the number of guesses that will be chosen for the parameter during a global fit. See the Global Fit button for details.

Parameter Coupling Mode

This section is used in conjunction with the ‘Change Parm Coupling’ button to couple one fit parameter to another. Parameters can be coupled together in one of two ways; they can be coupled by a constant ratio or they can be coupled by a constant offset. The coupling type is chosen by selecting either the “constant ratio” bubble or the “constant offset” bubble. When one of the coupling bubbles is selected, the current Couple To Pram # and Coupling Constant edit boxes will be used to set up coupling for the selected parameter or parameters. An example of this operation is described in a later sections. You must use the ‘Change Parm Coupling’ button to change coupling information; using the OK button will not change the parameter information.

Do not fit all parameters option

This check box gives you additional flexibility in selecting fit parameters when performing a normal fit. If this box is checked when you start a normal fit (use Fit|Normal_Fit), you will be presented with a dialog box containing all fit parameters currently defined in the model (or models, if more than one model is active). This list will include optical constants at each wavelength if the optical constants of one or more layers are directly defined as fit parameters. From this list you can choose
which parameters will actually be varied during a fit. For some complicated fits, you might find it easier to select the desired fit parameters from this list rather than checking or unchecking fit selection boxes throughout the model.

**Global Fit**

The global fit button is used to perform a global fit. A global fit is actually many small fits, each with different parameter starting values. The purpose of a global fit is to find the smallest MSE for a model when good starting values for the parameters (i.e. thickness, optical constants, etc.) are not known. The global fit is setup by putting minimum and maximum limits on the parameters and specifying a number of guesses for each parameter. Then, when the Global Fit button is pressed, an $N$ dimensional grid is setup consisting of guesses for each parameter where $N$ is the number of fitting parameters. The guess values are spaced at equal increments between the minimum and maximum parameter limits, where the increment is defined as the allowed parameter range (maximum – minimum) divided by the number of guesses. The Iterations edit box is used to specify the maximum number of fit iterations to perform at each grid point. After the fit, the parameter values resulting in the smallest MSE are entered into the model. See the section “Performing Global Fits” below for more detailed information.

**Delete all parms**

This button will immediately turn off all fit parameters and dismiss the dialog box. There is no warning message. For some complicated fits, you might find this an easy way of deselecting fit parameters from multiple layers and starting again.

**Range limits on fit parameters**

The primary reason for enforcing an allowable range on a fit parameter is to enforce some degree of physicality on the model. For instance, physical layer thicknesses can not be less than zero, so thicknesses are usually forced to be positive values. Also, most every material studied by ellipsometry will be either optically absorbing or transparent, but not amplifying. For that reason the imaginary part of a layer’s optical constants are usually not allowed to be less than zero. (A positive imaginary part is considered absorbing by WVASE®.)

WVASE® allows you great flexibility to set limits on the fit parameters. Each fit parameter has its own default limits, but you can change these limits using the Fit|Edit_Parms command. In the following example (Figure 10.19) the fit limits for parameters #0 and #1 (“Thick.1” and “Thick.2”) have been changed to a minimum of 0 and a maximum of 500. These values are in Å’s because the WVASE® thickness units have been set to Å’s using the |Global|Defaults command. The fit parameter list is a multiple selection list box, and in this case the limits for both parameters were changed together using the ‘Change Parm Coupling’ button.
Coupling fit parameters

Coupling fit parameters is not a commonly used feature but it can be a useful technique for some data analyses. The primary reason for coupling fit parameters together is to use extra knowledge you might have about a sample (or set of samples) to reduce the number of fitting parameters. You might want to couple a layer thickness from one model to another. Or you might want to couple the ratio of two thickness in a given model using extra knowledge you have about the sample preparation.

The Fit|Edit_Parms command is used to couple fit parameters which are not optical constants. Optical constants are coupled together when the model is built. For more details on coupling optical constants from one layer to another see “Model|AddLayer, Coupling of Layers”.

WVASE® allows you to couple one parameter to any other through a ratio or a constant offset. To set up coupling, you select the parameter you want to be dependent on another parameter. You select the dependent parameter (or parameters) from the parameter list in the Fit|Edit_Parms dialog box. Then you fill in the coupling constant and the identifying number of the independent fit parameter. In the following example (Figure 10.20) the value for parameter #1 (“Thick.1”) has been coupled to parameter #2 (“Thick.2”) by a factor of 0.7.
The value for parameter #1 (Thick.2) has been coupled to parameter #0 (Thick.1) through a constant 0.7. This coupling means that during a fit, the thickness of layer #2 will be set at 0.7 multiplied by the current thickness of layer #1. For each fit iteration, the thickness of layer #2 may change, but only as the thickness of layer #1 changes. The coupling dependence of fit parameters is only updated during a fit process. Using the Gen_Data|Generate_Data command does not update the coupling status; it simply uses whatever values are currently displayed in the model.

The fit parameter list is a multiple selection list box, and multiple dependent parameters could have been coupled to one independent parameter using the ‘Change Parm Coupling’ button. Note that the Coupled Parameter bubble is filled in, and this indicates that new limiting values are desired.

Do not fit all parameters option

This option allows you to fit only a subset of the currently selected fit parameters when performing a normal fit (Fit|Normal_Fit). When this box is checked in the Fit|Edit_Parms dialog box, you will be presented with a dialog box after you use the Fit|Normal_Fit command. This dialog box will show all currently checked fit parameters, and will look similar to the following.
In the figure above, 144 of the possible 154 fit parameters are currently selected for this fit. Parameters #4-#13 would not be fit if the OK button was used. Note that individual entries are included for the optical constants at different wavelengths.

**Parameter names**

This is the list of all fit parameters and their initial values for the fit. This is a multiple selection list box where you can use the mouse in conjunction with the <Shift> and <Ctrl> keys to select (highlight) parameters. Dependent coupled parameters are displayed in this list, however their selection status will not affect the fit.

**Total # of parms**

This is the number of parameters in the list on the left.

**Selected parms**

This is the number of parameters selected from the list on the left.

**Select all**

This button will select all parameters in the list.

**Performing Global Fits**

Global fitting is a powerful tool for use when analyzing spectroscopic ellipsometry data. It is particularly useful for situations where false minimums in the MSE can appear. Two typical cases where false minimums are common are complicated models with lots of parameters where sensitivity to some parameters is low, and for thick films where it is important to have good starting values for thickness and optical constants so the same number of interference effects appear in the simulated and experimental data. As global fitting is a powerful tool, several examples in the chapter “VASE Data Analysis Examples” are devoted to the topic.

**11.6 Fit|Fit_Studies menu**

![Fit|Fit_Studies menu](image)

*Figure 11-27. The Fit|Fit_Studies pull-down menu from the Fit window.*

**Fit|Fit_Studies|MSE command**

When the MSE command is selected, WVASE® returns the $MSE$ and $MSEO$, based on the weighting schemes described below. $MSEO$ is calculated from the same weighting equations as $MSE$; except that for the $MSEO$ calculation, $M$ (the number of fit parameters) is set equal to 0.

The Calculate MSE window also reports $NFit$ and $Ndata$. $NFit = M$, the number of fit parameters. $Ndata = 2N$ or $N$, where $N$ is the number of measured $\Psi - \Delta$ pairs. In most cases, $N$ equals the number of measured wavelengths times the number of measured incident angles.
Manually calculating the MSE may be done for various reasons. The most common application is a check the MSE for different ranges of experimental data. By doing this you can locate experimental spectral regions or measurement angles which contribute a disproportionate amount to the MSE. For a statistically uniformly fit, every subset of the experimental data can be expected to have the same MSE.

**Fit|Fit_Studies|Uniqueness_Fit menu item**

Often there is an issue as to whether there is real sensitivity to a fitted model parameter. One way to examine this question is to take the best-fit model, slightly change the parameter of interest and fix its value (i.e. do not fit), and then refit all the other parameters around this value. If the same, or essentially the same, fit quality is achieved with the changed fit parameter, there will not be sensitivity to that fit parameter, at least to level by which is was changed. Manually changing and fixing the parameter of interest can be tedious.

The ‘Uniqueness Fitting’ menu option will perform such an analysis for one parameter in an automated fashion. As an example, “Example 7: Silver Film on Fused Silica” (from Chapter 14) was analyzed. In this example both the ellipsometric and transmission-intensity are fit simultaneously – which de-correlates the thickness from \( n \) and \( k \). The resulting model and data-fit shown in the figure below. (See chapter 14 for further details).

![Figure 11-29. The final model and data fits for the Silver film on fused silica example (See Example 7, Chapter 14).](image)

Next the ‘Fit|Uniques Fitting’ menu option is selected, opening the dialog box shown in the figure below. In this example, the silver thickness (Thick.1) is selected as the parameter of interest. Twenty-one test values from 25 to 45 nm are
selected. The Maximum Iterations for the fit are set to 20. If the ‘Save Env Files’ option is selected, the fit results for each of the test fits are saved as an environment file. This allows the test fits to be reopened and examined as needed.

**Figure 11-30.** The Settings for Uniqueness Fitting dialog box.

The results are returned in an RTF viewing window (figure below, left). This RTF file can be saved, or the results can also be transferred to a spreadsheet or other data manipulation/plotting program. At the end of the RTF file, the mse0 and mse0rel vs. parameter (Thick.1 in this example) are plotted (as shown on the right side of the figure below). These plots can be copied and pasted into MS® Word, Excel and other programs.

**Figure 11-31.** Left: The first 19 lines and (Right) bottom graphs from the RTF file output from the Uniqueness fit. The mse0 and mse0rel graphs show a clear minimum for Thick.1 equal to 36nm.

The MSE values adjusted for the number of fit parameters (mse) and unadjusted (mse0) are both listed. An unadjusted, relative-to-column2 value (mse0rel) is also listed. (The assumption is that one would perform a normal fit just prior to the uniqueness fit to give good starting values.) The mse0 and mse0rel vs. parameter (Thick.1 in this example) are also plotted at the end of the RTF file.

The resulting fit parameters and fit parameter figure of merit (error bars) for each fit are tabulated in separate rows. Parameters that are not fitted have figure-of-merit values of -1.
Chapter 12 Data Acquisition Procedures and Strategies

12.1 Overview

In this chapter we provide tips on how to get the best experimental data, and hence the best analysis of a given sample.

In this chapter the procedures for acquiring various types of optical data with the VASE® instrument are reviewed. Procedures for the acquisition of ellipsometric and intensity data are given. Strategies for selecting data types and scan parameters for different types of samples are given, as well as tips for optimizing the ellipsometer setup to obtain the best possible data from different types of samples. It is assumed that the user is familiar with moving between the various windows in WVASE®, and has worked through the tutorial in chapter 11 - “Quick Start: VASE®”.

Note that the procedures for the power-up and initial inspection of the VASE® instrument are given in chapter 11 - “Quick Start: VASE®”, as are the procedures for mounting and aligning samples and calibrating the VASE® instrument. In this chapter we will assume that the user is familiar with these procedures, and that the VASE® system is on and calibrated.

12.2 General principles of VASE® data acquisition

Learn these procedures well, and remember to experiment freely!

Ellipsometric measurements are known to be very sensitive to many experimental factors such as surface quality, choice of spectral range and angles of incidence for data acquisition, and sample alignment. In this section we discuss some useful general principles involving many of these experimental factors to help users to optimize their ellipsometric experiments for the given type of sample under study. Specifically, we discuss in this section sample preparation, acquisition of appropriate experimental data, and building physically reasonable models for the sample. Keep in mind throughout that nothing in this document constitutes a ‘law of nature’, and that experimentation by the user is always encouraged.

12.3 Sample preparation

The condition of the sample surface may have a very strong effect on the measured ellipsometric data. In this section we discuss the preparation of samples for ellipsometric measurements. We also discuss means for eliminating reflections from the back surface of transparent substrates, and preparation of very thin transparent substrates (Mylar sheets, for example).
Sample cleaning

Common sense is the best possible advice for sample cleaning (this will be a recurring theme throughout). The VASE® technique is very sensitive to microscopic surface quality, but rather insensitive to the presence of macroscopic objects such as dust particles. Larger objects tend to scatter light away from the detector, while things like surface contaminant films and surface roughness may have a strong effect on the specularly reflected beam. The user should refer to the literature for appropriate cleaning techniques for the given material under study, and keep in mind that the surface of the sample (and to a lesser degree the back surface too if the substrate is transparent and not roughened) should be as clean and dry as possible. Commercially available ‘dust blowers’ are quite useful for removing room dust from samples, but care must be exercised to avoid organic residues left by the gas in the blower cartridge.

Roughening transparent substrates

Tip: Always roughen glass substrates if you can when characterizing films deposited on them.

In many cases it will be desirable to eliminate the component of the beam which is reflected from the back surface of the substrate of the sample under study. While there are a number of means of doing this, we have found roughening to be the easiest and most consistently effective means of eliminating the back surface reflection. For glass substrates we have found a miniature hand drill with a grinding bit to be very useful.

Roughen an area slightly larger than the size of the beam on the back surface of the sample, behind the intended measurement point, and remove the particulate residue from both sides of the sample. For plastic substrates we have found silicon carbide sandpaper to be a most effective means of roughening the substrate. Just about any size of grit will work, provided it leaves a rough, non-specular surface. It may also be helpful to finish with sandpaper after using a grinding bit initially to roughen the back surface of a sample.

Very thin transparent substrates

The case of very thin transparent substrates (Mylar or polyester sheets, cover glasses, for example) requires very special care. Cover glasses are nearly impossible to roughen without breaking, however they are rigid enough that they may usually be mounted without inducing significant sample curvature, and thin enough that the back surface correction algorithm in the WVASE® software usually works quite well. Thin plastic sheets (coated or uncoated) are quite difficult to mount on the ellipsometer without inducing significant curvature into the sample surface, and the plastics involved are often birefringent, requiring elimination of the back surface reflection for any meaningful analysis of the ellipsometric data.

The roughening of the back surface of the film can usually be accomplished by lightly buffing the back side with very fine grade (600 or 1200) sandpaper. One can also blacken the back side of the substrate with a marker if necessary. After roughening, the sample must be mounted such that the surface is flat. One user has found polished porous metal surfaces under vacuum to work fairly well in this application, although dimpling due to the pores in the metal can be problematic. We have achieved reasonable results on coated and uncoated Mylar and polyester films by roughening the back side of the substrate as described above, and taping a piece of the film over a piece of black construction paper on a microscope slide. With a bit of care and experimentation this technique will yield an easily mountable and alignable sample with a reasonably flat surface. Remember that the surface only need be flat over the area of the incident light beam.
12.4 Choice of data type and acquisition parameters

The VASE® instrument can acquire many types of optical data!

The VASE® instrument is capable of acquiring a wealth of data from any given sample, however it would be prohibitively time-consuming to acquire all possible optical data from every sample with the VASE®. We then are faced with the choice of what types of optical data to acquire to characterize a given sample, and what wavelengths (or photon energies) and angles of incidence to acquire the data at. Experience is a wonderful guide in this choice, but there are some general concepts involved which may save the user a lot of headaches when subsequently analyzing the data. In this section we discuss the choice of data types, spectral range, and angles of incidence for acquiring data. We also discuss means of optimally acquiring each type of data with the J. A. Woollam Co., Inc. VASE®.

Please keep in mind that if you are confused as to which angles and wavelengths to use, don’t be afraid to experiment. Try acquiring data over the full spectral range of the instrument (250-1700 or 250-1000 nm) at three angles of incidence (65°, 70°, and 75° are generically good angles if nothing is known about the sample). Examine the delta data, looking for spectral regions in which the data at all three angles of incidence are close to 0° or 180°. If delta is close to 180° for all three angles in some spectral region, try acquiring data at larger angles of incidence. If delta is near 0° for all angles acquire data at smaller angles of incidence. In the absence of strong interference effects delta at any wavelength will decrease towards 0° as the angle of incidence increases, as discussed in chapter 2 - “A Short Course in Ellipsometry”.

Try analyzing these data. If you are successful, experiment with reducing the range of data which is being fit (Range select option in the experimental data window) and repeating the analysis. In this way the user can determine the minimum data set required for a given sample structure to perform the desired analysis.

In many cases the optimal choice of data types and ranges of angles and wavelengths can be determined from knowledge of the sample structure, and we discuss means of performing this determination below.

Choice of spectral range

The choice of spectral range is dictated by two factors: the materials in the sample and the information the user wishes to get about the sample. If a user intends to only determine the layer thickness(as) of some layer(s) in the sample, a few well chosen wavelengths may be enough to perform this analysis. A good example is thermal silicon dioxide on silicon. The thermal oxide thickness can usually be determined from a single measurement at nearly any wavelength provided the optical constants of the silicon substrate and thermal oxide are known. Acquiring multiple wavelengths of data allows the overdetermination of this thickness, such that estimates as to the uncertainty of the measurement may be made.

If the user is attempting to obtain optical constants for a given material, data must be acquired at each wavelength at which the user wishes to obtain optical constants. Keep in mind that WVASE® will linearly interpolate optical constants between measured points for you, but if the optical constants are changing rapidly as a function of wavelength it is a good idea to acquire data at closely spaced wavelengths. Typically, for optical coatings or metals we use a wavelength spacing of 10 nm. For semiconductor work when attempting to resolve fine critical point structure it is common to scan as a function of photon energy in 0.01-0.1 eV steps.
Our technique when approaching most types of sample structure is to acquire data from 250-1000 nm and attempt the analysis. It is a very good idea whenever possible to acquire data in a spectral region where the film(s) on the sample is(are) transparent, as this eliminates the determination of the film absorption from the analysis, reducing parameter correlations. In many cases the infrared extension is very useful for this purpose, as it allows the acquisition of data out to 1700 nm.

Choice of angles of incidence

In general, try to work near the pseudo-Brewster angle of the sample, where $\Delta$ is within 30° or so of 90°.

The choice of optimal angles of incidence is not critical for the analysis of most samples, but in some cases it can be crucial in obtaining a useful analysis of a given sample. As a general rule it is a good idea to acquire data near the Brewster (or pseudo-Brewster) angle of the sample. For our purposes it is sufficient to define the Brewster (or pseudo-Brewster) angle as the angle (for a given wavelength) at which $\Delta$ is 90°. An error analysis of the VASE® instrument shows that the effect of systematic errors (calibration errors) and random noise on the measured data is minimized when the beam entering the detector is as close to circularly polarized (corresponding to a $\Delta$ value near 90°) as possible. Here is a plot of $\Delta$ at 633 nm plotted as a function of angle of incidence for a silicon wafer with 10 nm of thermal oxide on the surface:

![Figure 12.1](image1)

*Figure 12.1 Ellipsometric delta data calculated as a function of angle of incidence at 633 nm wavelength for a hypothetical sample of 10 nm of thermal silicon dioxide on crystalline silicon.*

On the left $\Delta$ is shown over the entire range of angles of incidence (0°-90°). Note that $\Delta$ is 180° at normal (0°) incidence, and drops smoothly to 0° at grazing incidence (90°). On the right we have blown up the range of angles of incidence from 70° - 80°. We see that $\Delta$ passes through 90° at around 75° angle.
of incidence (75.275°, to be exact). Thus, 75.275° is the pseudo-Brewster angle for this structure at 633 nm. It is not critical to acquire data exactly at the pseudo-Brewster angle, but it is good to be close. For this sample, three good angles of incidence would be 72°, 75°, and 78°, or 74°, 75°, and 76°.

Note that the pseudo-Brewster angle for a given sample may be a strong function of wavelength, and it may not possible to find a small range of angles which yields data near the pseudo-Brewster angle for all wavelengths.

We will point out optimal angles and spectral ranges for all types of samples discussed in the ensuing section. In the absence of advice for a given sample structure, do not be afraid to find the pseudo-Brewster angle of a given sample empirically by acquiring data at a few widely separated angles and examining the measured delta data.

### Choice of data types

The VASE® instrument is capable of measuring a rather wide variety of types of optical data:

- Ellipsometric data in reflection from the top of the sample.
- Ellipsometric data in reflection through the back of the substrate.
- Transmission ellipsometry, through the sample.
- Intensity reflectance, polarized or unpolarized, anywhere from ~12°-90° angle of incidence.
- Intensity transmittance, polarized or unpolarized, any angle of incidence.

All of these data types can be useful when analyzing samples, but usually only one or two may be required for a given sample, providing the one or two data types are wisely chosen.

Most analyses are performed with standard ellipsometric data acquired in reflection from the top surface of the sample. This measurement has maximal sensitivity to coatings at the top surface of the sample, and is most easily performed. The other four data types are primarily employed when a sample is so complicated that a unique solution to the desired optical model cannot be obtained from reflectance ellipsometry alone. A common example is the case of a thin metal film of unknown thickness. It is not possible to uniquely solve for the optical constants and thickness of the metal film from reflectance ellipsometry data alone, regardless of how many wavelengths and angles of incidence are used for acquisition. This problem can always be solved when the film is on a transparent substrate (glass, semiconductors at energies below the bandgap energy) by acquiring intensity transmission data at normal incidence and fitting these data simultaneously with the VASE® data (examples will be given further on). On an opaque substrate, this problem may sometimes be solved by acquiring reflectance data (polarized or unpolarized) at some oblique angle of incidence.

A useful general procedure when analyzing complex samples is to start with reflectance VASE® data and see if the desired analysis can be performed uniquely. If not, add more data. Take a transmission scan at normal incidence if the sample is transparent. If not, acquire p- or s-polarized reflectance (but not both) at the same angles of incidence that the VASE® data were acquired at. Note that only two of the three quantities (psi, p-plane reflectance, s-reflectance) at a given wavelength and angle are independent, as any one may be calculated from knowledge of the other two. If this is still not enough information to uniquely solve the desired model, you are out of luck if the substrate is opaque. In this case try simplifying the model...
and/or eliminating some fit parameters. If the substrate is transparent, try acquiring VASE® data through the substrate in reflection or transmission.

In the following sections we discuss means to optimize the acquisition of the various data types with the J. A. Woollam Co., Inc. VASE® instrument. In all cases what we are trying to do is acquire data with the experimental configuration as close to ideal as possible, while maximizing the signal-to-noise ratio of the experiment.

There are several experimental parameters which the user controls. These are:

- The wavelengths at which data are acquired.
- The angles of incidence at which data are acquired.
- The sample alignment and surface quality.
- The spectral bandwidth of the light beam, via the monochromator entrance slit. A good default for PTI monochromators is to open the screw two full turns from fully closed. The maximum default slit width for CVI monochromators is 2000 microns.
- The intensity of the beam via the sliders on the PTI monochromators.
- The diameter of the beam, by leaving the alignment detector in or out.

Leaving the alignment detector in reduces the beam size but also reduces the signal intensity.

- The size of the beam on the sample, through choice of beam diameter and angles of incidence. Very small or very non-uniform samples may force you to leave the alignment detector in and/or acquire data at low angles of incidence.
- The width of the aperture at the front of the detector-analyzer assembly.

A good default is to set this aperture slightly smaller than the size of the light beam.

In the following sections we discuss modifications to the above default settings for optimizing the acquisition of the different data types allowed by the J. A. Woollam Co., Inc. VASE® instrument.

12.5 Simulation of optical experiments with WVASE®

Simulating experiments in advance can save you a lot of time in the long run!

The ability of WVASE® to calculate most types of optical data from any optical model defined in the model window provides the user with a powerful means of optimizing the experimental data set for a given sample, provided the nominal structure of the sample is known. When this is the case, the user can build the nominal model in the model window and predict the expected psi and delta data (or reflectance, transmittance, or any other optical data type) for this model. If the true sample structure is reasonably close to the nominal model, the simulation of data for the nominal model can be used to locate angles of incidence where delta is close to 90°, and can also be used to estimate the sensitivity of the ellipsometric (or other optical) measurements to parameters in the model.

12.6 Ellipsometric data acquisition

In this section we review the procedures and strategies for acquiring the various types of ellipsometric data, both in reflection and transmission modes.
Reflection from the top of the sample

This is the most common mode of data acquisition. This is the most commonly acquired data type, and most sample analyses can be performed from reflection VASE® data alone. The default settings given above should be good in most applications. Note that the some trade-offs are available. Random noise in the data can be reduced by increasing the signal intensity. This may be achieved by opening the input slit to the monochromator further, at the expense of increased bandwidth of the beam. If the acquired data does not show strong dispersion this is a very good trade-off, but if there are sharp spectral features in the data they may be ‘smeared out’ by the larger bandwidth. Random noise in the data may also be reduced by acquiring data with the room lighting off, or with a hood of some sort over the instrument. This is particularly useful when attempting to acquire data from samples which exhibit very low reflectance or when acquiring data at very short wavelengths (<300 nm).

Note that although the VASE® instrument is only specified to work at wavelengths of 250 nm or longer, good data may often be acquired below this wavelength by acquiring the data with the room lighting off and averaging many cycles of the analyzer (75-100, typically). It may be helpful in this case to sacrifice some spectral bandwidth and open the entrance slit to the monochromator further as well in order to increase the signal magnitude at the detector.

Reflection from the bottom of the film, beam incident through the substrate

This data type is useful for metal films or multilayers on glass substrates.

This type of data can be very useful when examining coatings on glass or other transparent substrates with polished back surfaces. The acquisition is performed in exactly the same manner as standard ellipsometric data, except that the sample is mounted ‘upside down’ such that the coated surface of the substrate faces the sample chuck and the beam is incident on the back surface of the substrate. After the acquisition is complete, the ‘Change data type’ option from the Experimental Data window must be used to change the data type to ‘Ellipsometric from the reverse direction’, and the data should be saved.

When acquiring data from the back of a coated transparent substrate, two light beams will be visible in reflection from the sample (it is helpful to move the monochromator to ‘white light’ in order to see these beams). The first beam is reflected from the back surface of the substrate, which is the first interface that the light beam encounters. This beam contains no useful information, as none of the photons in it have ‘seen’ the coating on the back of the substrate. The second beam is reflected from the coated side of the substrate, and it is this beam that we wish to measure. This measurement is not trivial, however, as the two beams tend to overlap somewhat.

The best possible data are obtained when the substrate is thick enough that the two reflected beams do not overlap. In this case it is possible to collect only the second beam at the detector by translating the sample stage along the sample (see sample alignment procedures section in this manual) until the second beam is centered on the detector iris. When analyzing such data the ‘% of first reflection collected’ parameter in the options dialogue box from the Model window should be set to zero and not varied.

Useful data may also be obtained if the substrate is very thin (< 1 mm or so) such that the two beams completely overlap at all angles of incidence for which data are to be acquired. In this case only one beam will be visible in reflection from the sample, and the ‘% of the first reflection’ parameter in the ‘Options’ dialogue box.
from the Model window should be set to 100% and fixed. In both cases the number of back-surface reflections which are collected should be defined as a fit parameter.

The most difficult case is when the two beams reflected from the sample partially overlap at the detector. In this case it is not possible to isolate the useful second reflection, and the degree of overlap will change with angle of incidence. When this happens, it may be possible to analyze data acquired at a single angle of incidence, but the change in overlap with angle of incidence will preclude fitting more than one angle of incidence at a time.

Transmission ellipsometry

This data type is very useful for films or multilayers on glass substrates.

Transmission ellipsometry data can be very useful for decorrelating the analysis of multilayer films on transparent substrates and thin absorbing films on transparent substrates. It is a rather difficult measurement to perform, however, and may not yield accurate data if the substrate is thick (> 2 mm or so). To perform this measurement, set the sample stage and detector arm in the straight through position, as if you were going to perform a normal incidence transmission measurement. Mount and align the sample, and then rotate the sample stage by hand to the desired angle of incidence (you will only be able to acquire one angle of incidence at a time, as we do not want the detector arm to move). You may need to be somewhat clever in mounting the sample in order to get the transmitted beam through to the detector iris. Set the monochromator to white light and examine the beam incident on the detector iris. If the substrate is fairly thin, the beam should be close to centered on the iris. If the substrate is thick, diffraction of the beam by the sample results in an offset of the beam path from the true straight through path, and the center of the beam will be offset from the detector iris. DO NOT rotate the detector arm to center the beam on the detector iris. The displaced beam is still parallel to the original beam path, and rotating the detector arm will cause the beam to travel at an angle through the analyzer and detector, leading to bad data. About the best you can do in this case is to open the detector iris wider and hope to collect at least some of the transmitted beam.

When ready to acquire a scan, check the Hardware window to see what WVASE® ‘thinks’ the angle of incidence is. Acquire a spectral scan at this angle, such that WVASE® does not try to change angle of incidence. You can save yourself a lot of hassle by using the following procedure:

1. Put the arms in the straight through position.
2. Mount and align the sample at the desired angle of incidence.
3. Use the ‘Current motor settings’ option from the Hardware window to set the angle of incidence. If you aligned the sample at 70 degrees angle of incidence, for example, set the sample stage position (in the Current motor settings dialogue box) to 70 and the detector arm position to 140. This does not mean that the goniometers are at these positions, we are ‘fooling’ WVASE® into thinking they are. This is a very useful trick for performing custom optical experiments.
4. Acquire a spectral scan at the given angle of incidence (70 degrees for our example). WVASE® will not try to move the goniometers, as it thinks that they are already at 70 degrees, and the angle of incidence will be stored as 70 degrees for the experimental data.
5. Use the ‘Change data type’ option from the Experimental Data window to change the acquired data type to ‘Ellipsometric transmission’.
6. Save the data.
Note that if \textit{WVASE}® thinks the angle of incidence is different from the true angle between the sample normal and the incident beam, an incorrect angle of incidence will be stored with the data and you will find it very difficult to fit the acquired data (or worse you will fit the data and obtain incorrect results). Be very careful to check the stored data to make sure that the stored angle of incidence (second column of numbers in the data file) matches the angle at which you positioned the sample to acquire.

12.7 Advanced spectroscopic scans

These scan types are useful for acquiring very accurate data and handling non-ideal samples.

The spectroscopic scan dialogue box contains a button labeled ‘Change settings’. Clicking on this button will open a dialogue box which allows the user to select the type of spectroscopic scan which will be performed. There are two types available, and a bullet appears next to the selected type. The first type is the ‘standard’ spectroscopic scan, which is the default. This type of scan measures psi and delta using a single polarizer setting. This is very quick, and in most cases yields very clean data.

The second advanced scan type is the anisotropic calibration scan. This scan is the same as the second type, the standard calibration scan, except the calibration scans are fit to determine not only psi and delta, but ratios of the off-diagonal sample Jones matrix elements to the diagonal elements, effectively characterizing all four elements of the sample Jones matrix. Again, try using 9-15 points over a 180° range of the polarizer, and be prepared for very long acquisition times. See chapter 6 - ‘The Experimental Data Window’, in the section on data types, for an explanation of the generalized anisotropic data types generated by these scans.

12.8 Acquisition of dynamic data

Dynamic data are acquired as a function of time from a sample which is being processed or modified in some way.

The ‘dynamic scan’ option from the ‘Acquire data’ menu in the hardware window will allow the user to acquire ellipsometric data at one or wavelengths and angles of incidence as a function of time. Selecting this option opens the dynamic scan dialogue box, from which the user may select either one or more discrete wavelengths at which the data are to be measured or a spectroscopic range for acquisition as a function of time. The \textit{VASE}® will then acquire data at the specified angles and wavelengths, and will continually repeat the acquisition, plotting the results as a function of time on the screen until the user terminates the acquisition by pressing the <esc> key.

This type of acquisition is very useful for monitoring time dependant processes such as chemical reactions, photoresist curing, and oxidation of surfaces. See chapter 16 - ‘M-44® Data Acquisition Procedures and Strategies’ and chapter 17 - ‘Dynamic Data Analysis’ for more information on acquiring and analyzing dynamic (time dependant) ellipsometric data.

12.9 Acquisition of intensity transmittance data

Intensity transmission is very useful for samples with transparent substrates.

Next to standard \textit{VASE}® data, intensity transmittance at normal incidence is the easiest to acquire and most generically useful data type. This type of data may only be acquired from film/substrate systems which are not completely opaque. To acquire transmission data at normal incidence use the following procedure:
• Set the sample and detector stages to the straight through position. The light beam should pass through the hole in the center of the sample stage, and should not contact the edge of this hole.

• Place the alignment detector in its socket and leave it there. This reduces the beam diameter significantly.

• Open the detector iris completely.

• Minimize the ambient lighting as much as possible. Turn off room lights, reduce the intensity of any computer screens which are on, etc.

• Select ‘R&T’ data from the ‘Acquire data’ menu in the Hardware menu.

• Select the appropriate spectral range, and set the initial and final angles of incidence to zero, with some non-zero increment. Select ‘Baseline and data’, and 10-20 revolutions per measurement. Select Return (or ‘OK’) when all parameters have been correctly set.

• WVASE® will prompt you to put the arms in the straight through position (you should have already done this) for the background scan. Select ‘OK’ and WVASE® will measure the intensity of the beam without the sample present at each specified wavelength.

• You will be prompted to move the goniometers to whatever angles WVASE® thinks they were at before the acquisition. Ignore this message and leave the goniometers in the straight through configuration.

• You will then be prompted to mount the sample and translate the beam on the detector. All you need to do is mount the sample. Do not move anything else in the instrument. When the sample is mounted, select ‘OK’ or hit return. WVASE® will measure the intensity of the beam with the sample in place at each specified wavelength. It will then calculate the transmission from the ratio of these values to the background values.

• When done, WVASE® will ask you if you wish to save the data. The data will be saved as transmission data, so you do not need to change the data type before saving.

Note that there are three options available when the R&T acquisition option is selected. Acquiring a baseline scan will allow you to view the relative intensity of the light beam as a function of wavelength. This is an informative experiment to perform, as it is the product of this intensity with the sample reflectivity which determines the signal strength at the detector for a given wavelength. Select ‘baseline only’ and perform the scan with no sample in place, and then display ‘transmission’ from the graph window. The intensity of the light beam as a function of wavelength will be displayed.

If you need to acquire a lot of transmission scans quickly, the same baseline may be used for multiple samples. Acquire ‘baseline and data’ for the first sample, and then use the ‘data only, using previous baseline’ option to measure subsequent samples. Do not try this unless the system has been turned on for at least 30 minutes or so, as the light source requires about this much time to stabilize.
12.10 Acquisition of intensity reflectance data

Intensity reflectance may be a last resort when correlations are a problem for a sample on an opaque substrate.

The acquisition of intensity reflectance data with the VASE® instrument requires some care. Reflectance data may not be acquired at normal incidence, as the finite size of the source and detector arms prevents positioning at angles of incidence less than about 12°. Therefore, reflectance may only be measured at oblique angles of incidence. At oblique incidence, three types of reflectance data may be acquired, depending on the polarization state of the incident beam. P-polarized reflectance may be acquired when the input beam is linearly polarized with the beam polarization in the plane of incidence. s-polarized reflectance may be acquired with the incident beam polarized in the s-direction, and reflectance data may be acquired with the incident beam linearly polarized along any arbitrary direction specified by the user. The polarization type is specified by the user when the R&T acquisition option is selected from the Acquisition menu. Please note that for a given angle of incidence, the three measurable quantities psi (VASE® data), p-polarized reflectance and s-polarized reflectance are not independent, as knowledge of any two of these quantities is sufficient for calculation of the third, therefore it is pointless to acquire all three for a given sample. We usually acquire VASE® data and then p-polarized reflectance at the same angles as the VASE® data were acquired.

The procedure for acquiring reflectance data is similar to that used for transmission data in that a background scan must be acquired in the straight through configuration to determine the intensity of the incident beam.

The general procedure for acquiring reflectance data from a given sample is as follows:

- Use the ‘Change angle of incidence’ option to move the angle of incidence to whatever the lowest angle of incidence that you wish to acquire reflectance data is. For example, if you are going to acquire reflectance data at 60°, 65°, and 70° angle of incidence, move the angle of incidence to 60°.
- Set the sample stage and detector arm to the straight through configuration.
- Mount the alignment detector and open the detector iris all of the way.
- Turn the room lights out and reduce the ambient lighting as much as possible.
- Select ‘R&T data’ from the Acquire data menu from the hardware window.
- Select the appropriate wavelength range and range of angles of incidence in the dialogue box which appears. You will also need to specify the polarization of the input beam, either by selecting p- or s-polarized reflectance or by specifying a polarizer angle.
- Click on ‘OK’.
- The VASE® will acquire the background scan. When done, you will be prompted to return the sample and detector goniometers to the original position (which should be the first angle of incidence of your scan).
- Mount the sample, and translate the sample stage along the sample normal to center the reflected beam on the detector. You will need to close the detector iris in order to do this. When centered, open the detector iris all of the way and hit ‘OK’.
- The VASE® will acquire the reflectance data at each specified angle of incidence. When the acquisition is finished you will be prompted to save the data.
13.1 Introduction

Ellipsometry is an indirect experimental technique in that the measured quantities in an ellipsometric experiment are not directly physically significant. An ellipsometric experiment constitutes the measurement of the polarization state of a beam of light after reflection from (or transmission through) the sample under test. The measured ellipsometric data must then be modeled in order to infer useful information about the sample under test.

It is this modeling process that is usually the most intimidating to the new VASE® user. The analysis of ellipsometric data is (wrongly) considered by many to be more of an art form than a science, even though all principles and techniques involved are purely analytical. In the development of the WVASE® software, it has been our goal to provide the VASE® user with a user-friendly means of obtaining useful physical information from any sort of ellipsometric data. In this section we outline how to perform the analysis of the ellipsometric (or reflectance or transmission) data from any type of sample. Some useful general principles are presented first, followed by discussions of the analysis procedures used for many different types of samples.

13.2 Modeling of experimental optical data

There are three parts to any optical experiment, such as reflectance, transmittance, or ellipsometry. The first part is the experimental measurement of some optical quantity from a given sample, such as intensity reflectance, transmission, or the ellipsometric parameters of the beam reflected from the sample. This part of optical experimentation was discussed in the previous sections, with particular emphasis on the use of the J. A. Woollam Co., Inc. VASE® for these experiments. The second part involves the inverse problem of extracting physical information about the sample under study from the measured light intensities or polarization states. The third step, which is often neglected (often with disastrous results) is the determination that the physical model obtained from the second step is indeed unique. In other words, once a model has been found which fits the available optical data well, it is necessary to show that there are not other models which will also yield the same fit to the experimental data. In this section we discuss the modeling of optical data and the determination of uniqueness of a given model.
Building the ‘most physical’ model

It is a commonly held belief that the ellipsometer is an all-powerful instrument which can tell you everything about an unknown sample without any prior information as to the structure or composition of the sample. This belief has been bolstered by many who are happy to claim that the instrument can indeed perform such ‘blind’ analyses. In actual fact, it is generally necessary to have some knowledge of the structure and composition of the sample under study in order to obtain any useful information whatsoever about the sample.

The construction of an accurate optical model for the sample under study is a critical part of any optical experiment. This is an involved topic, and there is a huge body of literature devoted to the modeling of optical data. In the following sections we will discuss strategies for developing accurate models for many classes of materials and sample structures. There are some general guidelines which the user may find helpful, all of which may be summed up by the following general advice. Find out everything you can about the sample you are attempting to analyze. Useful information includes (but is by no means limited to) the following:

- What is the substrate? How was it cleaned and processed? Was any native oxide or residue removed prior to any depositions? Is the substrate rough, and if so, how rough?
- How many films or coatings are on the substrate? What are the coating materials? How were the coatings deposited, and was the sample processed (annealed, for example) after deposition.
- Are the coatings well segregated, i.e., are the interfaces in the sample abrupt, or is there a gradual transition from one material to another?
- Are the coatings homogeneous along the film normal? ITO and titanium dioxide films are almost invariably non-homogeneous, and data from such structures must be modeled in such a manner as to account for such inhomogeneity.

Keep in mind that all optical experiments are model dependent. Any inaccuracies in the fixed parameters in the optical model (substrate optical constants, for example) will lead to inaccuracy in the fitting results.

Correlation and uniqueness

The final stage of any optical experiment is to prove that the best-fit result obtained from the modeling process is unique. In other words, there is only one set of values of the model parameters which will best fit the experimental data. This seemingly obvious requirement is ignored in many of the ‘canned’ optical analyzers which are available on the market today. Non-unique results indicate that two or more of the parameters in the model are strongly correlated, and the parameter set must be reduced (or more independent experimental data must be added to the fit) in order to eliminate the correlations. The WVASE® software provides some powerful tools for the determination of uniqueness and the elimination of correlation problems in models.

Let us say that you have performed a fit to a given set of data, and now you wish to determine if the fit is unique and the parameters in the model are not strongly correlated. There are some easily identifiable symptoms of non-uniqueness and correlation which you may spot during the fit:

- The fitting algorithm makes a lot of iterations, each of which reduces the mean-squared error (MSE) only slightly. This is caused by strong parameter correlations, as the algorithm cannot determine which of the correlated parameters to
adjust, or how to adjust them. It will make slight adjustments at each iteration, which have a minimal effect on the MSE. If the parameter set is uncorrelated and the model is physically accurate for the given sample, the algorithm will usually minimize the MSE in a few iterations.

- The fit parameters change radically with each iteration, yet the MSE does not change very much. Common sense would indicate that if a large change to one of the variables does not significantly change the MSE, there is no well defined best-fit value for that parameter. This may be due to correlation, or the MSE may not be sensitive to the given parameter. Thicknesses are good to watch for this. Watch one of the thickness values during the fit. If it changes a lot between iterations but the MSE does not change, your best-fit model will not be unique.

- Use the ‘Stats’ (statistics) option from the Fit window to calculate the sensitivity correlation matrix and the confidence limits on the variable parameters after the fit. Any element in the correlation matrix (other than the diagonal elements, which are always 1) which approaches 1 or -1 indicates a very strong correlation between two of the parameters in the model. Also, any parameter which has an unreasonably large 90% confidence limit (for example a layer thickness of 50 ± 75.3 Angstroms) is either strongly correlated to some other parameter (which will also have an unreasonably large 90% confidence limit) or does not effect the experimental data (such as a layer thickness buried under a thick absorbing film).

Throughout the following sections we will indicate types of analyses which are often prone to strong correlation or uniqueness problems, and indicate ways to alleviate these problems.

### Interpretation of confidence limits

Determining appropriate confidence limits for the fit parameters can be a confusing issue because many assumptions are used in transforming the experimental uncertainties into fit parameter error bars. This section discusses the validity of these assumptions and the appropriate interpretation of confidence limits when the assumptions may be violated. The basic assumptions are as follows: (1) Measured \( \psi \) and \( \Delta \) values are independent, normally distributed random variables (meaning that the errors in \( \psi \) and \( \Delta \) describe a Gaussian distribution about zero) and accurate standard deviations of the measured quantities, \( \sigma_{\psi}^{\text{exp}} \) and \( \sigma_{\Delta}^{\text{exp}} \), are available. (2) The final fit is "good," in that the differences between the model-calculated values and the experimental values are random with a normal distribution and the same deviations as the measured values. (3) The derivatives of the mean-squared error with respect to the fit parameters (used to evaluate the correlation matrix and 90% confidence limits) are valid over a wide enough range that the experimental deviations can be linearly mapped over to the fit parameter deviations. (4) Correlations between the fit parameters are small enough that individual standard deviations can be assigned.

(1) The usual assumption of normally distributed random measurement errors is made because a \( \chi^2 \) minimization assumes it. In fact, this may be a reasonable approximation even for complicated measurement quantities like \( \psi \) and \( \Delta \), but it can not be universally true. For example, a normally distributed error in \( \psi \) is impossible if \( \psi_{\text{true}} \to 0 \), since \( \psi_{\text{meas}} \geq 0 \). In addition, confidence limit accuracy is directly related to the accuracy of \( \sigma_{\psi}^{\text{exp}} \) and \( \sigma_{\Delta}^{\text{exp}} \). For a rotating-analyzer ellipsometer, these values can be approximately measured using multiple analyzer revolutions. (Data are averaged over multiple revolutions in any case, to improve the signal to noise ratio.) Note that for a biased fitting procedure, only the relative
magnitude of the standard deviations is important; relatively noisy spectral regions 
(\(\Delta \approx 0.180^\circ\), or low light intensity) contribute less to the overall fit. If all the 
measurement standard deviations are scaled by the same amount, the same final set 
of fit parameters will be obtained, but the resulting calculated standard confidence 
limit will change. This is in contrast to our figure of merit, which would remain 
unchanged. Certainly, relatively weighted \(\sigma^\text{exp}_\psi\) and \(\sigma^\text{exp}_\Delta\) can be found for proper 
baised fitting, and with increasing measurement time, increasing absolute accuracy 
for \(\sigma^\text{exp}_\psi\) and \(\sigma^\text{exp}_\Delta\) can be obtained. The assumptions of normal distributions for, and 
independence of all \(\psi\) and \(\Delta\) measurements are difficult to prove when acquiring a 
large amount of data. However, our experience is that whatever assumptions are 
made about measurement errors, the analysis (fitting), described next, is the larger 
problem.

(2) The most questionable assumption is that the differences between 
experimental and calculated model values are normally distributed with the same 
standard deviations as the measurement process. The normal distribution assumption 
implies that there are no systematic errors in either the measurement process or in the 
parametric model. The acquired standard deviations deal only with measurement 
precision. Calibration errors, incident angle errors, monochromator offsets, finite 
optical bandwidth, detector nonlinearity, etc. are systematic errors and should not be 
mixed with the random noise errors. These systematic acquisition errors must either 
be reduced to insignificance (by improving the hardware) or included in the model 
calculation (by fitting a correction term such as the angle of incidence). The 
hardware correction is of course preferable, since the correction term may be 
imoossible to calculate, or the term may be correlated to other more desired 
parameters being fit. Other systematic errors, unrelated to measurement accuracy, 
appear due to incorrect model assumptions about fixed optical constants, interface 
quality, thickness uniformity, etc. (One can not fit for every possible model or 
measurement imperfection simultaneously.) Systematic model errors include 
propagated errors from previous optical constant measurements, and therefore may 
be more important than acquisition errors.

Systematic errors severely limit an objective determination of the "goodness 
of fit" based on the normal distribution assumption. If random measurement errors 
really are dominant then the "good" fit limit of our test function is 
\(\xi_2 \rightarrow \{\text{MSE}^2 \rightarrow 1\}\). However, this statistical test relies heavily on the absolute accuracy of the 
experimental standard deviations. If the standard deviations are scaled improperly, 
then unrealistic low (or high) test function values can be obtained. As pointed out 
earlier, however, an improper scaling does not change the final fit parameter values. 
If the standard deviations used are not directly acquired from the measurement 
process, then no objective "goodness of fit" is available. In any case, the final 
minimized \(\xi_2^2\) for a particular fit can be used in a relative sense when comparing 
results between fits with similar models and measurement conditions.

There are some simple tests for the presence of systematic errors based on 
the idea that when random measurement errors are dominant, the experimental data 
will tend to be randomly above and below the model fit. No localized spectral 
region should contribute excessively to the test function \(\xi_2^2\). However, in our 
experience, the vast majority of fits to spectroscopic ellipsometry (SE) data have 
some spectral regions that fit less well than others, where the experimental values 
tend to be either all above or all below the model fit. Even if the total number of 
points above the model equals those below over the whole spectrum, these groupings 
by wavelength are statistically so improbable, that they must indicate systematic 
errors not accounted for in the model. A more objective test for the presence of 
systematic errors is to acquire two spectroscopic scans at different signal integration
times. Measure $\psi$, $\Delta$, and the standard deviations, and then perform the same biased fit with both spectra. If both fits produce the same overall $\chi^2$, then the assumption of random errors dominating is probably acceptable. (This does not imply however that the standard deviations have the correct absolute magnitude for confidence limit calculations). If $\chi^2$ decreases as the integration time decreases, then systematic errors are dominant at long integration times when random errors are reduced by averaging. For shorter integration times, random noise dominates, leading to a $\chi^2$ closer to the ideal value of one. The consequences of systematic errors are that the confidence limits determined using the normal error distribution assumption are not accurate, and that the usual $\chi^2$ "goodness of fit" test indicates the model is very unlikely. This second point is exactly correct though, because systematic errors by definition imply that the model is incomplete. This however should not mask what may be an excellent set of model parameters, accounting for all of the important spectral features except for limited regions with systematic errors. The sheer complexity of fitting SE data makes a completely objective "goodness of fit" determination problematic.

(3) The linearity of the transform from experimental errors to parameter confidence limits is less of a problem. For very noisy experimental data, this assumption may be violated, but the analysis is not very meaningful in that case anyway. The experimental deviations can in principle be reduced arbitrarily by increasing measurement time. Thus this assumption does not impose a fundamental limitation.

(4) Assigning an independent confidence limit to a fit parameter does require that the parameter be uncorrelated. This is usually a simple matter of checking the two-parameter correlation coefficients given by

$$S_{jk} = \frac{C_{jk}}{\sqrt{C_{jj} C_{kk}}}.$$  

(13.1)

An absolute value of $r_{jk}$ near 1 indicates correlation between the $j$th and $k$th fit parameters. The correlation coefficients, computed from the same covariance matrix as the confidence limits, are much less dependent on the absolute magnitude of the standard deviations, because those terms tend to cancel in the ratio. Thus the correlation coefficient can be objectively evaluated even when the confidence limit cannot. This two-parameter correlation check may not, however, reveal correlation which involves three or more parameters.

From our experience of fitting SE data, we have adopted the mean squared error (MSE) to describe our confidence in the fit parameter. We specifically reserve the use of "confidence limit" to cases when all the necessary assumptions can be proved true. In those cases, our FOM reduces to the usual SCL anyway. Unlike other examples where the standard deviations are defined after an unbiased fit, our procedure includes the proper relative weighting between $\psi$ and $\Delta$, and among data pairs throughout the spectral region. Only at the end are the standard deviations rescaled, and then in a manner that leaves the final fit parameters unchanged.

Whereas "confidence limit" implies a direct connection to the sample under study, our FOM is more properly interpreted as describing the combined measurement and fitting process. Our FOM combines information about the sharpness of the fit minimum ($C_{ii}$) and the overall quality of the fit ($\chi^2$). Our FOM does give useful information when comparing fit parameters from within a single fit, or when comparing the fits from samples measured and analyzed in the same way. These are two important cases where our FOM’s are quite useful on a relative basis, if not in absolute magnitude. When fitting multiple parameters from a single set of data, one can correctly compare the FOM of two uncorrelated parameters to
determine which is more sensitive to the data. For example, a 5 nm surface oxide thickness will have a much smaller FOM than will the thickness of a nominal 5 nm layer of material A buried below 100 nm of material B in the same sample. In this case, the ratio of FOM's is a useful number. A second example of FOM utility is in the case of quality control for a group of samples with nominally the same structure measured under the same conditions. For example, if the last sample in a series of optical coatings indicates a change of 50% in thickness over a well established baseline value and the confidence limit as a percentage is unchanged, one can believe the fit-for thickness rather than suspect an error in the measurement/fitting procedure. The real test of obtaining "true" (absolutely scaled) confidence limits from the FOM would require a great deal of work with many data analyses on samples well characterized in other ways.

Errors due to random noise

The ellipsometer is a very precise instrument, particularly when the data are averaged over at least 30 cycles of the analyzer. As a result, the precision of the fit results will usually be very high, and the effects of random noise in the data on the results of the fit are usually negligible. Exceptions will occur when fitting directly for the optical constants of a film (or the index of refraction of a transparent film) at each measured wavelength. In this case, random noise on the experimental data may be mapped directly into the best-fit optical constants, such that random errors will occur in the optical constant values. This is particularly noticeable when fitting noisy data or data in which delta approaches 0° or 180° (for data acquired without the use of a variable retarder). Usually, structural parameters such as thicknesses, EMA fractions, and grading parameters will not be affected by the degree of random noise in the data.

If noise in the optical constants is problematic, there are two means of eliminating the noise. First, the data can be reacquired with the ellipsometer configured for lower noise. Ways to achieve lower noise in the data are:

- Open the monochromator slit further (manually on PTI monochromators, by increasing the default slit width for CVI monochromators) to increase the light beam intensity.
- Open the detector iris, but not larger than the beam.
- Average more cycles of the analyzer per measurement.
- Turn the room lights off.
- Acquire more angles of incidence, and try to make sure that for every wavelength there is at least one angle for which delta is not close to 0° or 180°.
- Use the advanced scan options button from the spectroscopic scan window to select standard calibration scans rather than standard VASE® scans. This is very time consuming but generates the best possible data.

If the data cannot be improved, or you simply do not have the time to try reacquiring the data, it is possible to eliminate noise from the optical constants by using a parametric model for the optical constants of the material under study. In other words, rather than fitting for the values of n and k directly at each measurement wavelength, we use a functional parameterization of n and k as functions of wavelength, and fit for parameters in the functions which yield n and k as functions of wavelength. A well chosen parametric function will be flexible enough to reproduce the true optical constants of the material, contain a relatively small number of variable parameters, and will be continuous such that abrupt fluctuations and
discontinuities cannot occur, eliminating the incorporation of random experimental noise into the resulting optical constants.

There are several optical constant parameterizations provided explicitly with WVASE®, and it is a simple matter for the user to enter their own functions for n and k and declare any parameter in these functions as fit parameters. The various types of parametric models for material optical constants are discussed later in this chapter. The parameterizations appropriate for different materials are listed below:

- Transparent materials: Cauchy or user-defined dispersion model.
- Transparent material with absorption edge in the UV: Cauchy with Urbach absorption, or user-defined dispersion model.
- Semiconductors: Lorentz oscillators or parametric semiconductor model.
- Alloy semiconductors: Various alloy models, with n and k parameterized as functions of the alloy ratio.
- Metals, other absorbing materials: Lorentz oscillators.

All of these parameterizations are discussed with examples of when and how to use them later in this chapter.

Systematic errors due to model deficiencies

The VASE® is a very precise instrument, but rigorously determining the accuracy of the VASE® instrument is not possible. The precision of the instrument is defined primarily by the repeatability of the experimental measurement, and to a lesser degree by the stability of the variable parameter set in the optical model used to fit the experimental data. For the VASE® instrument, the experimental data are usually very repeatable. As long as the model used to fit the data is unique and does not contain very highly correlated parameters or parameters to which the measured data are not sensitive (for example trying to determine the thickness of a film underneath a 1 micron aluminum film!), the results of the fit will be very reproducible as well, and the total results of the sample characterization will be of very high precision.

The accuracy of the VASE® analysis of a sample is also determined by both the VASE® instrument itself and by the model used to fit the experimental VASE® data. The accuracy of the measured psi and delta values will depend on the accuracy of the calibration parameters, the quality of the instrument, beam, and sample alignment, and on the stability of the instrument. These factors are controllable, and usually do not contribute significant inaccuracies to the measurement. One way to gauge the accuracy of the VASE® is to acquire a spectroscopic scan in the straight through configuration, with no sample, such that the light beam leaves the input arm and travels straight into the detector. If the calibration parameters are accurate, this will yield, for all wavelengths, measured psi values within a few hundredths of a degree of 45°, and measured delta data within a few degrees of 0°. Also, the difference between the measured psi and 45° should be random, as any offset of the measured psi from 45° that occurs over the entire measured spectral range is probably indicative of an error in the calibration of the polarizer axis.

The accuracy of the VASE® analysis of a sample is critically dependant on the accuracy of the optical model used to fit the experimental data. There are many assumptions and approximations required to build the optical model in WVASE®.

- The light beam entering the detector is completely polarized. Approximate corrections for depolarization due to back-surface reflection, film non-
uniformity, patterned films, non-zero monochromator bandwidth, and angular spread of the beam are included as options in the WVASE® optical model. Significant roughness (greater than 100 nm or so in any dimension) may cause depolarization which cannot be modeled with WVASE®.

- All interfaces between layers, the ambient, and the substrate are abrupt and perfectly flat. Anyone who has seen TEM (transmission electron microscopy) pictures of many thin films knows that this is definitely an approximation. There are approximate means of dealing with surface and interfacial roughness (using effective medium models) implemented in WVASE®.
- All films and the substrate (unless explicitly specified to the contrary) are uniform along the direction normal to the sample surface. Approximate means of grading the optical constants of a film are included in WVASE®.
- All films and the substrate (unless explicitly specified to the contrary) are isotropic.
- The optical constants used for any layer in the model or the substrate which are held fixed exactly describe the corresponding material in the sample.

The final assumption is usually the most important in determining the accuracy of the results of a VASE® analysis, and is also the most frequently and flagrantly violated assumption in the list. It is almost never possible to fit for more than one set of optical constants at a time (exceptions occur with very highly constrained parametric models), such that if the sample is more than just a bare substrate, some optical constants must be assumed for the substrate and/or one or more films in the sample. In some cases, the optical constants of a given material are very well known from prior measurements or from the literature. Examples of very well known optical constants are those of non-degeneratively doped crystalline silicon, amorphous silicon (non-hydrogenated), gallium arsenide, most crystalline semiconductors, and silicon dioxide grown thermally on silicon. In most cases, particularly for thin films, literature optical constants are not accurate, and the results of modeling experimental data using inaccurate optical constants for one or more materials in the model will be correspondingly inaccurate, even thought the 90% confidence limits may be very small.

For this reason, it is generally a good idea to approach multilayered structures by first characterizing single films of the materials in the structure to obtain thin film optical constants which should be accurate for the film in a multilayer. It is also wise to know as much about the sample structure as possible prior to modeling, such that you can construct an optical model which is as accurate as possible.

As a final point, the inaccuracies induced in the best-fit model parameters by errors in the model will generally scale with the thickness of the film under study. Results for the thickness and/or optical constants of a very thin film will be very strongly affected by even slight inaccuracies in the rest of the model, while results for the thickness and/or optical constants of a thick film will tend to be much less sensitive to inaccuracies elsewhere in the model.

Assessing the quality of a fit

Once a best-fit model is obtained, how do we tell whether the fit to the experimental data is adequate. In other words, does this model adequately describe the experimental data, or is further modification of the optical model required? This is a difficult question for which there are no set answers, but there are several general principles that are helpful when assessing the quality of a fit.
First, keep in mind that there is no arbitrary standard of fit quality, and the evaluation of a given model for a sample is with respect to other possible models for the same sample. Often, the best fit obtainable without strong parameter correlations in the model is the best model for the sample, however this model may be unphysical and as a result may not be acceptable. Try many different models (with and without surface and/or interfacial roughness, index grading, etc.) for the same sample and compare the fit quality (as represented by the final MSE) for each model.

Second, examine the best-fit calculated and experimental data in the Graph window. Are there features in the experimental data that are not evident in the calculated data? If so, the model is obviously deficient, and modifications to the model should be made to try and fit the features in question. It may not be possible to do so and still obtain a unique model, but it is always worth trying. Also, it is very helpful when comparing experimental and calculated data to use the ‘Difference between Gen. and Exp.’ option from the ‘Data’ menu from the Graph window. Selecting this option instructs WVASE® to subtract the experimental data from the calculated data and plot the result (note that the ‘Type’ menu from the Graph window is used to select whether psi or delta or some other data type is plotted). In the ideal case, a difference plot for psi or delta (or any other experimental data type) for the best-fit model should yield a very noisy spectrum which is randomly distributed around zero, as shown below.

If the model is deficient in describing the experimental data, the differences between the experimental and calculated data will show systematic trends rather than being randomly distributed about zero, as shown below.

Figure 13.1. The difference between the calculated and experimental psi data, shown for a very good fit. Note that the errors are approximately random and evenly distributed around zero.

Figure 13.2. The difference between the calculated and experimental psi data for a best-fit model which does not completely describe the sample. Note the systematic increase of the error towards the short wavelength end of the spectrum.

Again, it may not be possible to find a unique model which eliminates all systematic features in the differences between the experimental and calculated data, in which case you should try to find the unique model which minimizes the systematic deviations of the differences from zero.
Finally, the best-fit model must be evaluated to determine whether it is a physically reasonable description of the sample. This determination, as well as other checks on the best-fit model, are described in the next section.

Assessing the quality of a best-fit model

Once a unique best-fit model is obtained, we must examine this model to gauge whether it is physically reasonable. There are a number of factors which must be considered for this evaluation, but again there are no fixed rules, only general guiding principles, and much is left to the common sense of the user.

First, how do the resulting layer thicknesses match up to the nominal layer thicknesses? Are there any thicknesses which are very far from the nominal, and if so, is there a reasonable physical explanation for the thickness in question deviating grossly from the target value? This criterion must be applied with care, as depositions are notoriously imperfect (human error is often a factor here!), and a film thickness which differs greatly from the target value may actually be correct.

Second, if the optical constants of any material(s) in the sample were varied (directly or parametrically), is the magnitude and dispersion of the resulting optical constants physically reasonable. This is usually easy to determine for dielectric and semiconducting materials, as the index of these materials must decrease with increasing wavelength in spectral regions where the material is transparent. For metals and other opaque materials (semiconductors at energies greater than the bandgap energy, for example) it may be very difficult to make this determination, as the material may show complicated dispersion. In this case, compare the best-fit optical constants with those of the same material from the literature or from other analyses. Are they at least close, and do spectral features which appear in the literature constants appear in the best-fit optical constants as well? In other words, the best-fit optical constants for a given material should be at least qualitatively similar to those obtained from the literature for the same material.

Third, do the best-fit optical constants exhibit structure at spectral locations where there is associated structure in the raw experimental data? If so, this indicates that the model is somewhat deficient for the description of the given sample. A common case where this criterion is very useful is the case of thick transparent films which exhibit interference oscillations in the experimental data. The following figure shows simulated experimental data for a 500 nm film of silicon dioxide on silicon. The best-fit calculated data are also shown, from a fit in which we assumed the film thickness to be 475 nm and fit for the film index.

Figure 13.3. Ellipsometric psi data for 500 nm of silicon dioxide on silicon. Model fit data are from fit for the film index assuming the film to be 475 nm thick.
Figure 13.4. Ellipsometric delta data for 500 nm of silicon dioxide on silicon. Model fit data are from fit for the film index assuming the film to be 475 nm thick.

Here is the silicon dioxide film index we obtain from this fit, in which the silicon dioxide film thickness is known to be off by 25 nm. The original film index spectrum is also shown for comparison.

Figure 13.5. Silicon dioxide index spectra. The dashed line is the literature spectrum used to calculate the experimental data in the previous two figures, the solid curve is the spectrum obtained by fitting for the index with the film thickness fixed at 475 nm, 25 nm less than the true thickness of the film.

Note the ‘glitch’ in the best-fit index spectrum at ~710 nm, and note also that there is a peak in psi and a sharp valley in delta (a handedness change) at this wavelength. Handedness changes are very sensitive spectral features, and any optical constants which are fit directly will tend to exhibit features such as those shown above at the handedness changes unless the model is very accurate. Try incorporating roughness or index grading to eliminate these features.

Fourth, do the best-fit optical constants exhibit structure at spectral locations where other materials in the sample exhibit pronounced features in the optical constants? If the model is inaccurate, the optical constants which are being fit will tend to show features where other materials in the sample have strong structure. A very common example is the analysis of thin films on silicon wafer substrates. To demonstrate, we calculated ellipsometric data for a 30 nm film of diamond like carbon on silicon, with the thickness chosen to be small enough that the experimental data does not exhibit interference oscillations. We then fix the film thickness at 31 nm and fit the calculated set of ellipsometric data to determine the diamond like carbon film optical constants. A perfect fit to the ‘experimental’ (actually simulated) data was obtained, and the optical constants obtained from this fit are shown below.
Figure 13.6. Diamond like carbon index of refraction spectra. The dashed curve is the original (true) index spectrum, the solid curve was obtained from fitting data calculated for a 30 nm film on silicon assuming the film to be 31 nm thick.

Figure 13.7. Diamond like carbon extinction coefficient spectra. The dashed curve is the original spectrum, while the solid curve was obtained from fitting data calculated for a 30 nm film on silicon, assuming the film to be 31 nm thick.

Note the sharp features in the diamond like carbon index and extinction coefficient spectra obtained from fitting the simulated data with the wrong film thickness. Note the location of these features, and compare the location and shape of the features with the crystalline silicon optical constant spectra shown below.

Figure 13.8. Crystalline silicon optical constant spectra.

Even though the layer thickness we assumed when fitting for the film optical constants was only 1 nm away from the true thickness of the film, we see very strong features in the resulting film optical constants which occur at the wavelengths where the substrate optical constants exhibit very strong features. This can provide a sensitive test of the accuracy of best-fit models for samples on substrates which exhibit strong dispersion features, such as most semiconducting materials. In general, the more pronounced the features in the substrate optical constant spectra are, the more sensitive the film optical constants will be to the accuracy of the film thickness.
Fourth, if roughness or grading was used in the model, is the resulting roughness or optical constant grading reasonable? Roughness layer thicknesses commonly correlate strongly to other thicknesses in the model, and any roughness layer thicker than 10 nm or so is usually indicative of a correlation problem. In addition, the EMA model used for roughness is not expected to be valid if the dimensions of the roughness (horizontal or vertical) are greater than 100 nm or so. If a graded model was employed, is the grading monotonic or at least justifiable in terms of the deposition and post-deposition processing of the sample? Often when too many nodes are included in a grading, one or more of the node values may become very large, and the nodes may oscillate between positive and negative values from node to node. These are indicators of very strong correlations, and the grading should be simplified.

Finally, if anisotropic optical constants were fit for, are the resulting spectra reasonable? For transparent anisotropic materials, we expect the ordinary and extraordinary index spectra to exhibit about the same dispersion, and to be shifted slightly in magnitude. If the dispersion of one index is markedly different from the other, the model is probably not correct. Either the film is not actually anisotropic, the orientation of the anisotropy of the material has not been correctly specified, other aspects of the model are incorrect, or the anisotropic index parameters are very strongly correlated to other parameters in the model.

To summarize this section, it is very important to not only obtain a unique best-fit model for a given set of ellipsometric data, but also to establish that the best-fit model is physically reasonable, both structurally and in terms of any optical constant spectra determined from the fit.

13.3 Bare substrates

In this section we will discuss the characterization of optically thick samples. For our purposes, optically thick will mean there are no films, coatings, or surface layers (such as surface roughness and surface oxides) on the sample under test. This type of analysis is most often performed to characterize substrates for further analysis of thin films on similar substrates.

Opaque bulk samples

The characterization of optically thick samples (either bulk substrates of optically absorbing materials with no coatings or thick films of optically absorbing materials) is in some ways both the simplest and the most difficult of ellipsometric analyses. It is the simplest in that fitting the data merely requires ‘inverting’ the measured psi and delta values to obtain n and k values for the substrate. It is very complicated in that such systems do not often occur in nature, and nearly all ‘bulk’ samples actually have some sort of surface overlayer on them (native oxide or surface roughness usually). The neglect of this overlayer will yield optical constants which are not correct for the substrate. If these constants are then used for a coated substrate from which the oxide or overlayer was removed prior to film deposition, difficulties may be encountered in the subsequent analysis of the coating. An excellent review of techniques for eliminating the effects of surface layers from ellipsometric measurement of the optical constants of bulk solids is given in Palik’s first Handbook of Optical Constants of Solids (Vol. 1), chapter 5, ‘The Accurate Determination of Optical Properties by Ellipsometry’, by D. Aspnes. As a general piece of advice, it is not a bad idea to read as many of Aspnes’ papers on ellipsometry as possible, as he is one of the pioneers of modern spectroscopic ellipsometry.
The optical constant fits for opaque bulk systems are nearly always perfect when fitting data acquired from good quality (smooth) surfaces. Failure of a bulk model to fit the ellipsometric data well is usually indicative of one (or more) of the following:

- Coatings of some sort on the sample.
- Very rough sample surface.
- Patterned sample surface which is exhibiting diffraction effects (depolarization).
- Anisotropic material, usually due to non-centrosymmetric crystal structure or stress.
- Gross misalignment of the sample.

Transparent bulk samples

The problem of obtaining optical constants of bulk samples becomes somewhat more complicated when the material in question is transparent. This is the case for glass, most plastics, dielectric materials, and semiconductors below their bandgap energies. The problem with these types of samples is that two light beams may be incident on the detector. The first beam is reflected from the top surface of the sample, and contains information which allows us to determine the index of refraction of the transparent material under study. The second beam passes through the top surface of the sample, reflects from the bottom surface of the sample, and then passes back through the top surface of the sample. If the sample is more than 0.1 mm thick (typically) this second beam does not mix coherently with the first, and the result is a partially polarized beam entering the detector. There are a number of ways to deal with this problem, all of which will be discussed in this section. These techniques are listed from best (easiest and most accurate) to worst.

- ‘Spatially filter’ the second beam at the detector iris. If the sample is sufficiently thick, the second beam will be physically displaced from the first at the detector. If this is the case, the detector iris size may be adjusted to admit only the first beam reflected from the top surface of the sample. This is always the best way to handle the reflection of the beam from the back surface of samples, but can only be done for very thick samples or by using a very small incident beam diameter.

- Roughen the back surface of the sample. This is the best possible way to deal with this problem if the second beam cannot be excluded from the detector, but unfortunately this technique ruins the sample for many types of further measurements. If you are going to acquire transmission data from the sample under study, make sure and do it prior to roughening such that the VASE and transmission measurements can be acquired from the same physical location on the sample.

- Include the second beam in the mathematical model for the sample, using the ‘back-surface correction’ parameters in the ‘Options’ dialog box from the Model window. This mathematical model is rather approximate, however, and can lead to difficulties in fitting the experimental data.

- Index match the sample to a large piece (wedge shaped, preferably) of the same material (very effective for glass or plastic samples) or another material of nearly equal index of refraction. This is a difficult and messy technique, requiring the use of index matching fluid to fill the air gap between the sample under study and the wedge of material underneath. There are tables of the indices of a large number of common oils and fluids in the CRC Handbook of Chemistry and Physics, and these should be consulted when selecting an index matching fluid for a given
material. There are also commercially available index matching fluids. The idea is
to have nearly all of the beam incident on the bottom surface of the sample pass into
the large wedge underneath, which makes the sample effectively very thick such that
the second beam may be excluded from entering the detector. The closer the indices
of the sample, index matching fluid, and wedge are, the smaller the fraction of the
second beam that scatters back from the bottom of the sample will be.

**Glass**

Perhaps the most commonly encountered transparent substrates are pieces
of glass. Examples are microscope slides (a rather poor quality glass), optical flats
(usually made of fused quartz), and colored glass filters. VASE® data alone are
sufficient to determine the index of refraction of the glass sample, regardless of
which technique is used to eliminate the back-surface reflection, however if the
extinction coefficient of the glass is to be determined it is necessary to acquire
transmission data at normal incidence from the same location on the sample as the
VASE® data is measured. It is also necessary to determine the thickness of the glass
sample in order to obtain the correct extinction coefficient values from the
transmission data fit. This is a rare case where the thickness of the substrate must be
correctly specified.

**Glass with UV absorption edge**

Most glasses (other than fused silica) will exhibit an onset of optical
absorption as the wavelength becomes less than 300 - 350 nm or so. In this case, the
procedures previously described are sufficient for the determination of the glass
index of refraction. The extinction coefficient of the glass may be determined by
measuring the thickness of the sample and then acquiring transmission data at the
same wavelengths as the VASE® data (used to determine the glass index) were
acquired. With the glass index held fixed at whatever was determined from the
VASE® data, specify the correct substrate thickness, and declare ‘k’ as a fit parameter
for the substrate. Load the transmission data only into the Experimental Data
window, and perform a normal or point-by-point fit (either will work), which will fit
the measured transmission to determine ‘k’ for the glass. Note that the ‘k’ values
you determine will depend on the thickness specified for the substrate.

**Float glass**

Float glasses are a special type of glass fabricated by floating molten glass
on liquid tin, and will often exhibit non-zero absorption throughout much of the
spectral range. In this case, the same procedure described previously for glass with a
UV absorption edge will work for the determination of the glass extinction
coefficient spectrum, however a user-defined parametric model based on the use of
an ensemble of Gaussian oscillators is also useful to model the glass extinction
coefficient spectrum.

**Plastics**

The characterization of bulk plastics is formally identical to that of bulk
glass samples, with one additional complication. Plastic substrates are commonly
birefringent (due to stress), and as a result it is crucial to eliminate the back-surface
reflection from any VASE® (or other polarimetric) measurement. A good way to
detect birefringence due to plastic substrates is to acquire ellipsometric transmission
data through the sample at normal incidence. If the sample is not birefringent, you
should measure psi at 45° and delta at zero (or very noisy and close to zero) at every
wavelength. If psi deviates significantly from 45°, it is very likely that the substrate
is exhibiting birefringence. It is possible to use this type of measurement to quantify the birefringence of the substrate as well.

The best approach to characterizing an unknown bulk plastic sample is to first acquire normal incidence intensity transmission data at all wavelengths at which you wish to obtain optical constants. Next, roughen one side of the plastic substrate. Sandpaper works very well for this (usually), whereas mechanical grinding does not seem to be as effective, and often yields a buffed semireflecting surface. Acquire \textit{VASE}® data from the sample. If the sample was roughened, the analysis of the transmission and \textit{VASE}® data should proceed in the same manner as described in the previous section. If the substrate is significantly birefringent and was not roughened prior to the acquisition of the \textit{VASE}® data, you will not be able to fit the \textit{VASE}® data with the previously described model. If this is the case, acquire normal incidence ellipsometric transmission data as described in the previous paragraph to test whether the substrate is actually birefringent. If it is, you must roughen the substrate in order to characterize the given material.

**Semiconductors below the bandgap energy**

Bulk semiconductors present an interesting problem in that they can be optically opaque over some of the spectral range available to the \textit{VASE}® instrument and yet be transparent over other spectral ranges. If the back surface of the sample under study is frosted or roughened in some manner, this is not a problem and the \textit{VASE}® data may be simply inverted to obtain \(n\) and \(k\) values for the substrate. If both surfaces of a given wafer are polished, however, the reflection from the back surface of the wafer may come into play. This will usually be visibly evident in the experimental \textit{VASE}® data, as there will be an abrupt shift in psi and delta at the band edge as the wafer becomes transparent and the back-surface reflection begins to reach the detector.

Here is an example. The following data were calculated for a bare silicon wafer with 2 nm of native oxide. We show the data predicted with and without the inclusion of the reflection from the back surface of the wafer.

![Figure 13.9. Ellipsometric psi data for native oxide on silicon calculated with and without back-surface reflections.](image-url)
Figure 13.10. Ellipsometric delta data for native oxide on silicon calculated with and without back-surface reflections.

Note the large shift in psi and delta at ~1100-1200 nm, as the silicon becomes transparent enough to allow the light beam to traverse the wafer (assumed to be 1 mm thick). Here is the same plot for GaAs, assumed to have a 2 nm native oxide:

Figure 13.11. Ellipsometric psi data calculated for native oxide on Gallium Arsenide with and without back-surface reflections.

Figure 13.12. Ellipsometric delta data calculated for native oxide on Gallium Arsenide with and without back-surface reflections.

Probably the best approach when this problem occurs is to split the analysis into two parts. First, invert the data below the discontinuity (below 1100 nm for silicon, below ~900 nm for GaAs) directly to obtain the optical constants of the wafer in this spectral region. Then, fit the data above the band edge (above ~1200 nm for silicon, above ~950 nm for GaAs) using the techniques described previously for transparent bulk samples to determine the wafer index of refraction in this spectral range.

Note that simultaneous analysis of ellipsometric and transmission data (which works very well for glass samples with an absorption edge) does not usually work well for semiconductor samples exhibiting back-surface reflection effects.
This is due to the large mismatch in index between the sample and ambient, as well as the (usually) unknown condition of the surface of the back of the wafer.

**Very thin transparent bulk samples**

Thin, flexible substrates (Mylar tape or film, polyester film, etc.) present a very difficult problem to the VASE™ instrument. While this characterization is in principle identical to the characterization of glass or plastic bulk substrates, there are practical considerations which make it rather difficult. First, it is necessary to roughen the back surface of the film after acquiring transmission data and prior to acquiring VASE™ data. This may be critical as the thinner film substrates will often exhibit semi-coherent mixing of the front and back surface beams, such that the experimental data exhibits very dense interference oscillations. These type of data can be fit (very approximately) by using a Cauchy model to simply ‘average’ through the oscillations, but it is better (particularly when characterizing films deposited on such substrates) to eliminate the back surface reflection. The second problem is that the samples are usually very flexible, and it is very difficult to mount them such that they present a flat surface to the impinging light beam. We have tried taping the samples (after roughening) to microscope slides, and have achieved reasonable results with this method, although there is much room for improvement.

The following example illustrates several of these points. Here are VASE™ data acquired from a thin polyester sheet taped to a microscope slide.

![Figure 13.13. Ellipsometric psi data from a thin polyester sheet taped to a microscope slide, but not roughened.](image)

![Figure 13.14. Ellipsometric delta data from a thin polyester sheet taped to a microscope slide, but not roughened.](image)

Note the ‘jump’ in psi around 310 nm, indicative of the onset of back-surface reflection effects, and also indicating that the polyester substrate is opaque for wavelengths below 310 nm. Of more importance are the rough oscillations observed for both psi and delta. These oscillations are caused by coherent interference of top- and bottom-surface reflected beams entering the detector. Normally substrates are thick enough that the back-surface reflected beam loses
coherence during the passage through the substrate and back again, and coherent interference oscillations are not observed.

To eliminate both of these effects, we roughened one side of the substrate using very fine grade sandpaper. While this was probably sufficient to eliminate the back-surface reflection, we also colored the back side of the substrate black with a marker and mounted it on black paper on top of a microscope slide for measurement. The psi data acquired from this sample are shown below, and may be fit using the simple Cauchy model with \( A = 1.688, B = 1.322e^{-2}, \) and \( C = 5.88e^{-4}. \)

![Figure 13.15. Psi data from same polyester sheet, after roughening.](image)

Note that the jump in psi around 310 nm is gone, as are the rough oscillations in the data, both of which were due to beam components reflected from the bottom of the substrate.

**Anisotropic substrates**

**WVASE**\(^\text{®}\) has very sophisticated modeling capabilities for anisotropic materials, both films and substrates. The optical constants of an optically anisotropic material can vary, depending upon the light beam’s direction of propagation and/or polarization.

Data acquisition, modeling and analysis of anisotropic substrates and films is a complex subject, and will not be covered in great detail in this manual. A simple example of an uniaxial anisotropic film is described in the next chapter (see Example 6: Anisotropic organic film on silicon (•••)). Contact the Woollam Company if you have further questions.

**Modeling surface oxidation and roughness**

Usually when we characterize bulk samples of a material we are trying to obtain the optical constants of that material as accurately as possible. Most materials will oxidize in atmosphere, however, and the resulting thin overlayer must be included in the optical model in order to obtain accurate substrate optical constants from the analysis. Unfortunately, if we are fitting for the optical constants of the substrate it is not possible to fit for the thickness and/or optical constants of the overlayer, as this leads to very strong parameter correlations and a non-unique best-fit model. As a result, to include the overlayer in the model we must make some assumption as to the optical constants and thickness of the overlayer.

To include an overlayer in the analysis of a bulk sample, first try to make a reasonable guess as to the optical properties of the overlayer. For metal samples, use the optical constants of metal oxides, many of which are known (titanium dioxide, aluminum oxide, chromium oxide, etc). If all else fails, use silicon dioxide as the overlayer. Next, guess at the thickness of the overlayer. TEM pictures may be helpful, and if no other information is available 2 nm (20 Angstroms) is usually a
reasonable guess. Add this overlayer to the model and fit again for the substrate optical constants.

13.4 Single films - general principles

In this section we review important general principles which pertain to the analysis of single films of any material. Without question the most common usage of ellipsometry is for the characterization of single layers, or coatings, on known substrates. In this section we discuss the use of ellipsometry to determine the thickness and optical constants of thin films. The estimation of surface roughness at the top of the film is also discussed.

In order to understand the following analysis strategies, it is important to keep in mind the following unfortunate fact of life. It is not possible to uniquely determine the optical constants n and k and the thickness of an absorbing film simultaneously from VASE® data (or reflection ellipsometry data of any type, or reflectance data) alone. This is the classic example of parameter correlation. We will give many examples as proof of this statement in the following sections. As a result, much of our analysis strategies will be centered on ways to eliminate this correlation problem, and thankful there are several good ones.

What do we want to measure?

What information can we get from VASE® analysis of a single film? At the very least, we hope to obtain the thickness of the film, and at the most we will obtain the thickness and optical constants of the film, and possibly parameters relating to any grading of the film properties from top to bottom and the extent of the surface roughness on the film. It is possible to obtain other information about the film such as alloy fractions, hydrogen content, void fractions, percent crystallinity, etc., but this type of information is indirect in that it comes from the models for the optical constant spectra of materials as a function of these parameters. Any structural or physical parameter of a thin film which effects the optical constants of the film may be determined in principle from VASE® analysis, but the connection between the parameter of interest and the optical properties of the material must be known, such that a model exists which will either predict the optical constants a function of the film parameter(s) of interest or the parameter(s) of interest may be calculated directly from the optical constants of the material.

An example is the effective medium model used to determine the crystalline to amorphous ratio in polycrystalline silicon films. This model yields the crystalline to amorphous ratio of the film, but it can only do so because it contains the model necessary to calculate the film optical constants from the EMA model given a value for the crystalline to amorphous ratio. We say that we have determined this ratio, but we have actually determined film optical constants based on a model with the ratio as a parameter.

Opaque vs. transparent substrates

The analysis procedure employed for a given film will be strongly dependent on the type of substrate the film is deposited on, as will the quality of the results obtained from the analysis. Opaque and transparent substrates both have advantages and disadvantages, but as a general rule the very best characterization of thin film optical properties can be obtained from films deposited on transparent substrates (glass, most commonly) such that intensity transmission data may be acquired from the film in addition to ellipsometric data. This assumes that the back-
surface reflections may be eliminated from the ellipsometric data by spatial filtering
or back-surface roughening.

The disadvantages of transparent substrates are that back-surface effects
may be a problem, and the index of the particular substrate may not be exactly
known. Also, the very sharp absorption edge exhibited by many glasses in the UV
and the broadband spectral absorption exhibited by many soda-lime float glasses
may lead to difficulties fitting the measured transmission data.

Opaque substrates do not allow the measurement of transmission data, but
may be required by the process used to deposit the film under study. Also, several
common opaque (or semi-opaque) semiconductor materials provide excellent
substrates as their optical constants are very accurately known. Silicon is the best
example of this type of material.

Our general conclusion is that for thin films which are transparent within
the measurable spectral range, crystalline silicon wafers are generally the best
substrate for study of the film, while glass substrates (fused silica is the best) are
more useful for films which are absorbing everywhere in the spectral range (metals,
very low bandgap semiconductors).

Substrate characterization

In many cases the optical constants of the substrate material will be well
known, and it will be sufficient to use reference spectra to model the substrate. The
most common examples are silicon wafers (and most other semiconductor
substrates) and common glasses such as fused silica, Corning 7059 glass, and BK7
glass. In some cases, however, the optical constants of the substrate are not well
known, and it is necessary to obtain the substrate optical constant spectra from a bare
substrate prior to characterizing films on similar substrates. In most cases the
techniques in the previous section on bulk samples are sufficient for this
characterization. An exception is metal substrates, either bulk substrates or very
thick metal films with coatings on them.

The surface of most metal substrates and thick films is somewhat rough and
oxidized. A measurement on a bare metal surface will then usually yield optical
constants which are effective optical constants of the bulk metal plus the roughness /
oxide overlayer. Unfortunately, this effective model for the substrate may not work
very well to characterize films on the substrate, particularly if the film under study is
very thin, and it is usually not possible to fit for the substrate optical properties and
the film thickness and optical constants.

For the case of metal substrates, there are basically three choices for the
analysis procedure:

- Characterize a bare substrate as a bulk system, and use these optical
  constants for the substrate to analyze the film. This may or may not work well,
  depending on the surface quality of the metal substrate and the thickness of the film
  under study.

- Find an accurate Lorentz oscillator parameterization for the substrate, and
  then allow one or more oscillator amplitudes to vary (along with the film variables)
  as necessary to obtain a good fit. This only works for transparent films (or spectral
  regions where the film is transparent), and requires considerable care to find the
  minimum set of Lorentz oscillator parameters which will fit the data well and still
  yield a unique and uncorrelated solution.

- Perform a multiple sample analysis on a series of samples consisting of a
  bare substrate and identical films of as many different thicknesses as possible. This
may yield information about the substrate overlayer as well as substrate optical constants and film thicknesses and optical constants. This requires a large number of samples and is very time consuming however.

Finally, never expect reference optical constants for metals to accurately describe either films or bulk samples of the given metal. Most of the reference spectra for metals (in Palik’s *Handbook of Optical Constants of Solids*, vols. I and II, for example) were measured at unknown temperatures from crystalline or polycrystalline samples of the metal, possibly in high vacuum, and of unknown surface condition. We rarely see metal optical constant spectra which show more than a qualitative resemblance to the reference spectra found in the literature.

**Quick analysis with reference optical constants**

The simplest possible analysis of a single film is performed by employing known optical constants for the film material and fitting for the thickness of the film. This is a single parameter fit, and as such is very easy to perform quickly. As a result this type of analysis tends to lend itself more to cases where speed and simplicity of the analysis is important. As an added bonus, very little experimental data is required to determine a single parameter (the film thickness), and measurements at a few wavelengths and one or more angles of incidence are usually sufficient for this type of analysis.

The drawback of this approach is that a single given material may exhibit a wide range of optical constants depending on how the film was deposited, what it was deposited on, post-deposition annealing or other treatments, etc. There are few cases where this type of analysis will yield reasonable results. First, if a film deposited under identical conditions has been analyzed to obtain the ‘known’ optical constants of the material under study. Second, the classic case of thermally oxidized silicon wafers can nearly always be analyzed in this manner, as the thermally grown silicon dioxide optical constants are quite reproducible. Third, it is rarely possible to uniquely determine the thickness and index of very thin dielectric films (10 nm or less). In this case, optical constants must be assumed for the film and the thickness only may be determined.

As a final note, this type of analysis can also be useful to obtain a ‘quick and dirty’ estimate of the thickness of a given film.

**Optical constant determination with the film thickness known**

In many cases we wish to determine the optical constants of a film with the thickness of the film known. To do this, declare n and k of the film to be fit parameters (by clicking on the ‘n’ and ‘k’ check boxes in the film dialog box). Then, perform either a normal or point by point fit. The normal fit will vary all of the optical constants at once, and may take a while. The point by point fit will fit the data one wavelength at a time and is very rapid. Both types of fits may sometimes move to the wrong branch, and exhibit unphysical dispersion or discontinuities in the optical constants. If this happens, try the following:

- Try the other fit type.
- Point-by-point fit starting at the other end of the spectrum.
- Point-by-point fit with different starting values.
- Use the ‘edit n and k’ option from the dialog box accessed by the ‘Optical constants’ bar in the layer dialog box to change the offending optical constant values to something more reasonable, and then execute a normal fit. Sometimes if you get
the values reasonably close they will settle on the correct minimum rather than wandering into a different branch.

- Restrict the spectral region to include only the questionable optical constants, and try point by point fitting with different starting values and from different ends of the spectrum.

### Parameterization of the film optical constants

Parameterization of the film optical constants is an extremely useful technique by which we can drastically reduce the number of fit parameters required to obtain the film optical constant spectra, and in many cases reduce the strong parameter correlations normally encountered when fitting directly for the film thickness and optical constants at each measured wavelength. Simply put, we find expressions for the film optical constants as a function of wavelength, and vary parameters in these expressions to fit the ellipsometric data rather than vary the optical constants directly at each wavelength.

This is very useful for transparent or partially transparent materials for which k can be fixed to zero over some spectral range and the index only parameterized as a function of wavelength. Very simple parameterizations are usually sufficient to model the dispersion of the index in transparent regions, and usually only two or three fit parameters are required to model this dispersion. Several parameterizations useful for transparent films are implemented in the WVASE® software, and it is also a simple matter to input arbitrary functions of the user’s choice with any number of fit parameters via the user-defined dispersion layer.

Parametric models for absorbing materials are very useful, and such models can be made consistent with the Kramers-Kronig transformation integral, thereby adding constraints to the dispersion that the layer may exhibit. The Lorentz oscillator model and the parametric semiconductor model are examples of such Kramers-Kronig consistent models which may be used for semiconductors, metals, and other absorbing materials. The parametric semiconductor model works best for semiconductors and dielectric materials with absorption edges in the UV, while Lorentz oscillators work well for the optical constant spectra of metals.

### EMA models and surface roughness

Effective medium approximation (EMA) models allow the calculation of the optical constant spectra of mixtures of two or three materials of known optical constants, provided the volume fractions of the constituent materials and the physical geometry of the mixing are known. The Bruggeman and Maxwell-Garnett EMA models are implemented in WVASE®, along with simple linear interpolation of the constituent optical constants. These models are very useful for describing surface and interfacial roughness, partially crystalline materials, and index grading of films.

EMA models for surface and interfacial roughness are most useful when the film is transparent and the experimental data exhibit interference oscillations, as the shape of these oscillations are very sensitive to roughness. For films which are absorbing everywhere or thinner than ~ 30 nm, the roughness layer thickness will usually correlate very strongly to the film thickness, and it will not be possible to obtain both uniquely. Finally, never vary the roughness layer constituent fraction in addition to the thickness of the roughness layer, as this nearly always produces total correlation between these two parameters.
Film inhomogeneity

Often during the deposition of a film a process parameter may drift such that the properties of the film vary from top to bottom of the film. Similar grading often occurs due to post-annealing or processing of the film after deposition. *WVASE®* provides a number of very sophisticated models to describe such graded films, based on either the use of EMA models to describe the grading as a variation in the mixing of two constituent fractions, or on the use of alloy models to describe the grading as a variation of the alloy fraction through the film. The grading can be described either by a piecewise linear function with up to eight nodes, or by a continuous equation specified by the user and containing any number of variable parameters.

13.5 Single transparent or partially transparent films

Techniques are presented in this section for the analysis of single films which are transparent over the entire measured spectral range.

Analysis with standard optical constants

This is usually not a good idea, as we can usually obtain the index and thickness of the film unless it is very thin or very thick (see last two parts of this section - ‘Very thin transparent films’ and ‘Very thick transparent films’).

Direct fit for \(n\) and \(t\)

It is possible to fit for the film thickness and the index of the film at each measured wavelength. This is an instructive academic exercise, but is usually not advisable as any noise in the experimental data will be directly mapped into the index spectrum. Parametric models are forced to be continuous which eliminates the noise in the optical constant spectrum.

Cauchy parameterization to determine film thickness

This has been the most commonly used approach in the past for the parameterization of the index of transparent materials, although we tend to use modified forms of the Cauchy dispersion relation implemented in the user-defined dispersion layer more commonly now. The Cauchy dispersion relation is an inverse power series containing only even terms:

\[
n(\lambda) = A + B/\lambda^2 + C/\lambda^4 + \ldots
\]

(13.2)

where the wavelength \(\lambda\) is given in microns and A, B, and C are fit parameters. This series is implemented in *WVASE®* as *cauchy.mat*, and the *cauchy.mat* layer dialog box is shown below.
Figure 13.16. Cauchy layer dialog box. The first three parameters A, B, and C specify the index of refraction. The last three parameters, k Amplitude, Exponent, and Band edge, specify the shape of the absorption tail.

To use this model, add the layer cauchy.mat to the model as the film. Specify a value for the A parameter which roughly matches the index value expected for the film at 633 nm (or any wavelength at which you can make a reasonable guess for the index). Specify small positive values for B and C, and declare all three along with the film thickness as fit parameters.

There are two problems which may be encountered with the Cauchy parameterization. First, strong correlations may exist between the Cauchy parameters themselves. This will occur when the material under study does not exhibit strong dispersion over the spectral range being fit. Usually, the B and C parameters correlate strongly to each other, although occasionally strong correlation between the A and B parameters may be observed when the index of the material is nearly constant. Indications that strong correlations between the Cauchy parameters exist are large negative B or C parameters (less than -0.01), or a tendency of the fitting algorithm to perform many iterations which reduce the MSE by a small amount.

The second problem, which is often related to the first, is that the Cauchy parameterization can produce unphysical dispersion of the index of the material. In chapter 2 - “A Short Course on Ellipsometry” the Kramers-Kronig integral which relates the dispersion of the extinction coefficient to that of the index of refraction was discussed. We concluded that in a spectral range where the absorption of the material is zero, the index of refraction should not exhibit strong dispersion and should decrease monotonically with increasing wavelength. If the B or C (or both) Cauchy parameters are negative, the resulting index of refraction may decrease with increasing wavelength, which is not physically possible. This may occur due to strong correlations between the B and C parameters, but usually represents either a lack of sensitivity of the data to the index of refraction of the layer under study (as is the case with films less than approximately 10 nm thick) or a gross inaccuracy in the optical model used to fit the data (very inaccurate substrate optical constants, for example).

The existence of a negative B or C parameter does not always mean the resulting index spectrum is unphysical. If only A and B are used, a negative B parameter always yields unphysical index spectra. If, however, A, B, and C are all employed, a small negative B value may be compensated by a larger value of the C parameter, and vice versa. The user should visually examine the index spectrum resulting from a Cauchy fit to judge the physical likelihood of the results.
Here are some examples of reasonable and unreasonable spectra from Cauchy fits for the index of materials. First, we consider two-parameter fits in which A and B are varied and C is held fixed at zero. Here is the index spectra for \( A = 2.0 \) and \( B = \pm 0.01 \).

![Figure 13.17. Index of refraction predicted by Cauchy dispersion relation with \( A = 2.0, B = 0.01, \) and \( C = 0 \). This is a physically reasonable index spectrum.](image1)

Thus, when using a two-parameter Cauchy model, any negative value of the B parameter leads to an unphysical index spectrum for the film. When all three parameters are used, the distinction is not so clear. The next three figures show examples of reasonable physical dispersion obtained from a three parameter Cauchy dispersion relation.

![Figure 13.18. Index of refraction predicted by the Cauchy dispersion relation with \( A = 2.0, B = -0.01 \). This is not a physically reasonable index spectrum, as the index is increasing with increasing wavelength.](image2)

![Figure 13.19. Index spectrum predicted by the Cauchy dispersion relation with \( A = 2.0, B = 0.01, \) and \( C = 0.001 \). This is a physically reasonable index spectrum.](image3)
Figure 13.20. Index spectrum predicted by the Cauchy dispersion relation with $A = 2.0$, $B = 0.02$, and $C = -0.0005$. This is a physically reasonable index spectrum.

Figure 13.21. Index spectrum predicted by the Cauchy dispersion relation with $A = 2.0$, $B = -0.001$, and $C = 0.005$. This is a physically reasonable index spectrum.

A marginally acceptable spectrum is often obtained in which the index ‘rolls over’ at the UV end of the spectrum, as shown below.

Figure 13.22. Index spectrum predicted by the Cauchy dispersion relation with $A = 2.0$, $B = 0.02$, and $C = -0.001$. This is a physically reasonable index spectrum, but we expect an absorption edge in the UV to accompany the peak in index.

This is a physically reasonable index spectrum, and is often observed for dielectric materials, provided there is an absorption edge which begins near the wavelength where the peak in index occurs. If this type of spectrum is obtained, it is a good idea to either try to incorporate absorption in the Cauchy layer using the exponential tail parameterization for the extinction coefficient included in the Cauchy layer, or restrict the fitting range to exclude the peak in index (for the case shown above, restrict the data range to 400 - 1000 nm, for example).

The next figure show some physically problematic spectra obtained from three term Cauchy parameterizations.
The Cauchy parameterization of the index of refraction provides us with a very powerful tool for the determination of film thicknesses, provided there is some window in the measured spectral range where the film is transparent. If we can locate such a window, we can fix $k$ at zero in this window and fit for the thickness of the film and two or three Cauchy parameters for the film. This is a very stable and uncorrelated model unless the film is very thin (typically less than 10 nm). Once the thickness of the film is determined, we can then fix the film thickness and then fit for $n$ and $k$ over the entire measured spectral range.

To determine the spectral range where the film is transparent, make a guess as to the location of the absorption edge of the film, and restrict the spectral range to wavelengths longer than the wavelength at which you think the absorption edge might be located. Perform a normal fit for the film thickness and three Cauchy parameters (two if correlation problems occur). Note the final MSE and the quality of the fit. Now, restrict the data range further and repeat the fit. For example, if we originally restricted the data range to 400 - 1000 nm (or 400 - 1700 nm with NIR data), we would now restrict it to (say) 500 - 1000 nm (or 500 - 1700 nm with NIR data). If the final MSE decreases significantly and the quality of fit improves when you reduce the data range, the film is most likely still absorbing into the lower end of
the selected range. Keep reducing the data range by increasing the lower wavelength limit until the MSE does not improve when the range is reduced. If the fit to the experimental data is very good, you have located a transparent window in the film absorption spectrum.

The Cauchy layer also contains a simple exponential model for absorption tails. The user may specify three parameters for the absorption tail, however only two of these parameters are independent and may be varied together. The first parameter is the amplitude of the exponential tail, the second parameter is the exponent, which controls the shape of the tail, and the third parameter is labeled the band edge, and specifies the point at which the extinction coefficient will equal the amplitude parameter. The amplitude and band edge parameters should not both be varied, as they will always be 100% correlated to each other.

To disable the absorption in the Cauchy layer, set the amplitude parameter to zero and leave it fixed. Always try fitting the data first with the absorption disabled, and then add the absorption if necessary as a perturbation and see if it improves the fit. Once the Cauchy fit with no absorption is complete, there are two good indicators that absorption in the Cauchy layer may improve the fit. First, if an index spectrum with a peak in the UV is obtained, such as that shown in figure 12.22, it is likely that absorption in the Cauchy layer will help. Second, if the best-fit calculated and experimental data match closely everywhere in the spectrum except for the UV, and particularly if the fit appears to be diverging toward the UV end of the spectrum, addition of absorption in the Cauchy layer may improve the fit.

To fit for the absorption edge along with the Cauchy index parameters, first fit the Cauchy model with no absorption to get the model close (hopefully) to the best-fit result. Next, specify the amplitude parameter to be 0.001 and declare it as a fit parameter. Specify the exponent parameter to be 1.5, and declare it as a fit parameter as well. Finally, specify the band edge parameter to equal the smallest wavelength in the data fitting range, in Angstroms. For example, if you are fitting data from 300-1000 nm, specify the band edge to be 3000. The choice of the value of this parameter is not critical. Do not declare the band edge parameter as a fit variable.

Perform the fit again, this time fitting for the amplitude and exponent absorption parameters in addition to the Cauchy index parameters and the layer thickness. Several results may be obtained:

- The fit may be improved, with physically reasonable index and extinction coefficient spectra as results.
- The fit may be improved, with physically unreasonable dispersion obtained for the index and/or extinction coefficient. The amplitude and exponent parameters must both be positive for physically reasonable dispersion of the extinction coefficient. If a negative exponent was obtained, set the exponent to 1.5 and turn it off as a fit parameter. Try the fit again with only the amplitude varying. If a better fit is obtained with a non-zero amplitude, try fitting for both the amplitude and exponent again now that the model is (hopefully) somewhat closer to the best-fit minimum.
- The fit may not be improved. Absorption in the Cauchy layer is not helping, so set the amplitude to zero and turn the amplitude and exponent off as fit parameters.
- The fit may terminate with the message ‘Singular matrix error’. This happens when an amplitude parameter fits to zero, indicating that absorption in the model worsens the MSE. Fix the amplitude to zero and shut off both the amplitude and exponent as fit parameters. You may want to first try fixing the exponent at 1.5
and fitting for the amplitude only (along with the index parameters, etc.) and seeing if the amplitude fits to a non-zero value.

Here is a physically reasonable index and extinction coefficient spectrum obtained from a Cauchy dispersion model with the exponential absorption tail enabled.

![Index and extinction coefficient spectrum obtained from cauchy.mat](image)

**Figure 13.26.** Index and extinction coefficient spectrum obtained from cauchy.mat, with the index parameters \( A = 2.0, B = 0.01, C = 0.001 \), and absorption parameters: amplitude = 0.01, exponent = 1.5, and band edge = 2500.

It is a useful fact that this parameterization is not only confined to the file `cauchy.mat`. You can copy `cauchy.mat` to any filename of your choice (provided it has the file extension `.MAT`) and the new file may still be loaded by WVASE®️, and will still be the Cauchy parameterization with the exponential absorption tail. This is useful if you have more than one Cauchy layer in your model and wish to be able to couple other layers to one or the other Cauchy layer. Using different names for each Cauchy layer allows WVASE®️ to differentiate between the two when coupling layers together.

Finally, keep in mind that the index of refraction and extinction coefficient of the Cauchy layer may be directly varied at each wavelength by turning off all of the Cauchy index and absorption parameters as fit variables, and clicking on the ‘n’ and ‘k’ check boxes. We often use the simple Cauchy layer at first when we intend to actually directly fit for \( n \) and \( k \). In this case the Cauchy layer is used to get the model close to the final minimum, and to obtain reasonable initial values for the index and extinction coefficient.

### Lorentz oscillators - Drude model for free electron absorption

If we define a model consisting of a single Lorentz oscillator (using the Lorentz oscillator layer file `lorentz.mat`) and fix the energy of that oscillator to zero, the Lorentz model reduces to the Drude model for free electron absorption. This term is often required (with several other normal oscillators) for metal films, but the Drude model is particularly useful for modeling the IR absorption edge due to free carriers in transparent conducting oxide (TCO) films (such as indium tin oxide) and heavily doped semiconductors. As long as the spectral range being fit does not include the region of interband absorption, which is usually in the UV below about 400 nm for TCO’s, a simple three parameter model (\( e1 \) at infinity, amplitude, and broadening of one oscillator with energy of zero) is sufficient. Most TCO films are strongly graded, however, and some combination of index grading and the Lorentz model are required to fit the experimental data well.

The optical constants of a single Lorentz oscillator with \( e1 \) at infinity set to 4.0, and one oscillator of amplitude = 2.5 eV², broadening = 0.2 eV, and center energy = 0 eV are shown below. These are typical values for good quality indium tin oxide (ITO).
Figure 13.27. Optical constants from a single Lorentz oscillator with \( e_1 \) at infinity set to 4.0, the oscillator amplitude set to 2.5 eV, the oscillator broadening set to 0.2 eV, and the center energy of the oscillator set to 0 eV, which are typical values for ITO.

To fit TCO films, restrict the experimental data range to 400-1700 nm (NIR data are very helpful for this analysis) to exclude the UV interband absorption edge, and fit for the layer thickness, \( e_1 \) at infinity, and the amplitude and broadening of one oscillator with the center energy fixed at zero. Add surface roughness and/or grading as necessary to achieve a good fit. For heavily doped semiconductors the same procedure applies, but the lower wavelength limit of the data range must be adjusted to exclude the absorption above the bandgap of the semiconductor.

User-defined dispersion models

The user-defined dispersion model layer \( \text{user.mat} \) allows the user to incorporate arbitrary parametric functions for the optical constants and fit for any parameters in these functions. We have found this layer type to be particularly useful for dielectric films. For dielectric materials, the user-defined layer allows slight modifications to the Cauchy dispersion relation which yield functions which are able to reproduce known index spectra for transparent materials much more accurately than the three term Cauchy relation. This is particularly true for data acquired to 1700 nm and for very thick dielectric films (> 200 nm). There are two functional forms in particular which are useful:

\[
n(\lambda) = A + \frac{B}{\lambda} + \frac{C}{\lambda^2} + \frac{D}{\lambda^4} + \frac{E}{\lambda^6}.
\]  

(13.3)

\[
n(\lambda) = A + \frac{B}{\lambda} + \frac{C}{\lambda^2} + \frac{D}{\lambda^3} + \frac{E}{\lambda^4} + \frac{F}{\lambda^5}.
\]  

(13.4)

The first dispersion relation is simply the three term Cauchy dispersion relation with a single added term which varies as the inverse of the wavelength. This dispersion relation is very useful for describing dielectric material indices over the spectral range 250-1000 nm. The second relation is a six term inverse power series, the first, third, and fifth terms of which are the three term Cauchy relation. This parameterization is very useful for dielectric films over the range 250 - 1700 nm, but tends to be too strongly internally correlated to be useful for more restricted spectral ranges.

We illustrate the accuracy of these two user-defined parameterizations by fitting them to the index of refraction spectrum of fused silica, from the literature. Rather than show the fit in terms of the index spectra, we show the result as the difference between the literature index spectrum and the best-fit spectrum from the parametric model. The fit is performed by constructing a model consisting only of a substrate of \( \text{sio2.mat} \) (fused silica), generating data from this model, copying it to the
Experimental Data window, and then fitting the various models to the psi data in the Experimental Data window.

Here are the results for fits of the two and three term Cauchy relations and the four term relation in equation 12.3 to the fused silica index spectrum over the range 250-1000 nm:

Figure 13.28. Difference between best-fit calculated index from two term Cauchy dispersion relation and literature index of fused silica.

Figure 13.29. Difference between best-fit calculated index from three term Cauchy dispersion relation and literature index of fused silica.

Figure 13.30. Difference between best-fit calculated index from four term user-defined dispersion relation and literature index of fused silica.

Note that the four term user-defined relation fits the fused silica index almost exactly. The user-defined dispersion layer dialog box with this model implemented is shown below:
Figure 13.31. The user-defined dispersion layer with the four term modified Cauchy relation implemented and all four coefficients declared as fit parameters. The coefficients shown are the best-fit values from the fit to the literature fused silica index spectrum.

Next, we compare the fits to the fused silica index spectrum obtained from 250 - 1700 nm from the two- and three-term Cauchy relations, the four term user-defined dispersion relation, and the six term power series.

Figure 13.32. Difference between best-fit calculated index from a two term Cauchy dispersion relation and literature index of fused silica.

Figure 13.33. Difference between the best-fit calculated index from a three term Cauchy dispersion relation and the literature index of fused silica.
Figure 13.34. Difference between the best-fit calculated index from the four term modified Cauchy relation and the literature index of fused silica.

Figure 13.35. Difference between the best-fit calculated index from the six term inverse power series and the literature index of fused silica.

Thus, we see that the four and six term dispersion relations are much more effective in fitting the fused silica index spectrum over the ranges 250-1000 nm and 250 - 1700 nm, respectively. Here is a picture of the user-layer dialog box with the six term series implemented and all six coefficients declared as fit parameters:

Figure 13.36. User-defined dispersion layer dialog box with six term inverse power series implemented and all six coefficients declared as variables. Parameter values shown are best-fit values from the fit to the fused silica literature index spectrum over the range 250-1700 nm.

**Surface roughness**

Surface roughness on films may be modeled using an effective medium approximation layer consisting of 50% of the film material and 50% voids. To include surface roughness in a model, first obtain the best possible fit without the roughness. When this fit is achieved, add the layer ema.mat above the film, select the film material as ‘Material #1’, and select void.mat as ‘Material #2’. Set the
fraction of material #2 (voids) at 50%, and set the thickness of the EMA layer at 0.1 nm or 1 Angstrom, such that the model is only slightly perturbed from the previous best-fit configuration. Declare the EMA layer thickness as a fit parameter in addition to all previously declared fit parameters for the film, and perform a normal fit. To be believable, the surface roughness layer should yield a significantly better MSE and fit to a positive thickness. If the EMA layer thickness fits to zero (or 1.e-8), it is not improving the model and should be removed.

Do not attempt to vary the void fraction in the EMA layer along with the EMA layer thickness, as these two parameters will be 100% correlated. Also, be wary of large roughness thicknesses, as these are usually indications of a strong correlation between the roughness thickness and some other parameter in the model.

Index grading

Many films will exhibit non-uniform optical properties along the direction of the film normal. This may be due to drift of the deposition parameters during the deposition of the film, and may also be due to post-deposition processing of the film. Index grading may be realized in WVASE® through the use of the layer graded.mat. There are two means within this layer type of specifying the grading profile, and there are also two means of specifying how the grading will actually be performed.

The actual grading of the film may be accomplished either by mixing two materials together using an effective medium approximation (EMA), or by employing an alloy parametric layer and grading the alloy fraction through the film. The grading profile may be specified either by a piecewise linear function or by a continuous equation specified by the user. The graded layer dialog box is shown below, with the EMA model selected to realize the grading, and a piecewise linear function chosen to represent the grading.

Examine the above dialog box carefully. In this dialog box, we have selected ‘Discrete nodes’ for the profile definition and ‘EMA’ for the optical constant calculation. The grading profile is specified to have three nodes, two of which are automatically located at the top and bottom of the film. The third node is specified to be 50% of the way through the film, from top to bottom.

We are mixing two materials to describe the grading. The first material is a Cauchy parameterization. Note that parentheses appear around the word ‘cauchy’ in the ‘Material name’ box at the right of the graded layer dialog box. This means that the optical constants of material #1 are coupled to the layer cauchy.mat which occurs
below the graded layer in the optical model. The second material is voids, which have a constant index of unity and no absorption. Note that this does not necessarily mean that there are voids in the film, it is simply a mathematical artifice for shifting the optical constants of the Cauchy layer up and down.

In the above dialog box, we have specified the graded Cauchy layer to effectively contain no voids at the bottom of the film, 10% voids at a point halfway through the film, and 20% voids at the top of the film, corresponding to a film with increasing index toward the surface. The surface and midpoint void fractions are declared as fit parameters. Here is a plot of the depth profile of the index of this graded layer at 500 nm, with the graded layer thickness set at 200 nm.

![Depth Profile of Optical Constants at 500nm](image)

**Figure 13.38.** Depth profile of the graded layer from the dialog box in the previous figure.

Finally, note in the above dialog box that the selected EMA type used for calculation of the effective Cauchy / void mixture is ‘Linear’, representing simple linear interpolation between the Cauchy and void optical constants. For graded layer modeling, the results are usually not strongly sensitive to the choice of EMA model, and the linear EMA is much faster than the Maxwell-Garnett and Bruggeman EMAs. We have also set the number of slices per node to 5. Once a best-fit model is reached it is not a bad idea to increase this value and make sure the same fit is still obtained.

Here is the graded layer dialog box with a continuous equation specified for the grading profile and the alloy model selected for the optical constant calculation.

![Graded Layer Dialog Box](image)

**Figure 13.39.** Graded layer dialog box with a continuous equation specified for the grading profile, and the grading accomplished by varying the alloy fraction of the AlGaAs alloy layer.

In this dialog box, we have replaced the previous piecewise linear grading with an equation which specifies the AlGaAs alloy fraction (in %) as a function of depth in the film. The depth parameter, ‘d’, ranges from zero at the bottom of the film to one at the top of the film. The continuous equation we used is a simple four term polynomial, with the values as shown in the box above the equation. Clicking
on the ‘Operator List’ button will display a list of allowed operators and functions which may be used to specify the continuous equation.

The depth profile specified by this dialog box is shown below.

![Graph showing depth profile and index of refraction and extinction coefficient](image)

Figure 13.40.  Depth profile of optical constants at 500 nm from the graded AlGaAs film as specified in the previous figure.

There are four distinct classes of usage of the graded model for single films that we have encountered.

- Simple variation of the index of dielectric films through the film, usually sufficiently modeled by a two or three node linear grading.

- Strong variation of the optical properties of transparent conducting oxide films. Very difficult to model, and many different approaches yield roughly equivalent results. This will be discussed in great detail further on.

- Damage profiles in implanted samples. Such profiles can usually be modeled with either a fairly complicated piecewise linear grading or a Gaussian type of continuous function.

- Intentionally graded materials, such as Rugate filters or parabolic quantum wells. If the target grading is known, a continuous equation can usually be deduced to describe the grading and implemented in the graded layer dialog box.

There are some general principles which apply to the usage of all graded models:

- Add the grading as a perturbation. In other words, first fit using a non-graded model such as a Cauchy model. Once the best fit has been obtained in this manner, add graded.mat just above the Cauchy layer in the model. Set the graded layer thickness equal to the Cauchy layer thickness and declare it is a fit parameter. Select material #1 to be the Cauchy layer, and answer Yes when asked if you want to couple it to the existing Cauchy layer. Select material #2 to be void.mat. Finally, select a two node grading and specify the void fraction at the top of the film to be 0.01, and define this fraction as a fit parameter. You have now replaced the uniform Cauchy layer with a very slightly linearly graded layer of the same optical constants, and added the effective void percentage at the top of the film as a fit parameter in addition to the film thickness and Cauchy parameters. Finally, do not forget to set the thickness of the original Cauchy layer to zero, and switch it off as a fit parameter.

- Add complexity to the grading incrementally, and watch for the development of strong parameter correlations and/or unrealistic grading profiles, which will tend to occur when the parameter correlations are very strong.

- Do not be concerned by negative effective void fractions, as these merely represent a shift of the index of the original material upward.

- Always try to find the simplest grading which fits the model well.
It is often helpful to fit a single angle of incidence only to speed up the fitting process. Once a good fit has been obtained, expand the selected range to all angles and fine tune the fit.

Anisotropic films

WVASE® has very sophisticated modeling capabilities for anisotropic films and substrates. The most commonly encountered anisotropic films are oriented polymer films, which are usually transparent everywhere but the UV end of the spectrum. The anisotropic model created in “Example 6: Anisotropic organic film on silicon” from Chapter 14 works very well for these materials. Here are some useful general principles for the analysis of anisotropic films, and a figure from Example 6.

**c-axis perpendicular to the film plane**

In this case it is not possible to obtain the anisotropic optical constants of the film from ellipsometric data in spectral regions where the film is absorbing, regardless of how many angles of incidence are acquired. We then have two choices, either model the data in a spectral range where the film is transparent using the anisotropic Cauchy layer, or fit the data where the film is absorbing using an isotropic layer and fitting for the effective isotropic n and k values with the film thickness fixed.

When fitting data in a transparent spectral range, start with an isotropic Cauchy model and obtain the best possible fit in this manner. Then replace the Cauchy layer with the anisotropic Cauchy layer accauchy.mat. Set the anisotropic Cauchy layer thickness at the value obtained from the isotropic Cauchy model, and set the A, B, and C parameters of both Cauchy relations in the anisotropic Cauchy layer at the values obtained for A, B, and C from the isotropic Cauchy fit. Declare the anisotropic Cauchy layer thickness and both sets of A, B, and C parameters as variables (use only A and B if correlation problems between B and C are encountered).
Finally, for transparent anisotropic films you should generally obtain similar dispersion from both indices. If this is not the case, particularly if one or spectra are unphysical, the model is probably not physically accurate.

**c-axis in the film plane**

When the c-axis of the (uniaxially anisotropic) film lies in the film plane, it is possible in principle to obtain both index spectra in spectral regions and both sets of optical constants for the film in spectral regions where the film is absorbing. In order to do this we need to know where the c-axis of the film lies in the film plane, as it is necessary to be able to align the sample with the c-axis oriented parallel and perpendicular to the film plane. One means of determining the c-axis orientation is X-ray diffraction measurements, provided the anisotropy is due to the crystal structure of the film.

To determine the index spectra in spectral regions where the film is transparent, a single VASE® scan is required, with the c-axis oriented either parallel or perpendicular to the plane of incidence. The experimental data type of these data must be changed to ‘aEp: Ellips, opt-axis in sample plane, parallel to p-plane’ if the c-axis was parallel to the plane of incidence during the data acquisition, or ‘aEs: Ellips, opt-axis in sample plane, perpendicular to p-plane’ if the c-axis was perpendicular to the plane of incidence during the data acquisition. If the substrate is transparent and was not roughened, the data types ‘aEpb’ and ‘aEsb’ are appropriate, and indicate the same data types with back-surface reflections included.

To fit either type of scan in a spectral region where the film is transparent, use the acauchy.mat layer, and follow the instructions in the previous section to fit for both sets of Cauchy parameters and the film thickness. Again, it is a good idea to use the isotropic Cauchy model first to get an estimate of the film thickness and the Cauchy parameters. Note that it is possible in theory to determine the location of the c-axis by acquiring data from the sample at a number of positions and fitting the data to determine which position placed the c-axis closest to parallel or perpendicular to the plane of incidence. We have never tried this, but it should work.

Determination of both sets of n and k values for the film in spectral regions where the film is absorbing is somewhat more difficult. First, it is necessary to obtain the film thickness, either by fitting the anisotropic Cauchy model to the experimental data in a spectral region where the film is transparent, or by making an educated guess. Second, two VASE® scans are required, one each with the c-axis oriented parallel and perpendicular to the plane of incidence. Make sure to change the data type of each set of data appropriately and save the files with the new data type.

Load one of the two data files and then append the other file in the Experimental Data window. Next build the appropriate optical model and add the layer acauchy.mat for the anisotropic film. Specify the thickness of the acauchy.mat layer but do not vary the thickness, as this will introduce unacceptable correlations into the model. Define ‘n’ and ‘k’ in the acauchy.mat layer as fit parameters, and execute a point by point fit. WVASE® will fit for four parameters at each wavelength - the n and k values appropriate for the c-axis and for the a- and b-axes. To view the results in the Graph window, display the current layer optical constants (with the acauchy.mat layer as the current layer) and click on the ‘Anisotropic Optical Constants’ check box which appears. Both sets of optical constants will be displayed.
Very thin transparent films

The special case of very thin (less than 5 nm or so) transparent films usually cannot be solved for both the thickness and index of the film due to a very strong correlation between these parameters. This is a case where the use of literature constants for the film is usually required, such that the data is fit for the film thickness only. Keep in mind that the actual ‘measured’ quantity from such a fit is the optical thickness of the film, i.e. the product of the film thickness and index, and any change in the assumption of index for the film will subsequently yield a corresponding change in the best-fit thickness. For example, if we assume an index of 1.5 for a very thin film and fit for a thickness of 2.0 nm, we will obtain a thickness of 1.0 nm if we assume an index of 3.0 for the film.

Film thickness measurements on very thin transparent films (gate oxides, for example) can be very accurate provided the film index is accurately known (as is the case for thermal oxides on silicon). They will always be very precise and systematically correct provided a consistent value of the film index is used, but may not be accurate if the film index assumption is not accurate.

Very thick transparent films

At the other end of the thickness regime, very thick transparent films (greater than 5.0 microns or so) offer a very difficult challenge for the determination of thickness and index as well. In this case the interference oscillations observed in psi and delta are very dense, and many combinations of thickness and index can usually be found which fit the data reasonably well. Use of NIR data spread over a wide range of angles of incidence is helpful in determining a unique solution in this case. Again, if the film index is accurately known in advance, a very accurate film thickness measurement may be obtained.

13.6 Single absorbing films

In this section the analysis of VASE® data from single films which are optically absorbing everywhere in the measured spectral range is discussed. This is a very difficult problem, particular for films on opaque substrates. The best approach is always to find a spectral region where the film is transparent and follow the procedures given in the previous section, however some materials (metals, semimetals, very low bandgap semiconductors) are simply too absorbing over the VASE® measurement range to allow this type of analysis.

It is important to keep in mind that the light beam is attenuated as it propagates in an absorbing material. In order for it to be possible to measure the thickness of an absorbing film with an optical experiment, the light beam must be able to traverse the film at least twice and still retain enough energy to be detectable. As a result, it is not possible to measure the thickness of metal films beyond a certain thickness limit (typically ~50 nm), which is a function of the extinction coefficient of the metal. If you try and fit for an absorbing film thickness and the thickness repeatedly becomes very large, and perhaps generates the ‘Singular matrix’ error, the film in question is almost certainly optically thick, and you cannot expect to obtain the film thickness. In this case, either fix the film thickness at a very large value (1 micron, for example) or define the film to be the substrate (by deleting all films underneath it).
Opaque substrates vs. transparent substrates

Transparent substrates are very advantageous for the characterization of absorbing films, as they allow the acquisition of intensity transmission data through the substrate. The simultaneous analysis of VASE® and transmission data will usually yield a unique solution for the thickness and optical constants of a single absorbing film, whereas the analysis of VASE® data only will not yield a unique solution. It is particularly helpful to characterize absorbing films on fused silica substrates, as the substrate will not exhibit an absorption edge in the UV, which simplifies the modeling of transmission data considerably.

Single absorbing films on opaque substrates are extremely difficult to characterize, as we can acquire at most VASE® and reflectance data from such samples. The reflectance data are not as useful for eliminating model parameter correlations as they are similar in information content to the ellipsometric Ψ data, which are the square root of the ratio of the p- to s-reflectances. For the case of single absorbing films on opaque substrates, there are only a few choices for the analysis procedure:

- Assume a value for the film thickness and fit for the optical constants of the film only. Any error in the guess for the film thickness will introduce errors into the resulting optical constants.
- Use a highly constrained parametric model for the film optical constants with very few variable parameters which do not correlate to the film thickness. This requires considerable effort to develop a sufficiently restrictive and uncorrelated parametric model. Best results are obtained for substrates with very sharp features in their optical constant spectra which cannot be reproduced by the parametric model for the film.
- Perform a multiple sample analysis on several similar films differing only in thickness. This is tricky, requires several samples, and any dependence of the film material optical constants on film thickness will skew the results.
- For the special case of semiconductor substrates with sharp critical point structure in the substrate optical constants, a trick invented by H. Arwin and D. Aspnes sometimes helps. Choose values for the thickness of the film and fit for the film optical constants. Try to find a film thickness which yields film optical constants which do not show features at the substrate critical points. This is very time consuming and relies on arbitrary decisions by the user.

Analysis of VASE® and T data for films on transparent substrates

For absorbing films on transparent substrates, it is usually possible to uniquely obtain the film thickness and optical constants by simultaneously fitting VASE® and transmission data from the sample. You should first characterize an uncoated (identical) substrate in order to determine the substrate index, and, if the substrate exhibits any absorption, the substrate thickness and extinction coefficient spectrum.

Then, to characterize the coated sample, acquire the intensity transmission data first, and then (if possible) roughen the back surface of the substrate to suppress back-side reflections. Then acquire VASE® data from the same spot on the sample, making sure to acquire the data at the same wavelengths the transmission data were acquired at. If the sample was not roughened prior to the acquisition of the VASE® data, change the VASE® data type to ‘Eb - ellipsometric with back-side correction’ and resave the file. Load the ellipsometric data into the Experimental Data window, and then append the transmission data. Use the ‘Type’ menu from the Graph.
window to select the experimental quantities you wish to view, either psi, delta, or transmission.

To model these data, add the substrate layer to the model, and then add a layer which is as close to the actual film material as possible. For example, if the film is a nickel-chromium alloy, try starting with the nickel or chromium optical constants. If the film is a semiconducting material, try to find an optical constant file for that material or a similar material. Specify the layer thickness as a fit parameter, but not the optical constants of the layer. Perform a normal fit, and see how close you get with the assumed film optical constants.

Now define the layer optical constants n and k as fit parameters, along with the film thickness. Execute a normal fit again. If the substrate was not roughened, you will probably need to fit for the number of back-surface reflections which were collected as well. Hopefully, this fit will yield a very good (and unique) fit to both the ellipsometric and transmission data, and a physically reasonable set of optical constants for the film. If not, there are a number of things to try:

- Increase the weighting of the transmission data (from the ‘Defaults’ menu from the Fit window). This may help eliminate correlations, and will force the film extinction coefficient spectrum to match the transmission data. This is very helpful if noise in the VASE® data is causing very noisy optical constant spectra. Setting the transmission weighting to 500 or 1000 percent of the standard deviations will cause the transmission to be weighted roughly equally with the VASE® data, while setting the transmission weighting to a very large number (say 10000) will cause the model to lock on to the transmission data in one or two iterations. Try doing this and then relaxing the transmission weighting and repeating the fit.

- Check the back-surface reflection parameter. Try the following, with the number of reflections set to 0.5, 1.5, and 2.5. First set the back surface correction parameter (at 0.5, 1.5, or 2.5) but do not allow it to vary during the fit. Perform a normal fit for the film thickness and optical constants. When this fit reaches a best-fit result, declare the back-surface correction parameter as a fit variable (in addition to the film thickness and optical constants) and repeat the fit. Try this for all three values of the back-surface correction parameter. This parameter (due to its mathematical formulation) may not want to cross integer values (0, 1, 2) and you may have to manually shift it in this manner to find which interval it should lie in.

- Add a surface oxide layer to the film. This is tricky, as you will not be able to vary the thickness of the surface oxide or its optical constants without totally correlating the model. Try to use an oxide material which is reasonable for the film under study, and try fitting for the film thickness and optical constants with several different assumptions of the oxide thickness (1.5 nm, 2.0 nm, 2.5 nm, etc.). You may be able to identify an oxide thickness which yields good results.

- As a last resort, you may need to vary the index of the glass substrate if the initial substrate characterization did not yield an accurate result. This is most conveniently done if the Cauchy dispersion relation or one of the similar user-defined index parameterizations is used to describe the substrate index. In this case, try varying the constant term in the substrate index dispersion model along with the film thickness and optical constants. You will probably not be able to obtain a unique solution, but if this model fits the data very well and no other model did, it is probably worth going back and characterizing a bare substrate again.

**Lorentz oscillator models**

The Lorentz oscillator parametric model for optical constant dispersion is very useful for metal films and metal substrates (or optically thick metal films, which
are effectively substrates). For single metal films on transparent substrates, the direct analysis of \textit{VASE}® and transmission data is the best approach, however Lorentz oscillator models can be useful to eliminate random noise from being incorporated into the film optical constants. For metal films on opaque substrates, the Lorentz oscillator model is usually the only chance one has to obtain any reasonable results for the film thickness and optical constants. Lorentz oscillator models for metal films are particularly useful for multilayered structures containing metal films and for analyzing dielectric films deposited on metal films or substrates.

The Lorentz oscillator parametric model for the dispersion of the optical constants of materials is derived based on the assumption that the response of electrons in a material to a driving electric field (in this case due to the light beam) is similar to the response of a harmonically driven mass on a spring subject to a dissipative force. In this analogy, the mass corresponds to the electron, the spring represents the electrostatic forces on the electron due to all of the other electrons and nuclei in the solid, and the dissipative force (friction, for the mass on a spring) represents the electron energy loss due to emission of a photon. Note that this model is classical in that the electron is treated as a particle orbiting or propagating in the solid with a known trajectory, and may possess any amount of kinetic energy (as opposed to the allowed energy levels and bands of quantum theory).

Nevertheless, the Lorentz model can accurately describe the optical constants of many materials, and is particularly useful for resonant absorptive processes (dye absorption lines, vibrational bands in FTIR data, etc.). It also has the useful property of reducing to the Drude model for free electron absorption in the limit of an oscillator centered at zero energy, which is very useful for transparent conducting oxides and heavily doped semiconductors.

It was stated in chapter 2 - “A Short Course on Ellipsometry” that the imaginary part of the dielectric function at a given wavelength was proportional to the power per unit volume (energy per unit time per unit volume) absorbed at a point in a material from a monochromatic light beam of the given wavelength. To complete the mass on a spring analogy for the electron is a simple matter then of calculating the power absorbed by the mass from the driving force, using electromagnetic units appropriate to the analogy. The result of this calculation is the imaginary part of the dielectric function, to which the Kramers-Kronig transformation is applied to obtain the real part of the dielectric function. The result, which is the Lorentz oscillator model, is generally formulated as follows:

\[
\tilde{\varepsilon}(E) = \varepsilon_i(\infty) + \sum_{i=1}^{N} \frac{A_i}{E_i^2 - E^2 - iB_iE},
\]

where \(\tilde{\varepsilon}(E)\) is the dimensionless complex dielectric function as a function of photon energy, \(\varepsilon_i(\infty)\) is the value of the real part of the dielectric function at very large photon energies, \(N\) is the total number of oscillators. Each oscillator is described by three parameters. \(A_i\) is the amplitude of the \(i^{th}\) oscillator, which has units of (eV)^2, \(B_i\) is the broadening of the \(i^{th}\) oscillator, which has units of (eV), and \(E_i\) is the center energy (location) of the \(i^{th}\) oscillator, also in units of (eV). The \textit{VASE}® Lorentz oscillator layer \textit{lorentz} mat allows up to seven oscillators in the model for a single layer. The following is the Lorentz oscillator dialog box, with three active oscillators:
Figure 13.42. The Lorentz oscillator dialog box, from lorentz.mat.

Note that the number of oscillators may be specified by the user, with 1 - 7 oscillators active. The value of $\epsilon_1$ at infinity may be specified and fit, and the amplitudes ($A_m$), broadenings ($B_r$) and center energies ($E_n$) of each oscillator may be fit. Also, the optical constants of this layer may be varied directly by turning off all of the Lorentz oscillator parameters and $\epsilon_1$ at infinity as fit parameters and clicking on the ‘n’ and ‘k’ check boxes in the lower right corner of the dialog box.

Lorentz oscillators are primarily useful for describing resonant absorption peaks due, for example, to doping of a dielectric material with a dye, and for metal films. For resonant absorption peaks due to a single type of optical transition, a single Lorentz oscillator mixed with a Cauchy background (using an EMA layer to mix the two constituents) is often useful. For metal films, anywhere from three to seven oscillators usually suffice, depending on the complexity of the metal optical constant dispersion and the spectral range required.

When fitting Lorentz oscillator parameterizations for metal film optical constants, follow the following procedure.

- Try to get an estimate of the optical constants of the material to start with, using any other model which will work. As a last resort, pick a reasonable thickness for the film and fit for the optical constants of the film with the thickness fixed.

- Create a new model with a layer having the optical constants you obtained for the film in the previous step as the substrate. Generate data for this model, and copy the generated data to the Experimental Data window. Make sure the generated data covers the spectral range in which you wish to use the Lorentz oscillator parameterization.

- Delete the model and create a new model by adding the file lorentz.mat as the substrate.

- From the Defaults menu, set the light units to photon energy.

- Go to the Graph window, and plot $\langle e_2 \rangle$ (pseudo-imaginary part of the dielectric function).

- Look for obvious peaks in the ‘experimental’ $\langle e_2 \rangle$ (no more than three at this point). We will need an oscillator for each peak, so use the pointer to pinpoint the energy of any obvious peaks. If you hold down the left mouse button while pointing the arrow at a point on the graph, the x- and y- coordinates of the tip of the arrow are displayed above the graph. In this case the x-coordinate is photon energy.
• Go to the Model window, and open the Lorentz layer dialog box. Set the number of oscillators to the number of peaks identified in the \( e^2 \) spectra plus one, as we will add an oscillator for the background due to free electron absorption.

• Set the amplitude of each active oscillator to one, and set the broadening of each active oscillator to 0.3. If you are working with a metal, set the energy of the extra oscillator to zero, set its amplitude to 10, and its broadening to 0.5.

• Generate data from this model. Go to the Graph window and view the generated and 'experimental' \( e^2 \) again, with an eye toward how well the peaks match. Go back and forth between the model, generated data, and Graph windows, changing values of the various amplitudes and broadenings to try and get the peaks in \( e^2 \) to match up fairly well. Do not be afraid to experiment a bit in order to get a good feeling for how changing the Lorentz parameters affects the lineshape.

• If you cannot manage to get close at all, and you are working with a metal film, set the number of oscillators back to one, set the energy of the single oscillator to zero, set the amplitude to 10, and the broadening to 0.5. Declare the amplitude, broadening, and \( e^1 \) at infinity as fit parameters.

• If you were able to get reasonably close, declare \( e^1 \) at infinity and all oscillator amplitudes as fit parameters.

• Execute a normal fit.

• If one of the amplitudes goes to zero (or 1.e-8) set the amplitude to zero and turn it off as a fit parameter, then execute a normal fit again.

• Go to the Graph window and view the ‘experimental’ and calculated \( e^2 \) data.

• Hopefully at this point the two sets of data are fairly close. If not, try moving the oscillators around and trying again, or reducing the number of oscillators and refitting.

• Turn on the broadenings of the oscillators in addition to all of the previously defined fit parameters and perform a normal fit again. If a broadening goes to zero a 'singular matrix' error will occur. Fix that broadening to zero and turn it off as a fit parameter, then fit again. If an amplitude goes to zero (1.e-8), fix it at zero and turn it off as a fit parameter, then fit again.

• Keep an eye on \( e^2 \) in the Graph window. The match between the experimental and calculated data should be getting closer as we turn on more and more fit parameters, and we should be starting to match the obvious peaks fairly well.

• Once a minimum is found with all amplitudes and broadenings varying, add the energies of all of the oscillators as fit parameters and fit again. If an energy goes to zero, fix the energy value at zero, turn it off as a fit parameter, and fit again.

• We should now be at the best fit obtainable for the number of oscillators we are using. To get a better fit we will need to add more oscillators.

• Go to the Graph window and view the ‘experimental’ and calculated \( e^2 \) data again. Select ‘Type’ from the menubar and select ‘Difference between experimental and calculated’ from the menu which appears. The quantity plotted in the Graph window is now the difference between the experimental and calculated \( e^2 \), which is negative if the experimental \( e^2 \) is larger than the calculated \( e^2 \).

• This provides an easy way to locate places where the addition of another oscillator will help. Any place that the difference plot is negative requires additional absorption from the model in order to achieve a better fit. Look for pronounced
negative valleys in the difference plot, and identify the location of the valley center for the largest valley using the pointer.

- Go to the Lorentz layer dialog box. Increase the number of oscillators by one, and set the center energy of the new oscillator at the value determined for the valley center in the previous step. Set the amplitude of this oscillator to 0.01 and the broadening to 0.3. Declare the amplitude and broadening of the oscillator as fit parameters (in addition to all previously defined fit parameters) and perform a normal fit. If the fit is improved and the amplitude of the new oscillator does not go to zero, turn the energy of the new oscillator on as a fit parameter and fit again.

- Repeat the viewing of the difference plot for \( e_2 \) and the addition of new oscillators until either there are no pronounced valleys in the difference plot or you have used all seven oscillators. By this point a good fit should have been obtained.

- \( e_1 \) at infinity has a strong tendency in metals to correlate to oscillator parameters, particularly if the broadening of an oscillator goes to zero. If the value of \( e_1 \) at infinity drops below one, it is strongly correlated to another parameter, and you should fix \( e_1 \) at infinity to one and turn it off as a fit parameter.

- An oscillator broadening may drift to zero, with a non-zero amplitude and center energy. This is equivalent to the poles in the parametric semiconductor model, and represents a contribution to the slope of the index of refraction from an absorption process located outside of the measurement range.

- The amplitude, energy, and broadening may simultaneous drift to very large values, representing a nearly constant value of absorption across the entire spectral range. If this happens, fix the broadening and center energy of that oscillator and fit only for the amplitude.

- This type of fitting can be frustrating, but it is worth the time and effort to develop some experience with it. Once you have a reasonable fit, save the Lorentz oscillator dispersion parameters. Load the original experimental data from your film, and build an appropriate optical model with the new Lorentz layer for the film. Use your best estimate for the film thickness, and declare the thickness as a fit parameter. Perform a normal fit.

- Turn on the larger Lorentz amplitudes as fit parameters (any greater than 10). If \( e_1 \) at infinity is not one, turn it on as a fit parameter as well. The thickness should still be defined as a fit parameter. Perform a normal fit.

- Turn on the rest of the amplitudes and the broadenings as well. Fit again.

- Turn on the energies of all oscillators (unless they are zero) and fit again.

- By now you hopefully have a very good fit to the experimental data.

Here are Lorentz oscillator parameterizations for some common metals, as determined by fitting literature optical constant spectra.
Figure 13.43. Lorentz oscillator parameterization for literature optical constants of aluminum.

Figure 13.44. Lorentz oscillator parameterization for chromium.

Figure 13.45. Lorentz oscillator parameterization for stainless steel.
Figure 13.46. Lorentz oscillator parameterization for tantalum.

Figure 13.47. Lorentz oscillator parameterization for titanium.

Figure 13.48. Lorentz oscillator parameterization for titanium nitride (TiN).
Figure 13.49. Lorentz oscillator parameterization for silicon, from fit to Jellison’s optical constant spectra. Note the negative oscillator amplitudes - an indication that the Lorentz oscillator parameterization is not quite flexible enough to model silicon accurately.

Surface oxidation of the film

The principles discussed earlier for the modeling of thin surfaces oxides on bulk absorbing substrates apply to the case of absorbing thin films as well. For a single film analysis the only reasonable approach is usually to guess at reasonable optical constants and a reasonable thickness for the surface oxide, but not to vary these parameters. Only in cases of multiple sample analysis or analysis of several different optical data types from a single absorbing film will it be possible to obtain any information about the thickness or optical properties of the surface oxide.

Surface roughness

The inclusion of surface roughness is nearly equivalent in principle to the inclusion of a surface oxide film. In this case, we use the EMA layer to define an effective mixture of 50% of the film material (select the film layer file name for material #1 and allow it to be coupled to the existing film layer) and 50% voids, and we usually try to fit for the roughness thickness. In most cases the roughness thickness will correlate very strongly to the thickness of the film, and at best you will usually have to either not include roughness or fix the roughness thickness at some reasonable value. In a few cases, the VASE® data will be very sensitive to the surface roughness, and it may be possible to get both the surface roughness thickness and the film thickness. This will nearly always be the case if the film optical constants are known and held fixed during the analysis, such that you are fitting for the film and roughness thickness only, and no optical constants or optical constant parameters for the film.

13.7 Single films - special

There are a number of special techniques which have been developed for the analysis of data from films of specific materials or classes of materials. In this section we review alloy models for compound semiconductors, the usage of the Lorentz model for transparent conducting oxides, and the use of EMA models for polycrystalline silicon films.
Alloy models

Consider the case of a ternary compound semiconductor, such as Al\textsubscript{x}Ga\textsubscript{1-x}As, a very important material for GaAs based devices. First, say we grow films of different alloy compositions covering the entire range of alloy concentrations, and including the endpoints GaAs and AlAs. We then analyze these films to determine the optical constant spectra of the films. We now know the optical constants of the alloy system at a number of discrete compositions which cover the entire allowed composition range. We can now use a critical point shifting interpolation algorithm developed by Snyder et. al. (P. G. Snyder, J. A. Woollam, S. A. Alterovitz, and B. Johs, J. Appl. Phys. 68(11), 5925 (1990) to predict the optical constants of an alloy with composition between two of the known compositions.

This knowledge allows us to construct a single parameter model for the optical constants of the alloy system. Given the alloy fraction of an AlGaAs film, we can calculate its optical constants by interpolating between our sets of known optical constants, such that when analyzing an AlGaAs film we can fit for the alloy fraction rather than the optical constants of the film. This model is implemented in WVASE\textsuperscript{®} as alx\_gaas.mat, and the following figures depict optical constants for various compositions predicted by the alx\_gaas.mat layer.

Figure 13.50. Real part of dielectric function (\(e_1\)) as a function of photon energy for various alloy concentrations in the Al\textsubscript{x}Ga\textsubscript{1-x}As system, as predicted by the WVASE\textsuperscript{®} alloy interpolation layer alx\_gaas.mat.

Figure 13.51. Imaginary part of the dielectric function (\(e_2\)) as a function of photon energy for various alloy concentrations in the Al\textsubscript{x}Ga\textsubscript{1-x}As system, as predicted by the WVASE\textsuperscript{®} alloy interpolation layer alx\_gaas.mat.

Needless to say, these alloy parameterizations are extremely useful, particularly for lower bandgap materials which are absorbing over much or all of the measurable spectral range (HgCdTe, for example). They are also extremely useful for analysis of time dependant in-situ data acquired during the growth of structures containing alloy layers.
Transparent conducting oxides

Thin films of transparent conducting oxides (most commonly Sn doped indium oxide, or indium tin oxide - ITO) present a difficult challenge to ellipsometry and optical experiments in general. There are two reasons for this. First, the films show absorption in the UV due to interband optical transitions, but also exhibit an absorption edge in the IR due to optical absorption by free carriers in the film. Second, the films are nearly always strongly graded due either to the deposition method used for the film or to the post-deposition processing (annealing, usually) performed on the film. Most researchers and commercial characterization instruments ignore the grading of the film, achieve poor to mediocre fits to the experimental data, and publish the results, claiming to have achieved a simple characterization of the film (spectroscopic reflectometry proponents are notorious for this).

There are major problems with ignoring the film grading, however, as the resulting ‘simple’ model will contain large (potentially huge) systematic errors due to the tendency of parameters in the simple model to adjust to try and compensate for the grading effects in the film. Unless the grading of the film (and any roughness on the film) is treated properly, the resulting value of the film thickness and the resulting film optical constants cannot be expected to be even approximately accurate.

All this having been said, we must point out that even with WVASE® it is only possible to approximate the true grading of ITO (and other TCO) films. Consider a strongly graded film of ITO, such that at the top of the film the ITO material is highly conducting (low resistivity) and at the bottom of the film the ITO film is not very conducting (high resistivity). The material at the top of the film will exhibit a very strong Drude absorption edge in the IR end of the spectrum, such that its optical constants may look like this:

![Figure 13.52. Hypothetical optical constants of highly conducting ITO, from single Lorentz oscillator. For the oscillator, eI at infinity was 3.5, the oscillator amplitude was set at 3.5 eV², and the oscillator broadening was 0.2 eV.](image)

Now, at the bottom of film, where the ITO is not highly conducting, the Drude absorption edge will be considerably diminished, and the optical constants of the ITO might look like this:
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Figure 13.53. Hypothetical optical constants for poorly conducting ITO, from a single Lorentz oscillator model. For the oscillator, $\varepsilon_1$ at infinity is 3.5, the oscillator amplitude is 0.5 eV, and the oscillator broadening is 0.05 eV.

Note the difference between the magnitude of the extinction coefficient for the two sets of constants, and note especially the difference in the shape of the index and extinction coefficient curves between the two sets of spectra. The standard grading model relies on being able to reproduce the optical constants of the film material at any point in the film by using the EMA model to mix the optical constants of two constituent materials together. This model is simply not accurate for ITO films where the conductivity of the film (and hence the shape and magnitude of the Drude absorption edge) is actually varying through the film.

Nevertheless, reasonable results can usually be obtained for ITO films by using the standard grading model or by using multiple thin Lorentz layers to approximate the grading. It is possible that a researcher with sufficient patience could construct an alloy interpolation model based on optical constant spectra for ITO material of a broad range of conductivities, where the interpolation parameter would be the film conductivity rather than an alloy fraction, but this has not been done to this point in time.

Finally, it is usually necessary to include surface roughness to achieve a good fit for ITO films, although it is unclear whether this roughness actually exists or whether the roughness layer just provides one additional parameter to help compensate for the approximate nature of the graded model used for the film.

Polycrystalline silicon

There are three possible approaches for the analysis of polycrystalline silicon thin films. The simplest analysis consists of modeling the film as an effective mixture of either amorphous and crystalline silicon or amorphous silicon, crystalline silicon, and voids. In this case we fit for the film thickness and the fraction of a-Si (and voids, if present) in the film. It is always necessary to include the native oxide on the surface of the film, with the oxide thickness as a fit parameter. The surface oxide is usually found to be 3 - 5 nm thick.

The EMA model has the advantage of yielding a physically useful quantity (the a-Si concentration), but is not very accurate unless the a-Si is close to 0% or 100%. We can also characterize the film using standard techniques described for partially transparent films - first use a Cauchy model to determine the film thickness by fitting in the infrared end of the spectrum, then fix the film thicknesses and fit directly for the film optical constants. The Cauchy fit will probably require that you fix the top oxide thickness to eliminate strong correlations between the oxide and poly-Si thicknesses.
13.8 Single films - advanced modeling techniques

The techniques outlined in the previous sections are adequate in nearly all cases for the analysis of VASE® data from single films. In many cases, the accuracy of the analysis can be improved by the use of the advanced modeling techniques described in this section. There are also single film cases which will require the use of these advanced techniques in order to obtain any results whatsoever from the analysis. In this section we discuss the benefits of parameterizing the optical constants of the film under study and the parametric semiconductor model for describing the optical constants of thin films. This section concludes with a discussion of the analysis of non-ideal films, specifically covering the cases of graded, non-uniform, and patterned layers. Note that the final section of this chapter also contains a discussion of advanced modeling techniques applicable to both single films and multilayer structures.

Optical constant parameterization

The usefulness of parametric dispersion models for the optical constants of materials cannot be overstated. Parametric dispersion models (as opposed to varying the optical constants directly at each measured wavelength) assist the modeling process in several ways. First, they are inherently continuous, and cannot exhibit random noise in the optical constants due to random experimental noise. Second, a constrained parameterization may reduce strong correlations in the optical model. Finally, they may provide systematic means for comparing the optical properties of different films (by comparing parameters from film to film) which may provide insight as to the physical origins of difference between the films.

There are a number of parametric dispersion models explicitly implemented in WVASE®:

- Effective medium approximations (EMA).
- Alloy semiconductor models.
- Cauchy dispersion relation, with exponential absorption tail.
- Lorentz oscillators.
- The parametric semiconductor model.

Also, the user-defined dispersion layer (user.mat) allows the user to specify any dispersion relation for the optical constants and fit for parameters in this dispersion relation.

Note that these models range from very highly constrained models with very few parameters (EMA, alloy semiconductor), to moderately constrained with a moderate number of variable parameters (Cauchy, Lorentz oscillators), to relatively unconstrained with (potentially) a large number of variable parameters (parametric semiconductor model). The particular model used will depend on the type of material under study and the problem the user is encountering which the parametric relation is being employed to solve.

As a general rule, try to obtain film optical constants directly to begin with (fix the film thickness and fit directly for n and k, for example). Generate ellipsometric data from a bulk model with these constants as the substrate, and fit the parametric model to the generated bulk data first to determine the initial parameterization. Then, fit the original experimental data from the film using the parametric model. It can be very difficult to fit the parametric model directly to experimental data unless the initial guesses of the parametric model parameters are
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Try to identify which parameters have the strongest effect on the optical constants, and which have little effect on the optical constants. Parameters which do not strongly affect the optical constants can often be fixed, thereby potentially reducing model correlations. Diamond-like carbon, for example, may be described over a reasonable range of bandgaps by the parametric semiconductor model with only three variable parameters.

If the optical constants of the film under study are not correlated to the film thickness, neither will the parametric model parameters. If, however, there are strong correlations between the film optical constants and other model parameters, it is quite likely that parameters in a dispersion model will also correlate to other model parameters. In this case, try to find the minimum set of film parameters which will still fit the data, and keep fixing parameters until an uncorrelated model is obtained (if possible).

Non-ideal films

The ideal thin film (perfectly flat top and bottom surfaces, homogeneous, etc.) is an abstraction required for the construction of optical models, but rarely occurs in the real world. The most commonly encountered film non-idealities are roughness at the top and/or bottom of the film, thickness variations with position in the film, variation of the optical constants from top to bottom through the film, and incomplete coverage by the film (unintentional or intentional, such as patterned films). In this section we discuss the modeling of optical data from non-ideal films, specifically addressing the cases of graded, non-uniform, and patterned films. Surface and interfacial roughness was treated previously (via the use of EMA models) and will not be covered here.

Graded dielectric films

There are many physical mechanisms which may lead to variations in the optical properties of a thin film along the direction normal to the film (vertically through the film). Most commonly, such variations are due to drifting of process parameters during the deposition of the film, or are induced by post-deposition processing of the film (annealing, implantation, etc.). This is a case where extensive knowledge of the deposition process and any post-deposition treatment are very helpful in constructing the optical model, as well as deciding whether or not a graded best-fit model is physically reasonable.

To truly model graded films well, it is important to understand the physical mechanisms which lead to grading of the film optical constants. For many dielectric materials, the grading is due to slight changes in the stoichiometry of the film and can normally be adequately modeled by simple grading profiles which merely shift the index up or down through the film. In many cases, however, the grading of the film optical constants is tied to variations in a primary optical absorption mechanism through the film, and the resulting change in the dispersion of the optical constants through the film cannot be modeled simply by shifting the optical constants up and down with the EMA type grading.

This is a very important point, which we will illustrate with some examples. First, in the simplest case, consider an off-stoichiometric silicon dioxide film, deposited (most commonly) by chemical vapor deposition (CVD), and let us assume that the stoichiometry of the film is changing slightly through the film. In this case, as long as the film does not get too close to silicon monoxide, the film will be
transparent from 250-1700 nm. Now, since the absorption edge of silicon dioxide (and the off-stoichiometric oxides near this composition) is much deeper into the UV than 250 nm, the index will show little dispersion from 250-1000 nm. As a result, even though the index will change slightly through the film, the dispersion of the index will not change significantly, and the simple EMA grading model will adequately describe this material. Here are the index spectra we might observe at the top and bottom of the film.

Note that a negative void fraction of -10% was used to calculate the shifted curve in the above figure. Negative void fractions are commonly encountered in graded models for dielectric materials, and are not problematic. The EMA model with voids is being used only to shift the index up and down, and has nothing to do with whether there are actually any voids in the film or not. Negative void fractions will always shift the index higher, while positive void fractions shift the index lower.

A very common approach to graded dielectric films is to use a Cauchy model to describe the index of the film and then allow the film to be graded. In many cases this allows the determination of the index and grading of the film. To perform this type of analysis, first fit the standard Cauchy model to the experimental data (this may be done over a restricted spectral range). Try adding surface roughness, and if it helps (without correlating the model) leave the surface roughness in the model. To test for grading, we now add the potential for grading in the model without (initially) perturbing the model significantly from the result of the non-graded Cauchy fit.

To add grading, move the active layer arrow in the Model window next to the Cauchy layer in the model and select ‘AddLayer’ from the menu bar, thus adding a layer above the Cauchy layer. Select graded.mat, and the graded layer dialog box will open. Make sure the EMA type of model is selected under ‘OptConstCalc’. Select cauchy.mat for material #1, and reply ‘Yes’ when asked whether to couple to the existing layer. This forces the optical constants of one constituent of the graded layer to be the same as those of the Cauchy layer already in the model. Select void.mat for material #2.

Now specify the grading. Always start simple and add parameters incrementally to the model. If you initially specify a 5 node grading and fit for all of the parameters, the odds are good that the grading parameters will wander and the model will drift very far from the true best-fit model, causing you to have to start over (or use the ‘Reset’ command from the menu bar in the Fit window to reset all of the variable parameters). To begin, make sure that ‘Discrete nodes’ are selected under ‘Profile Definition’ and set the ‘# of Nodes’ to two (2). Set the value of the top node to 0.1, and declare this value as a fit parameter.
Next, specify the thickness of the graded layer to be equal to the thickness of the Cauchy layer, and declare the graded layer thickness as a fit parameter. Then set the thickness of the Cauchy layer to zero, and turn the Cauchy layer thickness off as a fit parameter. When done, the graded layer dialog box would look like this:

![Graded layer dialog box, for graded Cauchy layer fit.](image)

We have now allowed a linear grading of the index of the film, with the dispersion of the film index described by the Cauchy layer (of zero thickness). The use of layers of zero thickness for coupling into graded or EMA layers is very common. Execute a normal fit, and see if the grading parameter moves significantly away from zero. If so, and the fit is considerably improved, the film is probably graded. Fit the model to a minimum, and check for correlation. If the film seems to be graded strongly (grading parameter at top greater than a few percent), try adding another node halfway through the film, guessing its value at half of the top node value, and fitting for the middle node value as well. If this improves the fit, try varying the center node position as well. Nodes may be added one at a time, and their values and positions varied as necessary to fit the experimental data.

In practice, use of more than three nodes usually leads to very strong correlations in the model and often to very strange grading profiles in the film. Be very careful when using graded models to establish that you have truly found the best-fit minimum (not a local minimum) in the MSE, and that the final best-fit model is unique and not strongly correlated.

Finally, it is very important when fitting for the index and grading of the film simultaneously to make sure that the EMA fraction at least one node is not varied. Normally, the fraction at either the top or bottom of the film is set to zero and not varied, such that the optical constants at this point in the film are exactly described by the Cauchy layer (or whatever layer is used to describe the film material). If there is no fixed node, the Cauchy A parameter will be 100% correlated to all of the node values, as the index of the film may be shifted uniformly in exactly the same way by either changing the Cauchy A parameter or changing all of the node values by the same amount.

Several examples of the analysis of graded dielectric films are given in chapter 18 - “VASE® Data Analysis Examples”.

**Graded absorbing films**

Life is considerably more difficult when dealing with graded films which are not transparent over much of the measured spectral range. In this case, there is usually much stronger dispersion of the optical constants of the film material, and the change in film properties will often lead to changes in the optical constant.
dispersion. Grading with voids will shift the film optical constants uniformly, but cannot model grading of the dispersion of the film material.

The best example of this type of grading are transparent conducting oxide (TCO) films, most commonly indium-doped tin oxide (ITO). The optical constants of a typical ITO film are shown below.

Figure 13.56. Optical constants of a typical low resistivity ITO film.

There are two optical absorption processes which shape the dispersion of the ITO optical constants. Interband absorption in the UV leads to the absorption tail observed for wavelengths less than 300 nm, while free electron absorption yields the strong absorption tail in the IR, with the accompanying ‘twist’ in the index of refraction spectrum.

The interband absorption does not usually change significantly through the film, however, the free electron concentration in the film may change drastically from top to bottom of the film, with accompanying drastic changes in the optical constant spectra from about 800 nm on up. The spectra in the previous figure were obtained from highly conducting ITO, and should be compared to the following spectra, from a film of much lower conductivity.

Figure 13.57. ITO optical constants, low conductivity film.

While the spectra are reasonably similar in the UV, where interband transitions are dominant, they are markedly different in the IR, with the low conductivity film exhibiting a much smaller absorption tail and an index spectrum resembling that of normal dielectric materials. Note also that the extinction coefficient is non-zero over the entire spectral range. This is an unfortunate artifact of the Lorentz oscillator model. The onset of absorption in the UV is due to direct transitions in ITO, such that the absorption edge should go abruptly to zero. The Lorentz oscillator model is simply not capable of reproducing this feature, and a tail in the absorption at the band edge is always present when using Lorentz oscillators to model the UV absorption edge.

Now, if the free electron concentration is changing through the ITO film, the magnitude and location of the IR absorption tail will be changing.
correspondingly, as will the dispersion of the index of the film in the IR. Only in rare cases (very weak grading or very thin films) will EMA type grading models be adequate to describe this type of grading.

There are several ways to attempt to analyze this type of grading. First, it may be possible to use Lorentz oscillators to define two sets of ITO optical constants and grade between them. This works for thin films, but will not usually work if the film is very strongly graded or is thicker than a few tens of nm. The other possibility is to not use the graded model at all, but split the ITO film into multiple uniform films (via Lorentz oscillators) and try to fit for the optical constants of each film.

In all cases, it is helpful to simply avoid the UV absorption edge of the film by fitting the data from 500 - 1700 nm only, where a single Lorentz oscillator with a fixed center of zero will describe ITO very nicely. In this case, fit for $\epsilon_1(\infty)$, and the amplitude and broadening of the oscillator.

As a final note, we point out that the ideal means of modeling graded ITO (and other graded absorbing films) is to construct a model for the optical constants of the material in terms of parameters which are related to the film property which is graded, and grade these parameters directly through the film. For the case of ITO, this would require the ability to grade the three Lorentz oscillator parameters ($\epsilon_1(\infty)$, amplitude, and broadening) through the film, which would correctly reproduce the change of the dispersion of the optical constants through the film. This type of model is not currently available within WVASE®.

### 13.9 Two layer systems

The VASE® technique can be very powerful for the characterization of double film systems, and in many cases is the only technique capable of yielding useful results from double filmed structures. In this section we discuss general principles applicable to the characterization of double films, and explicitly treat the cases of dielectric/dielectric, metal/dielectric, dielectric/metal, and metal/metal film systems. We close with a brief discussion of double film samples in which one or both films are anisotropic.

#### General principles

There are some general principles which are important when characterizing double film systems, which are discussed in this section.

**Opaque vs. transparent substrates**

For double films on opaque substrates, it is only possible to acquire VASE® data in reflection from the sample (and intensity reflection, which adds very little information). For double films on transparent substrates, it is usually a good idea to acquire intensity transmission data at normal incidence first, and then acquire VASE® data from the same spot on the sample. It is very helpful to roughen the back side of the sample prior to the VASE® data acquisition in order to eliminate back-surface reflections.

For structures (on transparent substrates) in which one or both films are absorbing, it may be necessary to ’pile up’ as much information on the sample as possible. In such cases, acquire normal incidence transmission, reflection VASE® data, transmission SE data, and, if possible, reflection VASE® data through the substrate. Append all of the sets of data and force the model to fit them all together. This may solve correlation problems for absorbing films.
Characterization of reference films

Whenever analyzing multilayer structures it is always helpful (but not required) to first characterize single films of the materials in the multilayer structure in order to obtain their optical constants. The thickness of the single film should be as close as possible to the thickness of the corresponding film in the multilayer in case the given material exhibits thickness dependent optical constants. When possible, try to obtain parametric models (Cauchy, user-defined, Lorentz, parametric semiconductor model) for the given film optical constants such that parameters in the optical constant model rather than the optical constants directly can be varied (if necessary) for the double film analysis.

Surface and interfacial roughness

Surface and interfacial roughness are both modeled with the effective medium approximation (EMA) layer. Surface roughness should be modeled as an EMA of 50% of the top film material and 50% voids, while interfacial roughness should be modeled as 50% of each film material. Note that if you are fitting for the top film optical constants (directly or via a parametric model) you will have to set the top film to zero thickness, add the interfacial roughness EMA layer above it (and couple one constituent of the EMA to the zero thickness layer), and then add the top film layer above the EMA, coupling it to the lower (zero thickness) layer, and specifying the original top film thickness. For example, a model for a silicon dioxide film on a silicon nitride film on a silicon wafer, with interfacial roughness between the two films, would appear as shown in the following figure. In this model, we are using literature optical constants for the nitride film and a Cauchy model for the silicon dioxide film.

![Figure 13.58. Model for silicon dioxide (Cauchy layer) on silicon nitride on silicon, with interfacial roughness between the silicon dioxide and silicon nitride films.](image)

Indistinct interfaces between the films

There are many cases where the interface between the two films may not be abrupt, but may be smoothed out over a transition region of non-zero thickness. A good example of this type of case are silicon dioxide films grown by thermal oxidation of silicon nitride films in oxygen. In most cases, the interfacial roughness model described in the previous section is adequate to model non-abrupt interfaces. If this model does not fit the data well and you suspect a broad transition between the films, it may help to replace the interfacial roughness layer with a graded layer. Set the graded layer up as an EMA grading with the two film materials as the constituents (this may require the use of a zero thickness layer, as shown in the previous figure). Choose the bottom film material as ‘Material #1’ and the top film material as ‘Material #2’. Choose a two-node grading, and fix the bottom node to zero and the top node at 100%, such that the graded layer optical constants vary smoothly from the bottom film to the top film. Specify a small thickness for the graded layer and fit for the graded layer thickness in addition to any other parameters in the model.

In any case, whether using standard EMA models or graded models for surface and interfacial roughness, be very careful to avoid strong correlations. In all cases, varying the fraction of one constituent in roughness layers in addition to...
thickness will yield 100% correlation between these parameters. Also, roughness layer thicknesses will commonly correlate very strongly to other thicknesses in the model, particularly if one or both films are less than ~30 - 40 nm thick. The most successful use of roughness layers will occur when one (or preferably both) films are transparent and at least a quarter wave thick. In this case interference features will be present in the data, and the shape of the interference oscillations will be very sensitive to surface and/or interfacial roughness.

**Dielectric / dielectric / substrate**

Two layer systems consisting of two dielectric films (or two films which are both transparent over an appreciable part of the measured spectral range) are usually the simplest two film systems to model. Best results are generally obtained by employing a Cauchy model (or similar dispersion model for the index) for one or both films and fitting for the thickness of both films along with any dispersion model parameters.

This type of approach may fail for a number of reasons. First, if the films are fairly thin (say 10-20 nm each) it will usually not be possible to determine both thicknesses and both film indices due to strong parameter correlations. Second, if the films have very similar index spectra it will be nearly impossible to distinguish between the two films, and the sample may be modeled as a single film of some effective index. Third, if the lower film optical constants are similar to those of the substrate, it may not be possible to sense the lower film, and again a single film model may be appropriate.

As a general rule, the thicker both films are, the better the results will be. Also, the thicker the films or the more likely it is that there will be appreciable sensitivity to surface and interfacial roughness, index grading of one or both films, and anisotropy in one or both films.

**Dielectric / metal / substrate**

The dielectric / metal / substrate system is commonly encountered in many applications, and presents a difficult challenge to the VASE® user, particularly if the substrate is opaque. In the best case, we would hope to obtain the dielectric film optical constants and both film thicknesses from this analysis, although in some cases where the substrate is transparent it may be possible to obtain the metal film optical constants as well. In either case, it is very helpful to first characterize a single (identical) metal film without the dielectric top layer in order to obtain the metal film optical constants. This can be complicated if the metal film is very thin or exhibits significant surface roughness or surface oxidation. Note that the Lorentz oscillator parameterization is very useful in this case. First obtain the metal film optical constants directly (see previous sections for relevant procedures), then generate data from a bulk model with these optical constants, and fit Lorentz oscillators to these optical constants to obtain a Lorentz oscillator parameterization for the metal film optical constants. This will allow us to vary the metal film optical constants somewhat in the analysis of the double film structures (if necessary) by varying a few carefully chosen Lorentz oscillator parameters for the metal film, rather than directly varying the metal film optical constants at each measured wavelength.

If the substrate is opaque, try to fit VASE® data from the double film structure to determine both film thicknesses and the index of the dielectric film (in the spectral region where it is transparent) via a Cauchy or user-defined dispersion relation. If this fit does not work well, try including interfacial roughness (EMA of
50% metal and 50% dielectric, fit for thickness), surface roughness (EMA of 50% dielectric and 50% voids, fit for thickness), or possible index grading of the dielectric film.

For dielectric / metal film structures on transparent structures, VASE® and normal incidence transmission data should be acquired from the sample at the very least (characterize a blank substrate first to determine the substrate optical constants, if possible). Transmission ellipsometry data at oblique angles of incidence and reflection ellipsometry through the substrate from the back side of the film structure may also be helpful.

Fit all of the data acquired from the sample simultaneously, and try initially to fit for both film thicknesses (with the substrate and metal film optical constants fixed) and parameters in a dispersion model (Cauchy or user-defined) for the dielectric film index. Note that if the sample was not roughened, or if you are fitting transmission or reverse direction ellipsometric data you will need to use the back-surface correction parameters as well. Once a minimum is reached, try varying the metal film optical constants (via Lorentz oscillators or directly) in addition to all other parameters. This will probably yield a very good fit, but you must be careful to check that this fit is unique (no strong correlations in the model). If a good fit is not obtained, try adding (one at a time!) surface and/or interfacial roughness, index grading in the dielectric film, or anisotropy, if appropriate for the dielectric film material.

**Metal / dielectric / substrate**

The case of a metal film on a dielectric film on a thick substrate can also be quite challenging, although in special cases it is rather simple and provides an invaluable means of obtaining metal film optical constants. The metal film, of course, must not be optically thick, or the sample can be treated as a bulk system with the metal film as the substrate.

If the substrate is transparent, the techniques suggested in the previous section for dielectric / metal film systems on transparent substrates are applicable. Note that the dielectric film index may match the substrate index very closely (silicon dioxide film on glass, for example) in which case it will be very difficult to obtain the dielectric film thickness and index spectrum.

Opaque substrates present a very difficult analysis of the dielectric film is thinner than ~50 nm or so. In this case, either predetermined optical constants or optical constant spectra from the literature should be used for both films, and the thicknesses of both films should be fit. Attempting to fit for optical constants of either film directly or via parametric models (in addition to one or both thicknesses) will usually result in very strong parameter correlations and non-unique models.

If the dielectric film is thick enough to exhibit interference oscillations, and the metal film is thin enough that these oscillations are not completely damped out, we can perform a very powerful analysis of the sample. This analysis requires ellipsometric spectra acquired at least two (preferably three or four) angles of incidence, and the angles should be spread over a range of at least 10°. In this case, provided we know the index spectrum of the dielectric film we can uniquely determine the thickness of the dielectric film and the thickness and optical constants (either directly or via a parametric model such as Lorentz oscillators) of the metal film. If the dielectric film is silicon dioxide grown by thermal oxidation of the silicon wafer, the literature silicon dioxide index spectrum will accurately describe the dielectric film index. If the dielectric film consists of any other material a single film of the dielectric material should be characterized first to obtain the dielectric film optical constants.
Finally, to obtain best results it may be necessary to include an oxide layer at the surface of the metal film. This can be problematic, as the optical constants of many metal and metal alloy oxides are unknown, and the thickness of the oxide layer is usually not known. Try to find optical constants for a metal oxide which should be close (iron oxide for iron alloys, etc.), assume a thickness for the oxide layer (2 - 3 nm is usually a good guess), and fit the VASE® data for the dielectric and metal film thicknesses and the metal film optical constants. Varying either the oxide thickness or the oxide optical constants (directly or parametrically) will yield very strong parameter correlations and non-unique solutions. In this case we are simply trying to improve the accuracy of the model in order to obtain more accurate results.

**Metal / metal / substrate**

Double metal films are the most difficult of the double layer systems to characterize, as the optical constants of at least one and usually both films must be known in advance. In particular, if the substrate is opaque, all we can do is assume optical constants (from previous analysis of single films of each metal, hopefully) for each metal and fit for both thicknesses.

If the substrate is transparent, acquire as much data as possible from the sample (VASE®, transmission, reverse and transmission ellipsometry). Fit all of the data simultaneously, assume optical constants for each metal (from the literature or from previous characterization of single films) and fit for both film thicknesses (and back-surface correction parameters if appropriate). Try varying the optical constants of one or both metal films (parametrically if possible, directly otherwise) and see if a unique fit is obtained. Lorentz oscillators are invaluable for this type of analysis.

### 13.10 Multilayer structures

The VASE® technique can be an extremely powerful means for characterizing multilayer structures, provided the acquisition of data is carefully planned to provide a maximally useful data set for fitting, and the modeling of the data is performed carefully. As was the case for double layer films, it is always helpful (and often required) to characterize single films of the constituent layers in the multilayer of interest first in order to obtain optical constants for the various materials in the multilayer (in parametric form, preferably) prior to the characterization of the multilayer. In this section, strategies for the analysis of samples with three or more layers on a thick substrate are discussed.

**Opaque vs. transparent substrates**

Transparent substrates (particularly fused silica, which shows no absorption edge in the measurable UV region) are always advantageous for multilayer characterization, as they allow the acquisition of intensity transmission, reverse direction ellipsometric data, and transmission ellipsometry data. All of these data may be fit simultaneously, and will often yield a considerable amount of information about even fairly complicated multilayer structures. If possible, acquire normal incidence transmission, transmission ellipsometric data, and reverse direction ellipsometric data first, then roughen the back side of the substrate and acquire the standard VASE® data.

Opaque substrates may be somewhat less amenable for the analysis of multilayers, as we are limited to standard VASE® data and perhaps p- or s-polarized reflectance data from such samples. Crystalline semiconductor substrates (silicon, germanium, gallium arsenide, indium phosphide, etc.) are the most useful, as
literature optical constant spectra are usually adequate to model these substrates. Metal substrates are very difficult to handle, as it is difficult to obtain accurate optical constants for the substrate due to the presence of surface oxides on bare substrates.

Regardless of the type of substrate, it is a very good idea to obtain the substrate optical constants from the analysis of a bare substrate prior to the analysis of the multilayered structure.

**Choice of optimal experimental data**

For multilayers on opaque substrates, we are limited to standard VASE® data in reflection and intensity reflectance (p- or s-polarized) data only. Acquire the VASE® data first (make sure to get at least two and preferably three angles of incidence), and then attempt the analysis. If you cannot obtain a unique solution for the parameters you wish to determine by fitting the VASE® data only, acquire p- or s-polarized reflectance (but not both) at the same angles of incidence at which you previously acquired VASE® data. (Note that the ellipsometric psi equals the square of the ratio of the p- and s-polarized reflectances, thus any two of these quantities is sufficient to calculate the third, and we are wasting time measuring more than two of these data types). The VASE® and reflectance data should then be fit simultaneously, and in many cases the reflectance will eliminate some of the correlations in the optical model.

For multilayers on transparent substrates, begin by acquiring intensity transmission data at normal incidence. Depending on the complexity of the multilayer you may wish to also acquire transmission ellipsometry at one or more (oblique) angles of incidence, and you may also wish to acquire reverse ellipsometry data (through the substrate, reflecting from the bottom of the film stack). Then, roughen the back surface of the sample (if possible) and acquire standard VASE® data from the same location on the sample. Note that all of these sets of data should be acquired over the same range of wavelengths (photon energies) and with the same wavelength (photon energy) spacing if the optical constants of any material in the structure are going to be directly varied. It is difficult to tell in advance of the data analysis which experimental data types will be required, but in most cases the normal incidence transmission and standard VASE® data contain most of the information available from optical analysis of the sample, and these two data types are always a good place to start. Do not be afraid to experiment!

**Transparent layers**

There are two approaches to modeling transparent layers in multilayer structures. The first, which may be used for any type of layer, is to use fixed optical constants for the layer, obtained either from the literature or from the previous characterization of a similar film. In this case we would expect to fit for the layer thickness. The second approach is to parameterize the index spectrum of the layer, such that we can fit for the film index by varying 1-3 parameters in a suitable dispersion model (Cauchy, user-defined, or parametric semiconductor model, for example). It is often helpful to start with a Cauchy parameterization for a given material which is obtained from previous analysis of a similar film or from fitting the Cauchy relation to literature spectra for the given material. We can then vary only the constant (A) term of the Cauchy relation, allowing the film index to shift up and down but holding the dispersion of the index constant, or we can fit for all of the Cauchy parameters, thus allowing the dispersion and magnitude of the index to change.
The trick of varying the constant term only is particularly helpful in eliminating parameter correlations when the film is expected to be similar to the film from which the original Cauchy parameters were obtained. In this case it is reasonable to assume that shifting the film index up or down by a small amount while holding the dispersion of the index constant is a reasonable model for the index of the film. This trick is also very helpful for modeling glass substrates when the glass index spectrum is not exactly known.

The parametric semiconductor model, which is described in the final section of this chapter, is also a very powerful means of parameterizing the optical constants of films in multilayer stacks.

If the same transparent material appears more than once in the multilayer, define a Cauchy (or other) parameterization for the lowest film in the stack, and then couple the other films of the same material to the first film. This will allow you to vary the index of the material in question, and will force each film of this material in the multilayer to have the same index spectrum.

Superlattices and other periodic structures

Many multilayer samples consist of two or more layers repeated multiple times. Such structures are called repeated periodic structures, and when they consist of crystalline semiconductor films are usually referred to as ‘superlattices’. WVASE® has an option from the Model window called ‘Superlattice’, which will allow you to repeat any set of two or more films in the model any number of times. A single model may contain one or two repeated periodic structures.

For example, consider a structure consisting of a silicon wafer substrate, on top of which is deposited a 100 nm film of titanium dioxide, followed by a 150 nm film of silicon dioxide. These two films are then repeated ten times, such that there is a total of twenty films on the silicon substrate. To build an optical model for this structure, start with crystalline silicon for the substrate, then add the titanium dioxide film (we will use a Cauchy layer for this film in this example), and finally add the silicon dioxide film (we will use the literature silicon dioxide optical constants). The model should now look something like this.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Material</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 si</td>
<td>1 mm</td>
<td></td>
</tr>
<tr>
<td>1 cauchy</td>
<td>100 nm</td>
<td></td>
</tr>
<tr>
<td>2 sio2</td>
<td>150 nm</td>
<td></td>
</tr>
</tbody>
</table>

Figure 13.59. Starting model for the ten-period repeated periodic structure described in the text.

Next, from the Model window, select the ‘Superlattice’ option. The superlattice dialog box will appear. Click on the check box next to ‘Superlattice #1 Enabled’ to enable the first superlattice, enter ‘1’ as the starting layer for superlattice #1, enter ‘2’ for the ending layer, and specify the number of periods to be ten. The resulting dialog box is shown below.
Figure 13.60. Superlattice dialog box, with the bilayer consisting of layers #1 (Cauchy layer for titanium dioxide) and #2 (silicon dioxide) being repeated ten times, for a total of twenty layers.

Click on ‘Ok’ to close this dialog box. A bracket will now appear to the right of the model in the Model window, indicating which layers are being repeated and how many times they are repeated. The model for our example of ten periods of a silicon dioxide on titanium dioxide bilayer is shown below.

Figure 13.61. Model for ten periods of silicon dioxide on titanium dioxide, with the titanium dioxide films described by a Cauchy dispersion relation.

We may now define either (or both) film thickness(es) as fit parameters, and we may also fit for the Cauchy parameters for the titanium dioxide film (or any optical constants or optical constant parameters for either film). The twenty layer structure has been effectively reduced to a two layer optical model, and this reduction of the number of variables may yield unique solutions where explicit modeling of the full structure may not. This model will usually fail, however, if there is significant variation of the layer thicknesses through the structure, or if the optical constants of different films of the same material differ through the structure.

Use of parametric models to suppress correlation

In the simplest analysis of a multilayer, we assume fixed optical constants for each material in the multilayer and fit for thicknesses only. Even this simple model may not yield a unique solution if there are many layers, particularly if the assumed optical constants for one or more film material(s) are not accurate. In the most complicated case, we could fit for the optical constants and thickness of each film in the structure, but this model will always be 100% correlated, as there are far too many fit parameters for the available experimental data. We may also assume optical constants for all films in the multilayer and then fit for the thicknesses of the films and the optical constants of one film in the model, but even this simplification nearly always fails to yield a unique best-fit model due to strong parameter correlations.

So, to simply state the problem, how do we vary optical constants in a multilayer model without introducing unacceptable correlations between the model parameters? The answer is to parameterize the film optical constants which we intend to vary, such that we can vary a few parameters in the optical constant
dispersion model rather than varying the optical constants directly at each measured wavelength (photon energy). The simple Cauchy parameterization for transparent materials was discussed in the previous sections for transparent films (in all or part of the measured spectral range), but absorbing films often appear in multilayers as well, and parameterization of the absorbing film optical constants may be required in order to allow these optical constants to vary.

The simplest parameterization of absorbing materials is the alloy model for compound semiconductors such as AlGaAs, InGaAs, etc. In this case the optical constants of the alloy are parameterized in terms of a single variable, the alloy fraction of one constituent of the alloy. Thus, we can vary the optical constants of an alloy semiconductor layer by varying a single parameter - the alloy fraction. This is particular useful when characterizing semiconductor superlattices and quantum well structures.

For metal films, Lorentz oscillators are probably the best approach. Try to obtain an initial set of Lorentz oscillator parameters by characterizing a single film of the metal in question, or by fitting to literature spectra for the given metal. When using the Lorentz oscillator parameterization in a multilayer, try fitting only the largest amplitudes (and perhaps the value of the dielectric function at infinity) while leaving the remaining amplitudes and all broadenings and center energies fixed. This will allow adjustments to the metal optical constants, but will constrain the locations and broadenings of the individual oscillators. Depending on the sample structure, you may be able to fit for quite a few of the LO parameters and still obtain a unique model, or you may not be able to fit for any of the LO parameters without obtaining very strong correlations. Experiment with the LO parameters to find out which most strongly affect the data, and try to find the smallest possible set of LO variables which will a good fit and a unique best-fit model.

Finally, the parametric semiconductor model can be very helpful for the analysis of multilayer structures. This model is discussed in detail in the next section.

13.11 Advanced modeling techniques

In this section we conclude the chapter on analysis strategies by discussing some advanced techniques for modeling optical data. It is not possible to comprehensively review all of the available advanced techniques without writing a multi-volume series, so we will concentrate on useful concepts and general techniques, leaving the specific implementation of many of these techniques to be described by example in the next chapter - "VASE® Data Analysis Examples". Throughout all of this, remember to never be afraid to experiment, as even failed modeling attempts are usually quite educational.

Partial polarization effects and other non-idealities

To this point we have assumed that the ellipsometer itself and the sample under study are ideal. There are many non-idealities of the ellipsometer and the sample which may affect the measured ellipsometric data (or other optical data), the most common of which may be modeled with WVASE®. All of the non-idealities discussed in this section have a common property - in each case the non-ideality of the sample or the instrument leads to a beam entering the analyzer which is not completely polarized, but rather exists of two or more component beams, each of which exhibits a different (but well defined) polarization state. In this case the VASE® instrument (or M-44®) will measure well defined psi and deltas, but the
model will not correctly predict these values unless the non-ideal aspects of the instrument and/or sample are included in the model calculation.

**Back-surface reflection**

The most commonly encountered sample non-ideality is the collection of light reflected from the back surface of the substrate in addition to the desired beam which was reflected from the front of the substrate. This is shown schematically in the following figure.

![Figure 13.62. Schematic illustration of the reflection of light from the back surface of a transparent substrate.](image)

The problem with collecting the beam reflected from the back of the substrate in addition to the beam reflected from the front is that these two beams will not usually add coherently at the detector. Even though each individual beam (front- and back-surface reflected) has a well defined polarization state, the resulting beam entering the detector does not have a single well defined polarization state, rather it is partially polarized, meaning that it may be decomposed into a number (two in this case) of constituent beams of well defined polarization state.

Any number of the beams reflected from the back surface of the substrate may enter the detector in addition to the front-surface reflected beam, however the back-surface reflected beams usually decay very rapidly in intensity, as most of the beam is transmitted through the interface at each reflection from the bottom of the substrate. When modeling the number of back surface reflections which enter the detector, we use a real variable which may take on any positive value. This parameter may have non-integer values when only part of a back-surface reflected beam enters the detector. WVASE® allows the user to implement the back-surface correction algorithm by changing the data type of the experimental data to an appropriate back-surface corrected type. Two parameters may be varied in the back-surface correction model. The ‘# of back-surface reflections collected’ parameter allows the user to directly vary the number of back-surface reflected beams which are assumed to enter the detector when calculating data from the model in the Model window. The ‘% of first beam collected’ parameter allows the user to vary the amount of the first back-surface reflection which is collected, which is useful for analyzing reverse direction ellipsometric data.

It is preferable to eliminate the back-surface reflection by excluding it from entering the detector or by roughening the back of the substrate, but in many cases neither of these approaches is possible. You will usually know that back-surface reflections are being collected from the structure of the sample. Any sample on a glass substrate which is not opaque will exhibit back-surface reflection effects unless the substrate is so thick that the front and back reflected beams are well separated at the detector. Any substrate which is transparent in some part of the measured spectral region and has a reflecting or semireflecting back surface will also exhibit back-surface reflection effects. Common examples are silicon and GaAs wafers, which will exhibit very strong back-surface reflection effects at photon energies below the bandgap energy when the back surface of the wafer is polished.
It is particularly simple to detect the presence of back-surface reflection effects in ellipsometric data for bare substrates and samples with thick transparent films which exhibit strong interference oscillations (and hence handedness changes in delta) in the experimental data. For a bare transparent substrate, delta should be either 0° or 180°, and any systematic offset of delta from either bound usually indicates back-surface reflection effects, as shown below.

Figure 13.63. Ellipsometric delta calculated at 60° angle of incidence for a bare fused silica substrate. Data are shown for calculation both with and without back-surface reflection effects. The curve for the case where no back-surface reflections are collected is identically zero.

For thick transparent films which exhibit interference oscillations, the collection of back-surface reflections will smooth out the sharp handedness changes in delta, as shown below.

Figure 13.64. Ellipsometric delta data calculated for a 250 nm film of amorphous silicon (a-Si) on fused silica. Data were calculated at 70° angle of incidence, both with and without back-surface correction.

If you are uncertain as to whether back-surface reflections were collected for a given set of data, try changing the data type, starting the # of reflections parameter at a small value (say 0.01) and fitting for this parameter in addition to the other model parameters. If the fit is significantly improved and is still unique, it is probable that back-surface reflections were collected.

In most cases trying to vary both back-surface correction parameters simultaneously will yield a 100% correlation between them. Exceptions are reverse direction ellipsometry where the first reflection may be intentionally excluded from the detector. As a general rule, leave the % of the first beam collected fixed at 100% and fit for the # of back surface reflections. The back-surface reflections die out quickly, such that a value of 3 or so for this parameter is equivalent to infinity, and the # of back surface reflections should simply be fixed at three if it fits to this or a larger value. Note that the correction algorithm may be somewhat ill-behaved as this parameter approaches integer values, as the derivative of the correction is singular at integer values of the # of back-surface reflections collected. As a result, the fit algorithm may resist allowing this parameter to cross the integers one and two, and it is a good idea to try starting the fit with several different initial values of the # of reflections collected, such as 0.5, 1.5, and 2.5. Usually one initial value will yield a
considerably better fit, and the fit will converge to the same result for any initial value which lies between the same two integers.

**Film thickness non-uniformity**

A common sample non-ideality is variation of one or more film thicknesses across the sample surface. If a film thickness varies over the width of the light beam, the resulting reflected beam will be partially polarized, as the beam may be divided up into thin slices, each of which effectively ‘saw’ a film of slightly differing thickness. These beams must be properly added at the detector in order to correctly predict the measured psi and delta values. *WVASE*® allows the user to specify that the film structure on a given sample is non-uniform, such that all films in a multilayer are assumed to exhibit the same non-uniformity. The user must specify the percentage variation in film thickness across the probing light beam, and may fit for this percentage.

The measured data will not be very sensitive to film thickness variations unless there are spectral features in the measured data which are very strongly dependant on the film thickness, most commonly interference oscillations in psi and delta and sharp handedness changes in delta. For thinner films, non-uniformity of the film will simply lead to the determination of an effective thickness of the film which is roughly an average value over the illuminated area. For thicker transparent films, the film non-uniformity will tend to smooth out the sharp handedness changes in delta, as shown below.

![Figure 13.65. Ellipsometric delta data calculated for a 200 nm film of silicon nitride on silicon. The dashed curve was calculated for a uniform film, while the solid curve was calculated for a film exhibiting a 5% variation of the film thickness over the illuminated spot.](image)

**Patterned films and structures**

An extreme case of a non-uniform film is a film which only partially covers the substrate. Such films are commonly encountered due to patterning of the film into device structures. If the dimensions of the patterning are considerably greater than the wavelength of the light used in the *VASE*® instrument, diffraction by the patterned structures may be ignored, and this case may be treated by dividing the incident beam into components which either strike the film or strike a region with the film removed. The resulting beams yield a partially polarized total reflected beam.

*WVASE*® allows the user to specify one film in the sample which is patterned, and fit for the percentage of the illuminated area from which the film was removed.

**Monochromator bandwidth effects**

If the psi and delta data for a given sample show very sharp spectral features, a partially polarized beam may be obtained at the detector due to the non-zero bandwidth of the light beam leaving the monochromator. This bandwidth is usually very small (2 nm or so), such that the change in psi and delta over the band is
not significant. For very thick transparent films which exhibit very sharp handedness changes, or other structures which exhibit very sharp spectral features, psi and delta may change significantly over the spectral band of the incident beam.

We treat this case by dividing the beam into monochromatic components with wavelengths spanning the range specified by the monochromator bandwidth parameter, calculating the reflected polarization state of each component, and summing the reflected beams at the detector. The monochromator bandwidth parameter is specified in the current light units, and may be varied.

Note that the bandwidth of the VASE® system is usually 2-3 nm, while the M-44® ellipsometer has a fixed bandwidth of 12 nm, which should always be included in the model (but not fit) when analyzing M-44® data.

**Angular spread of the beam entering the detector**

If the sample surface is slightly curved or the VASE® light beam is very poorly collimated, beam which enters the detector will consist of component beams which were incident on the sample over a range of angles of incidence. In this case, WVASE® allows the user to specify the angular range and fit for it as well. This non-ideality is very rarely encountered, and is most commonly helpful when analyzing data from very thin Mylar or polyester sheet samples, which are very difficult to mount in a manner which yields a flat surface.

**Use of multiple optical data types**

There are many cases where the desired analysis of a sample cannot be performed uniquely with VASE® data alone. In some cases it is possible to reduce parameter correlations in complicated models by adding other types of optical experimental data from the sample to the fitting procedure. This is primarily the case for samples on transparent substrates, as this allows the acquisition of many additional data types (transmission, ellipsometric transmission, reverse direction ellipsometry). For samples on opaque substrates, we can only augment the VASE® data with reflectance data.

For samples on opaque substrates, acquire VASE® data first and try the analysis. If correlation of parameters in the model is problematic, try acquiring p- or s-polarized reflectance (but not both) from the sample at the same angles of incidence as the VASE® data were originally acquired. Fit both data sets simultaneously, and check to see if the addition of the reflectance data reduces the parameter correlations in the model.

For samples on transparent substrates, acquire normal incidence transmission and VASE® data initially (the transmission may be omitted for very simple systems) and try the analysis. If parameter correlations are problematic, try adding transmission ellipsometry data to the fit. If correlation is still a problem, try adding reverse direction ellipsometric data. The reverse direction ellipsometry data is particularly helpful if the bottom film (next to the substrate) is metallic, as the ellipsometric data through the substrate will help to pin down the optical constants of the metal film.

As a final note, when acquiring multiple data types from the same sample, try to acquire all data sets from the same physical location on the sample. If one or more films on the sample are non-uniform, acquiring data from different locations may lead to data sets which simply cannot be simultaneously fit. The acquisition of all data from the same spot may be difficult if you plan to roughen the back side of the sample prior to VASE® data acquisition. If this is the case, acquire all of the other data types first, then roughen the back-surface and acquire the VASE® data.
Fit parameter coupling and limiting

*WVASE®* will allow the user to couple fit parameters together and/or specify upper and lower bounds on any fit parameter by using the ‘Edit Parms’ option from the Fit window. The bounding of parameters should be used with extreme caution, as more often than not any parameter which fits to its upper or lower bounding value is very strongly correlated to some other model parameter. It is usually best not to bound the fit parameters unless you have a very good reason for doing so.

Parameter coupling is most useful for multiple sample analyses, but has several applications for the analysis of single samples as well. In samples where a given layer is repeated more than once, we may wish to couple the thicknesses of each of the similar films together, such that they effectively become one fit parameter. To couple parameters together, select the ‘Edit Parms’ option from the Fit window. This causes a dialog box to appear containing a list of all of the currently defined variable parameters. To couple parameters together, select the parameter to be coupled, click on the ‘Coupled Parameter’ button to the right of the parameter list, specify the number of the fit parameter you wish to couple the selected parameter to, specify a coupling constant, and press <enter>. The text ‘Coupled to parameter ###’ will appear next to the parameter you selected, and it will be held equal to the parameter it is coupled to times the coupling constant during any fit. For example, the following dialog box shows several thicknesses in the model coupled together.

![Edit Fit Parameters Dialog Box](image)

Figure 13.66. 'Edit Parms' dialog box from the Fit window, displaying several thicknesses coupled together as single fit parameters. The thicknesses of layers 4, 5, and 6 are coupled to the thickness of layer 2, and the thicknesses of layers 3 and 4 are coupled to the thickness of layer 1.

Note that any fit parameter may be coupled to any other fit parameter, although unpredictable results may be obtained if dissimilar parameters are coupled, such as, for example, a thickness being coupled to an optical constant or Cauchy parameter.

**Multiple sample analysis**

A very potent means of eliminating strong parameter correlations from complex models is the technique of multiple sample analysis. Any time two or more samples are known to have some physical property in common, the analysis of both (or all) samples may be performed simultaneously, with the common physical property coupled across the models for the different samples. For example, if we have two samples consisting of thin aluminum films on silicon wafers, in which the
aluminum films are nominally identical but of differing thickness, we can fit the VASE® data from both samples simultaneously, varying the aluminum film thickness on each sample and a single set of aluminum optical constants, forced to be identical for both films.

WVASE® will allow the user to load up to ten sets of experimental data and specify up to ten models. The experimental data may consist of any combination of the optical data types supported by WVASE®. The various models and experimental data sets may be accessed either through the ‘Select’ option from the menubar of the Model window, or by using the hotkey sequence <alt>-#, where # represents the number keys 0-9, with 0 selecting model #10. When a given data set and model are selected, the title bars on the model, experimental data, and Generated Data windows will show the number of the current sample set.

For example, to set up a three sample multiple sample analysis, we would first load the experimental data for the first sample into the Experimental Data window, then create an appropriate model for the first sample in the Model window (the first model should be selected). Then, select the second model either by using the ‘Select’ option from the Model window or by pressing <alt>-2. Load the experimental data for the second sample into the Experimental Data window (which should show ‘Experimental Data #2’ on the title bar), and create an appropriate model in the Model window. Press <alt>-3 to select the third model, load the experimental data for the third sample into the Experimental Data window, and then specify the model for the third sample in the Model window.

The reason why we wish to fit more than one sample at a time is that we can force parameters in the optical model for the various samples to be identical for more than one sample, thereby hopefully eliminating correlations which prevent the unique determination of the desired model for a single sample alone. For example, we cannot usually uniquely obtain the thickness and optical constants of thin metal films on opaque substrates, but we can usually obtain a unique solution for the two thicknesses and one set of optical constants of two thin films of the same metal on opaque substrates. In order to take advantage of this feature we need a means by which we can couple parameters in the optical model for one sample to parameters in the optical models for other samples.

WVASE® provides two means for parameter coupling within the multiple sample analysis. First, any time a layer is added to models 2-10, WVASE® checks to see if that layer is present in the first model. If it is, WVASE® offers the option of coupling the layer being added to the identical layer in the first model. If this option is chosen, the optical constants of the layer which is added are always held identical to those of the same layer in the first model, even when these optical constants are fit, either directly or parametrically (via a Cauchy, Lorentz, or other dispersion relation). Note that WVASE® only checks the first model, such that any layer you wish to couple other layers to must appear in the first model, although it may have zero thickness if not actually present in the first sample.

A second means of coupling parameters between models is to use the ‘Edit Parms’ option from the fit menu as described in the previous section. When multiple samples are being analyzed, the sample number will appear after the parameter name in the displayed list, separated by a hyphen. The following ‘Edit Parms’ dialog box shows a possible parameter list in which two Cauchy parameters for film #1 on the second sample are coupled to two Cauchy parameters for film #1 on the first sample.
When fitting multiple sample data sets, you must tell WVASE® which models are being fit by using the ‘Select’ option from the Model window. The following dialog box will appear.

The applications of multiple sample analysis are too numerous to list. Several examples ranging from very simple to very complex are given in the next chapter - “VASE® Data Analysis Examples”.

13.12 The parametric semiconductor model

A recurring theme throughout this chapter has been the usefulness of parametric dispersion models for the optical constants of materials to reduce parameter correlations and enforce continuity and/or Kramers-Kronig consistency on the optical constants of the material under study. In this section we discuss the most powerful and sophisticated parametric dispersion model available within WVASE®,
The primary purpose of the PSEMI model is to reproduce complicated dielectric functions. The PSEMI parameter values that define the model have no direct physical interpretation.

The primary purpose of this parametric model is to accurately reproduce the optical constants of materials, especially semiconductors with complicated critical point structure in the optical constant spectra, using a reasonably well-parameterized function. The parametric semiconductor model is very successful in this respect, and has the added bonus of being Kramers-Kronig consistent.

The PSEMI model’s primary contribution to the understanding of the physical properties a material is in the optical constants it generates, not the internal parameters that define the model. The PSEMI parameter values have no direct physical relationship to critical point parameters, such as energy and broadening, that one might obtain from a derivative or other type of analysis.

Because it is a highly flexible curve, the PSEMI is usually not a unique model. Therefore the final parameter values depend upon how the various oscillators are initially configured, which means that more than one PSEMI model will produce essentially the same dielectric function and equally good fits to the data, even though they have different parameters. For the same reason, one should be cautious when comparing PSEMI parameters from one model to another. It should only be attempted when the PSEMI models are similarly constructed, and should only used to model optical constants with similarly organized features (as one might find in an alloy system like AlGaAs).

The optical function generated by the PSEMI model can be subjected to a derivative analysis. WVASE® does not currently perform derivative analyses, although graphs of derivatives can be displayed (see “Plot derivatives,” section 10.6 on page 10-20). The derivative values from that plot can be output as text files (see “Copy Data to Clipboard” and “Output Data points to text file” in section 10.2, pages 10-5 and 10-7).

The primary drawback of this model is its complexity; effective use usually requires some study and practice. Also, its parameters can be strongly correlated to other parameters within the same model. These difficulties can be overcome, and for certain situations this model is worth the time and effort.

Mathematical description

The parametric semiconductor model begins with the treatment used to derive the Kim and Garland’ parametric dispersion model and most other oscillator type dispersion models. The complex dielectric function is defined as
\[ \tilde{\varepsilon}(E) = 1 + i \int_0^\infty W(E')\tilde{\Phi}(E, E')dE' \] (13.6)

The dielectric function is defined as a function of the photon energy E. The variable E’ is a dummy integration variable. The joint density of states is included in W(E), the unbrodened absorption spectrum. The broadening function \( \tilde{\Phi} \) is typically either Lorentzian or Gaussian.

\[ \tilde{\Phi}(E, E') = \int_0^\infty e^{i(E-E'+iy(s))} d\gamma - \int_0^\infty e^{i(E+E'+iy(s))} d\gamma \] (13.7)

\[ \gamma(s) = \Gamma \text{ for Lorentzian broadening} \]
\[ \gamma(s) = 2\sigma^2 s \text{ for Gaussian broadening} \]

Kim and Garland observed that something like Gaussian broadening is required to produce the proper value of \( \varepsilon_2 = 0 \) below the direct bandgap of a material like GaAs. Thus, for this model we have chosen pure Gaussian broadening. Note that \( \tilde{\Phi} \) is a complex valued function and for Gaussian broadening it involves \( \text{erf} \) (the ‘Error’ function) of imaginary arguments. The Kramers-Kronig consistency for the model is built into this broadening function \( \tilde{\Phi} \).

Equation 12.8 is derived from equation 12.6 to represent the finite extent for which data is available by restricting the integration range and adding zero-width oscillators which can describe higher energy or restrahlung band absorption. (For the zero-width poles, the form of broadening is unimportant.) Also the \( W(E) \) function (which includes the joint density of states) is broken into pieces which have an associated constant broadening parameter. The Kim/Garland approach has the broadening parameter linearly change between CP’s. In this aspect, our model is more similar to the oscillator ensemble where each component has a single broadening parameter.

\[ \tilde{\varepsilon}(E) = 1 + i \sum_{j=1}^m \int_{E_{mn}}^{E_{mn+1}} W_j(E')\Phi(E, E', \sigma_j) dE' + \sum_{j=m+1}^{m+p+1} A_j \left( \frac{1}{E - E_j} \right) \] (13.8)

Only certain functional forms for \( W_j(E) \) are allowed if we wish to be able to evaluate the broadening integral analytically. For Gaussian broadening, delta functions

\[ W_j(E) = \delta(E - E_j), \] (13.9)

and bounded polynomials

\[ W_j(E) = \sum_{k=0}^N p_{j,k} E^k u(E - a_j) u(b_j - E). \] (13.10)

are possible because look-up tables can be constructed to evaluate the integrals. Attempting to make \( \sigma \) a function of energy as Kim and Garland have done would require two-dimensional look-up tables. The broadening parameter is primarily a local property at the CP energy and between CP’s there is little sensitivity to the broadening.

The parametric semiconductor model does not just use polynomial coefficients, \( p_{j,k} \) as the fit parameters. Rather, each component of our model is more like an oscillator, but the underlying delta function has been generalized to become a polynomial background, centered at an energy, \( E_c \), with amplitude, A, and
broadening parameter B. The polynomial background is a collection of 4 polynomials which span a bounded spectral region. The structure of the background before broadening is defined by 7 structure parameters and 2 bounding energies. Figure 12.70 shows a generalized component before broadening with the defining parameters. We have adopted the term CP structure for these components since in our modeling scheme, one component is typically assigned to fit the spectral feature associated with one CP. The relationship between the center energies of the CP structure and CP energies determined by the more standard critical-point parabolic-band lineshape (CPPB) fitting procedure will be described later.

The 13 defining parameters for a CP structure are as follows: center energy \( E_C \), upper bounds energy \( E_U \), lower bounds energy \( E_L \), center amplitude \( A \), broadening \( B \), amplitude discontinuity \( \text{Disc} \), upper and lower mid-positions \( U_{\text{mid}}, L_{\text{mid}} \), upper and lower mid-amplitudes \( U_{\text{amp}}, L_{\text{amp}} \), and upper and lower second order polynomial factors \( U_{2\text{nd}}, L_{2\text{nd}} \). From these parameters, polynomials in energy, \( F_I, F_{II}, F_{III}, F_{IV} \), are defined using constraints that connect \( F_I \) and \( F_{II} \) (\( F_{III} \) and \( F_{IV} \)) smoothly and force \( F_I \) and \( F_{III} \) to 0 at the boundaries. The discontinuity in amplitude at the center is based in part on the fact that the joint density of states can be discontinuous at CP’s. However, in our model, Disc is more just a shape fitting parameter than a physically meaningful quantity.

![Diagram of CP structure parameters](image)

Figure 13.69. A generic, unbroadened CP structure composed of 4 component polynomials, \( F_I, F_{II}, F_{III}, F_{IV} \). Defining parameters and values derived from them are shown.

While the lower, center, and upper energies and the amplitude and discontinuity have obvious physical significance, the remaining 6 structure parameters have no obvious physical significance and are similar to the polynomial coefficients in the Kim/Garland model. However, these 6 parameters are defined as normalized values which have sensible physical limits. If \(-1<U_{2\text{nd}}(L_{2\text{nd}})<1\) then \( F_I, F_{II}(F_{III}, F_{IV}) > 0 \) over the defined spectral region, and in this way the resulting dielectric values can not be the result of the difference between large internal values. The more physically relevant parameters, \( E_C, A, B \), are certainly not the same as the CPPB model would define them, but they are related. More importantly, comparisons of corresponding parameters can be made between models for different materials. Our model also assumes the bounding energies \( E_U, E_L \) are themselves the center energies for other CP structures. This connection of CP structures to one another is an important aspect for making the model “stretchable,” in that a CP energy can be moved relative to the others and the model still produces a plausible dielectric function.

**Parametric semiconductor model for GaAs**

The literature optical constant spectra for crystalline GaAs were fit using the parametric semiconductor model, with the result as shown below. Note that the parametric semiconductor accurately reproduces the tabulated spectra from the
literature, including the subtle features near the direct energy gap, as well as the first, second, and third energy derivatives of the tabulated spectra.

Figure 13.70. GaAs dielectric function. The legend gaas_tab denotes the tabulated spectra from the literature, while gaas_prm denotes the spectra calculated from the best-fit parametric semiconductor model for GaAs.

Figure 13.71. GaAs dielectric function near the direct energy band gap. The legend gaas_tab denotes the tabulated spectra from the literature, while gaas_prm denotes the spectra calculated from the best-fit parametric semiconductor model for GaAs.

Figure 13.72. Second derivative of the imaginary part of the dielectric function with respect to photon energy, for crystalline GaAs. The dashed curve is the second derivative of the tabulated data from the literature, while the solid curve is the second derivative of the best-fit spectrum from the parametric semiconductor model for GaAs.
The entire list of parameters used to model the GaAs dielectric function is given in Table I. Each line represents the definition of a single CP structure (like Fig. 70) in the order presented within the WVASE® software. The “set” column indicates that this row is active. (In a WVASE® parametric model layer, up to 20 CP structures are allowed, but in this model only 7 are used. Also, this text has used the convention “U” for upper while the WVASE® layer presently uses “R” for right in naming some of the parameters.) The conL and conU contain the CP structure numbers whose center energies are the lower and upper bounding energies respectively. For example, CP#2 is positioned at 2.896 eV and spans the spectral region from 1.414 eV (E#0) to 4.64 eV (E#4). The connection scheme used in Table I has been used with minor modifications for 8 III-V binary materials and the HgCdTe II-VI system. The first 2 CP lines correspond to the E₀ and E₀+Δ₀ CP’s. (The data did not provide sufficient sensitivity to these broadenings to fit them.) Also note that these CP’s are one sided; they are connected to themselves on the low energy side. If E_L ≥ E_C or E_C ≥ E_U, the respective side does not contribute to the dielectric function. Lines #2 and 3 describe the contribution associated with E₁ and E₁+Δ₁. Lines #4 and 5 describe the E₂ CP region. For GaAs, there are actually 3 discernible CP’s when performing a CPPB derivative analysis. However, for this work, the derivatives are unavailable for the fitting process and there is very little structure in the measured ψ and Δ values to fit extra model CP structures.

Furthermore, to maintain consistency with the other III-V material models for latter alloy model development, similar CP groupings and connections are required for the binary endpoints. Line #6 holds a “dummy” CP which is outside the range of available ellipsometric data. This contribution to the model absorption is necessary to allow a physical model for ε₁ to exist out to 6 eV. If the absorption model was abruptly cutoff at 6 eV, the K-K relationship would produce a very sharp, unphysical feature. The CP structure for this line is very simple because there is almost no data with which to fit the parameters. The absorption above 6.5 eV is lumped into a single zero-width oscillator with parameters given on the first row of Table I.

The shaded parameters in Table I were determined from a preliminary multi-material analysis for GaAs, AlAs, InAs, InP, and GaP. Once these “global” III-V values were determined, the remaining model parameters for the individual materials were fit to their final values. (These “global” values have also proven useful in describing the HgCdTe II-VI system.) For a given material, there would considerable correlation between the various structural parameters, but much of that correlation is removed by establishing the global III-V parameters. Forcing this group of 20 parameters to be the same for multiple materials greatly constrains the possible configuration and concentrates the structural information for a particular material in the remaining

Table I: Parametric model for GaAs.

<table>
<thead>
<tr>
<th>gaas.mat</th>
<th>Pole Pos</th>
<th>Pole Amp</th>
<th>set</th>
<th>con L</th>
<th>con U</th>
<th>E(eV)</th>
<th>A</th>
<th>B(meV)</th>
<th>Disc</th>
<th>Lpos</th>
<th>Lamp</th>
<th>L2nd</th>
<th>Upos</th>
<th>Uamp</th>
<th>U2nd</th>
</tr>
</thead>
<tbody>
<tr>
<td>#0</td>
<td>1</td>
<td>0</td>
<td>2</td>
<td>1.414</td>
<td>0.43</td>
<td>1.7659</td>
<td>0.0936</td>
<td>40</td>
<td></td>
<td>0.4</td>
<td>0.75</td>
<td>0.</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>#1</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>2.896</td>
<td>11.989</td>
<td>33.0977</td>
<td>0.2</td>
<td>0.75</td>
<td>0.1968</td>
<td>1.</td>
<td>0.8</td>
<td>0.4</td>
<td>0.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>#2</td>
<td>1</td>
<td>0</td>
<td>4</td>
<td>3.1701</td>
<td>13.1907</td>
<td>45.2828</td>
<td>-0.1</td>
<td>0.3</td>
<td>0.03</td>
<td>0.</td>
<td>0.1</td>
<td>0.0455</td>
<td>0.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>#3</td>
<td>1</td>
<td>0</td>
<td>4</td>
<td>4.6405</td>
<td>22.3793</td>
<td>154.1036</td>
<td>-0.35</td>
<td>0.4</td>
<td>0.1365</td>
<td>0.</td>
<td>0.9</td>
<td>0.4</td>
<td>0.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>#4</td>
<td>1</td>
<td>3</td>
<td>6</td>
<td>4.8915</td>
<td>42.2217</td>
<td>164.7492</td>
<td>-0.7251</td>
<td>0.8</td>
<td>0.06</td>
<td>0.</td>
<td>0.1</td>
<td>0.0243</td>
<td>0.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>#5</td>
<td>1</td>
<td>3</td>
<td>6</td>
<td>6.5</td>
<td>5.8</td>
<td>200.</td>
<td>0.5</td>
<td>0.5</td>
<td>0.</td>
<td></td>
<td></td>
<td></td>
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<td></td>
<td></td>
</tr>
</tbody>
</table>

The shaded parameters in Table I were determined from a preliminary multi-material analysis for GaAs, AlAs, InAs, InP, and GaP. Once these “global” III-V values were determined, the remaining model parameters for the individual materials were fit to their final values. (These “global” values have also proven useful in describing the HgCdTe II-VI system.) For a given material, there would considerable correlation between the various structural parameters, but much of that correlation is removed by establishing the global III-V parameters. Forcing this group of 20 parameters to be the same for multiple materials greatly constrains the possible configuration and concentrates the structural information for a particular material in the remaining...
structure parameters. This reduction in correlation is essential in establishing parametric models that can be interpolated parameter-by-parameter to form dielectric function groups. The 5 adjustable structure parameters control the shape of the dielectric function when spanning the larger ranges between CP groupings. The L_{amp}#2 establishes the shape of the long tail from E_1 down to E_0. The R_{amp}#3 and L_{amp}#4 control the shape in the region between E_1+Δ and E_2(1). The R_{amp}#5 and Disc#5 control the long tail out to 6 eV where the available ellipsometric data ends.

Figures 12.74 and 12.75, respectively, show the ε_2 spectra associated line #0 (E_0) and line #2 (E_1) before and after broadening. Figure 12.76 shows how the component CP structures combine to generate the GaAs ε_2 spectra.

Figure 13.73. Contributions to the GaAs ε_2 spectrum due to CP#0 (a, E_0).

Figure 13.74. Contributions to the GaAs ε_2 spectrum due to CP#2 (b, E_1).
A CPPB analysis was performed on the derivative of $e_2$ from the GaAs parametric dielectric model. The corresponding energies and broadenings are given in Table II. To obtain accurate CPPB parameters, a tabulated dielectric ellipsometric analysis is preferred because it provides the most accurate information for calculating dielectric function derivatives. The parametric model can, as just demonstrated, be used to determine appropriate layer thicknesses and then allow a wavelength-by-wavelength dielectric function extraction with the thicknesses fixed. The results in Table II indicate that there is some relationship between the parametric model parameters and the CPPB parameters, but those model values can of course only be assigned importance to the GaAs if the parametric model fits the derivative spectra as well.

### Table II: Comparison of Parametric Energies and Broadening Values with a CPPB Analysis

<table>
<thead>
<tr>
<th>CP</th>
<th>model E(eV)</th>
<th>model B(meV)</th>
<th>CPPB E(eV)</th>
<th>CPPB B(eV)</th>
<th>CPPB dimension</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_0$</td>
<td>1.414</td>
<td>20 (not fit)</td>
<td>1.410</td>
<td>6.3</td>
<td>3-d</td>
</tr>
<tr>
<td>$E_0$+$\Delta_0$</td>
<td>1.766</td>
<td>40 (not fit)</td>
<td>1.775</td>
<td>32.7</td>
<td>3-d</td>
</tr>
<tr>
<td>$E_1$</td>
<td>2.896</td>
<td>33.1</td>
<td>2.908</td>
<td>42.4</td>
<td>2-d</td>
</tr>
<tr>
<td>$E_1$+$\Delta_1$</td>
<td>3.170</td>
<td>45.3</td>
<td>3.137</td>
<td>65.2</td>
<td>2-d</td>
</tr>
<tr>
<td>$E_2(1)$</td>
<td>4.641</td>
<td>154.1</td>
<td>4.531</td>
<td>114.1</td>
<td>2-d</td>
</tr>
<tr>
<td>$E_2(2)$</td>
<td>4.892</td>
<td>164.7</td>
<td>4.909</td>
<td>164.8</td>
<td>2-d</td>
</tr>
</tbody>
</table>

### Parametric semiconductor model fits to other materials

To demonstrate the exceptional flexibility of the parametric semiconductor model, fits were performed to optical constant spectra determined directly (without the use of a parametric optical constant model) from films of the given semiconductor. These fits are shown below. Note that fits from the Forouhi and Bloomer oscillator model are shown for InP for comparison. Note that the...
parametric semiconductor model reproduces all of these optical constants very accurately.

![Image](https://example.com/image1.png)

**Figure 13.76.** Parametric semiconductor model fit to tabulated spectra for AlAs from the literature. The dashed lines denote the literature spectra, while the solid lines are the parametric semiconductor model fit.

![Image](https://example.com/image2.png)

**Figure 13.77.** Parametric semiconductor model fit to tabulated spectra for InP from the literature. The literature spectra (inp_tab) and the best-fit parametric semiconductor model spectra (inp_prm) are nearly indistinguishable. The best-fit obtainable with the Forouhi and Bloomer oscillator model is also shown (inpfb).

![Image](https://example.com/image3.png)

**Figure 13.78.** Parametric semiconductor model fit to tabulated spectra for InAs from the literature. The dashed lines denote the literature spectra, while the solid lines are the parametric semiconductor model fit.

We see from the above figures that the parametric semiconductor model accurately reproduces a wide variety of semiconductor optical constant spectra. In the following sections we discuss how to use the parametric semiconductor layer within the **WVASE®** software for ellipsometric data analysis.

**Using the parametric semiconductor layer within **WVASE®**

A default parametric layer can be obtained by adding *p_semi.mat* as a new layer. The resulting parametric layer, which is shown in Figure 12.80, can be manipulated just like other layers; the amount of information presented is just much greater. The most immediate difference is the manner in which model parameters
are edited. Instead of typing directly into the display, a row (or group of rows) is first highlighted in the parameter list box (in Figure 12.80, the row corresponding to CP structure #2 has been highlighted). When highlighted, the parameter values for the selected row can be edited in the row of boxes at the top of the list. This row is also where the fit status of each parameter is established. After changes have been made to the selected parameter values (and fit status), it is very important to click on the ‘Change’ button to update the parameters in the list. The pole position and amplitude boxes are on the left and above the main parameter listing. In practice it is much easier to modify an existing parametric file than start from scratch. The meaning of the parameters has already been described. There are, however, certain hints for using the parametric layer to fit real data.

![Parametric semiconductor layer dialog box.](image)

Here are some tips for getting the most effective use from the parametric semiconductor model.

1) If you are working with III-V or II-VI semiconductors, do not try to fit the shaded parameters in Table I without a very compelling reason. (The Lamp#3 parameter is sometimes needed to fit materials with large $\Delta_1$ values, like InAs and the antimonides.)

2) There are reasonably good starting values already available for GaP, InP, AlAs, GaAs, InAs, AlSb, GaSb, InSb, In(.53)GaAs/InP, Al(.48)InAs/InP, HgTe, CdTe, so do not spend a lot of time creating them from scratch.

3) When starting work on a new material, try starting with a similar binary material that already exists. Then “eyeball” the energies near their new values. Next, fit only the amplitudes (including pole amplitude) to get closer. Then start fitting whatever parameters you want. There is no absolute technique that works, but as a general rule try fitting with as few of the structure parameters as possible.

4) Si and Ge are distinct in structure from the III-V materials and have a separate CP structure connection strategy.

5) Figure 12.81 shows the GaAs dielectric function and points out where some of the structure parameters have their greatest influence.

6) Sometimes it is helpful to change the ‘Fit Defaults’ option (in WVASE®) for Fit Weighting to ‘<c2> only’ when initially fitting the parameterized model to existing optical constants (be sure to turn off the ‘pole’ fitting parameters). Switch back to standard or psi&delta fit weighting after you have adequately fit the model to...
the $\angle e_2$ spectra. At this point, you can also fit for the ‘pole’ parameters, to adjust for any offset observed in the $\angle e_1$ spectra.

The dielectric function of indirect gap semiconductors, such as Si and Ge, can also be modeled with the parameterized model. Figures 12.82 - 12.84 show the data fits to Ge, Si, and an intermediate composition of Si$_x$Ge$_{1-x}$. A CP connection scheme was chosen that is simultaneously compatible with both the Si and Ge endpoints, and its compositional alloys. The parameters for the Si dielectric function are shown in Table III. A simplified parameterized model for Si can be found, if compatibility with the Ge dielectric function is not required (the Ge dielectric function spectra exhibits some CP structures which are degenerate or not observed in the Si dielectric function).

The dielectric function of indirect gap semiconductors, such as Si and Ge, can also be modeled with the parameterized model. Figures 12.82 - 12.84 show the data fits to Ge, Si, and an intermediate composition of Si$_x$Ge$_{1-x}$. A CP connection scheme was chosen that is simultaneously compatible with both the Si and Ge endpoints, and its compositional alloys. The parameters for the Si dielectric function are shown in Table III. A simplified parameterized model for Si can be found, if compatibility with the Ge dielectric function is not required (the Ge dielectric function spectra exhibits some CP structures which are degenerate or not observed in the Si dielectric function).
Figure 13.82. Experimental data fit for SiGe alloy, using the parametric semiconductor model.

Figure 13.83. Experimental data fit for crystalline silicon, using the parametric semiconductor model.

Table III: Parameters for the Si dielectric function

<table>
<thead>
<tr>
<th>set</th>
<th>con L</th>
<th>conR</th>
<th>Amp</th>
<th>Br</th>
<th>En</th>
<th>Disc</th>
<th>Lpos</th>
<th>Lamp</th>
<th>L2nd</th>
<th>Rpos</th>
<th>Ramp</th>
<th>R2nd</th>
</tr>
</thead>
<tbody>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>#1</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>c0.554</td>
<td>50</td>
<td>a3.2636</td>
<td>1.12</td>
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<td>c256.584</td>
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<td></td>
<td>0.1497</td>
<td>0.2843</td>
<td>0</td>
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<td>0.6157</td>
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<tr>
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<td>1</td>
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<td>5.0291</td>
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<td>#7</td>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*a*Set equal to En#4  
*b*Set equal to En#3  
*c*Taken from multi-sample with a_gen1,sin1,sg_487n1  
Italics established before fits  
Shaded established in k1 multi-sample with Ge  
Bold fit to Si only
The parametric Si model was also used as a starting point for fitting the dielectric functions of heavily doped Si samples. By allowing only a few (10) parameters to vary (selected CP broadenings and energies, and a few ‘shape’ parameters), the dielectric functions of the heavily doped Si samples were accurately described by the parametric model (Figures 12.85 - 12.86). By interpolating between the dielectric function model parameters, it should be possible to generate physically reasonable dielectric functions for arbitrary doping concentrations, in this heavily doped regime.

![Doped Si Parametric Model](image1)

Figure 13.84. $\varepsilon_1$ spectra for doped silicon, determined with the parametric semiconductor model.

![Doped Si Parametric Models](image2)

Figure 13.85. $\varepsilon_2$ spectra for doped silicon determined using the parametric semiconductor model.

While we have pointed out several uses of the parametric semiconductor model in this section, we have hardly scratched the surface of the useful applications of this model. Many examples of the analysis of thin films and multilayers and multiple sample analyses using the parametric semiconductor layer are given in the next chapter - “VASZ® Data Analysis Examples”.

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Chapter 14 Ex Situ Data Analysis Examples

14.1 Overview

In this chapter we present examples of the analysis of static optical data with WVASE™. The experimental data used for these examples was obtained from measurements on actual samples at the J. A. Woollam Co., Inc. It is not possible to give examples of every type of data analysis which may occur, but the examples presented here should be sufficiently general as to provide suggestions for the analysis of nearly all types of samples. Examples are first presented for the analysis of bare substrates and other bulk samples. Examples are then given for a variety of single film systems, double film systems and multilayers. Finally, an example of the powerful multiple sample analysis technique are presented.

It is important to understand that the techniques presented here are by no means the final answer for the analysis of data from the various types of samples. Our knowledge of analysis techniques comes from years of extensive experimentation with the data analysis, and we cannot recommend strongly enough that you experiment freely with the analysis capabilities available within WVASE™. Many of the most useful analysis ‘tricks’ in our repertoire were suggested by our customers from their experiences with the data analysis.

The following example data analyses are presented in this chapter. Note that the number of dots next to each example represents the difficulty of the example, with one dot (●) representing the easiest examples and five dots (●●●●●) denoting the most difficult examples. Note that multilayers are indicated by listing the layers from top to bottom, separated by slashes (/), with the substrate always given last. For example, the designation ‘poly-Si / SiO₂ / silicon’ denotes a sample consisting of a poly-silicon film on a silicon dioxide film on a silicon substrate.

1. Bare silicon wafer. (●)
2. Optically thick chromium film. (●)
3. Bulk HgCdTe with surface roughness. (●●)
4. Bare glass cover slip. (●●●)
5. Organic film on silicon. (●●)
6. Anisotropic organic film on silicon. (●●●)
7. Silver film on fused silica. (●●)
8. Indium tin oxide (ITO) film on glass. (●●●●)
9. Diamond-like carbon (DLC) film on glass. (●●)
10. GaAs / AlGaAs / GaAs. (●)
11. Polycrystalline silicon (poly-Si) / silicon dioxide / silicon. (●●●●)
12. TiN / silicon dioxide / silicon. (●●)
13. Five layer hi-lo stack on silicon. (●●●●)
14. SiO\textsubscript{2} / Si\textsubscript{3}N\textsubscript{4} / SiO\textsubscript{2} / poly-Si / SiO\textsubscript{2} / silicon. (●●●●)
15. Multiple sample analysis of thermal oxides on silicon. (●●●●●)

The following list is a breakdown of the major analysis topics covered in these examples:

Data types which are analyzed:
- Standard ellipsometric - All examples.
- Transmittance - Examples 4, 7, and 9.
- Reflectance - Examples 9 and 11.
- Analysis of multiple data types - Examples 4, 7, and 9.

Analysis procedures and techniques:
- Obtaining substrate optical constants - Examples 1, 2, 3, 6, and 15.
- Obtaining index and thickness of films which are transparent over the full measured spectral range - Examples 13 and 15.
- Obtaining optical constants and thickness of films which are transparent over some of the measured spectral range - Examples 5, 6, 8, 11, and 14.
- Obtaining optical constants and thickness of films which are optically absorbing over the entire measured spectral range (metals and low bandgap semiconductors) - Examples 7, 9, 10, and 12.
- Point-by-point fit - Examples 2, 5, and 6.
- Layer coupling - Examples 8, 13, and 15.
- Fit parameter coupling - Examples 8 and 15.
- Multiple sample analysis - Example 15.
- Cauchy fit for film thickness and index - Examples 5, 6, 13, and 15.

Parametric optical constant dispersion model layers:
- EMA layer -Examples 3, 7, 8, 9, and 14.
- Alloy layer - Examples 3 and 10.
- Cauchy layer - Examples 4, 5, 6, and 13.
- Anisotropic Cauchy model - Example 6.
- Lorentz oscillator model - Example 8.
- User-defined dispersion model - Examples 8, 13, and 15.
- Parametric semiconductor model - Examples 11 and 14.
Sample, instrument, and model non-idealities:

- Surface oxidation - Examples 1, 2, and 11.
- Surface roughness - Examples 3, 7, 8, and 9.
- Index grading - Example 8.
- Monochromator bandwidth correction - Example 6.

At the end of each example we have provided a list of additional educational experiments which may be performed on the data used in the example. We do not provide complete procedures for these experiments, but hope to encourage the user to learn the operation of WVASE™ and gain a fuller understanding of the analysis of optical data by trying as many analysis options as possible. These additional suggested experiments range from very simple to very complex, and the new user should move on to the other examples if a particular suggested experiment is problematic. In all cases the ‘best’ modeling procedure for the sample is given explicitly in the example, and the suggested further experiments are intended more to stimulate learning than to provide better results.

We recommend two approaches to using the examples in this chapter. The first approach is recommended for the novice user (but is very educational for the expert as well), and consists of working through all of the examples in order of difficulty (starting with the easiest). The second approach is to use this chapter as a reference by trying to find an example which is similar to the sample you are trying to characterize.

### 14.2 Important WVASE™ procedures

*Learn these procedures well!*

In this section we review a number of important procedures which are used during data analysis with WVASE™. You should be familiar with all of these procedures before attempting the examples given below, as they are used throughout the analysis examples which follow. Try each procedure before proceeding onward, and consult chapter 13 - ‘Analysis of Static Optical Data’ for further details on analysis procedures.

#### Activate a WVASE™ window

There are two ways to activate one of the WVASE™ windows. To activate a window using keystrokes, use the following procedure.

- Select ‘Window’ from the menubar.
- Select the desired window from the list which appears.

To activate a window with the mouse:

- Click anywhere on the desired window.

For more information about the WVASE™ windows and how they are used, consult chapter 3 - ‘Navigating WVASE™’.

#### Loading an experimental data file

- Activate the Experimental Data window.
- Select ‘File’ from the menubar.
- Select ‘Open’ from the menu which appears.
- Select the directory containing the file you wish to load.
- Select the file you wish to load from the displayed list of files.
- Select ‘Ok’.

For more information about experimental data files and the Experimental Data window, consult chapter 6 - ‘The Experimental Data Window’.

**Saving an experimental data file**

- Activate the Experimental Data window.
- If you have previously used ‘Range Select’ from the Experimental Data window menubar to restrict the data range for fitting and plotting, only experimental data within the selected range will be saved. Use ‘Range Select’ to set the spectral and angle of incidence ranges for which the experimental data will be saved.
- Select ‘File’ from the menubar.
- Select ‘Save’ from the menu which is displayed.
- Select the directory in which you wish to save the experimental data.
- Type the name of the file you wish to save in the box provided in the upper left area of the File Save dialog box. You do not need to specify a file extension, as the extension ‘.dat’ will automatically be added to the name you specify.
- Select ‘Ok’, and the file will be saved in the selected directory.

For more information about experimental data files and the Experimental Data window, consult chapter 6 - ‘The Experimental Data Window’.

**Adding a substrate to the model**

- Activate the Model window.
- If layers are already present in the model, use the up and down arrow keys to position the current layer arrow in the Model window (‘>’, on left side of model) just below the lowest film.
- Select ‘AddLayer’ from the menubar.
- The Add Layer dialog box will be displayed.
- Select the layer you wish to add. You may need to select the directory in which this layer is stored as well.
- Select ‘Ok’ when you have chosen the desired layer filename.
- The layer will be added to the model as the substrate, with a default thickness of 1 mm.

For more information about models and the Model window, consult chapter 7 - ‘The Model Window’.
Adding a layer to the model

- Activate the Model window.
- Use the up and down arrow keys to position the current layer arrow in the Model window ('>', on left side of model) next to the layer (or substrate) above which you wish to add a layer.
- Select ‘AddLayer’ from the menubar. The Add Layer dialog box will be displayed.
- Select the layer you wish to add. You may need to select the directory in which this layer is stored as well.
- Select ‘Ok’ when you have chosen the desired layer filename. The dialog box appropriate for the chosen layer type will be displayed.
- Specify the thickness of the layer, and declare any desired fit parameters within the layer.
- Click on ‘Ok’. This will close the layer dialog box and display the layer in the appropriate place in the model.

For more information about models and the Model window, consult chapter 7 - ‘The Model Window’.

Viewing the optical constants of a layer

There are two ways to view the optical constants of a layer. The Graph window may be used to view the optical constants of any layer, or the optical constants of all layers currently in the model. Also, the optical constant plots may be exported from the Graph window to the Windows™ Clipboard such that they may be pasted into other applications. The layer dialog box (accessed within the Model window) may be used to view the optical constants of the layer as well, and may also be used to examine and/or modify the numerical values of the layer optical constants.

To view the optical constants of a layer within the Graph window, use the following procedure.

- Activate the Model window.
- Use the up and down arrow keys to position the current layer arrow ('>', on the left side of the model) next to the desired layer.
- Activate the Graph window.
- Select ‘Data’ from the menubar.
- Select ‘Current Layer Opt. Con.’ from the menu which is displayed. The Current Layer Optical Constants dialog box will be displayed.
- Select the optical constant spectra you wish to view for the chosen layer. You may select ‘n & k’ (plot both n and k together), ‘n only’ (plot only the index of refraction), ‘k only’ (plot only the extinction coefficient), or ‘Absorption Coefficient’ (plot the absorption coefficient only, equal to 2π time the extinction coefficient divided by the wavelength).
- Do not select ‘Graph Anisotropic optical constants’ unless you are viewing the optical constants of an anisotropic layer.
- Click on ‘Ok’. The specified optical constant spectra for the chosen layer will be displayed in the Graph window. Use the ‘Edit’ menu
from the Graph window to customize the plot (change titles, axis labels, etc.)

To view the optical constants of a layer from the layer dialog box in the Model window, use the following procedure.

- Activate the Model window.
- Click on the layer whose optical constants you wish to view, or use the up and down arrow keys to move the current layer arrow (‘>’, on the left side of the model) next to the layer whose optical constants you wish to view and press <Enter>.
- The appropriate dialog box for the chosen layer will be displayed.
- Select ‘Optical Constants’ from the layer dialog box. The Optical Constants dialog box will be displayed.
- The tabulated optical constants for the chosen layer are given on the left side of this dialog box. Click in this list and use the up and down arrow keys to view the table of optical constant values.
- A plot of the optical constants is displayed on the right side of this dialog box.
- If the optical constants of the layer (‘n’ and ‘k’) are explicitly declared as fit parameters, the ‘Edit n & k’ button will be active. Select a row from the tabulated list of optical constants and click on the ‘Edit n & k’ button to alter the optical constants at the selected wavelength.
- If the optical constants of the layer (‘n’ and ‘k’) are explicitly declared as fit parameters, the ‘Smooth Opt. Const.’ button will be active. Click on this button to perform a polynomial smoothing of the optical constant spectra.
- Select ‘Save’ to save the optical constants of the layer.
- Select ‘Cancel’ when you are done viewing or altering the optical constants of the chosen layer.

For more information about layers, layer types, models and the Model window, consult chapter 7 - ‘The Model Window’.

**Saving the optical constants of a layer**

- Activate the Model window.
- Click on the desired layer in the model, or use the up and down arrow keys to position the current layer arrow (‘>’, to the left of the model) next to the desired layer and press <Enter>. The dialog box for the selected layer will be displayed.
- Click on the ‘Optical Constants’ button. The layer optical constant dialog box will be displayed.
- Click on the ‘Save’ button in the layer optical constant dialog box.
- If the layer whose optical constants you are saving is a function-based layer (Cauchy, Lorentz, user-defined, parametric semiconductor) you will be asked ‘Save dispersion model parameters?’ Select ‘Yes’ to save the parametric representation of the optical constants (Cauchy parameters or Lorentz oscillator parameters, for example) or select ‘No’ to save a tabulated list of optical constants calculated from the
dispersion model contained in the chosen layer. If you select ‘No’, optical constants will be listed in the saved file at every wavelength (within the selected spectral range) for which data (of a currently selected type) is present in the Experimental Data window.

- Choose the directory in which you wish to save the optical constants, and specify a name for the file. You do not need to specify the file extension, as the extension ‘.dat’ will automatically be appended to the file name you specify.
- Click on the ‘Ok’ button to save the file and close the file save dialog box.
- Click on ‘Cancel’ to close the layer optical constant dialog box.
- Click on ‘Ok’ to close the layer dialog box.

For more information about layers, layer types, models and the Model window, consult chapter 7 - ‘The Model Window’.

**Saving a model**

- Activate the Model window.
- Select ‘File’ from the menubar.
- Select ‘Save’ from the menu which appears. The standard file save dialog box will be displayed.
- Choose the directory in which you wish to save the model.
- Specify a file name for the model. You do not need to specify the file extension, as the extension ‘.mod’ will automatically be appended to the file name you specify.
- Click on the ‘Ok’ button to save the file and close the file save dialog box.
- **WVASE**™ may ask you whether you wish to save the optical constants of one or more layers in the model (usually if their optical constants have been altered). This is a good opportunity to save the optical constants of layers in the model.

For more information about models and the Model window, consult chapter 7 - ‘The Model Window’.

**Loading a model**

- Activate the Model window.
- Select ‘File’ from the menubar.
- Select ‘Open’ from the menu which is displayed. A standard file open dialog box will be displayed.
- Choose the directory in which the model you wish to load is stored, and select the model file name from the list of available model files.
- The model file will be read, and the model will be displayed in the Model window.
Changing data types

- Activate the Experimental Data window.
- Select ‘Change Data Type’ from the menubar.
- Select the desired data type from the displayed list.
- Select ‘Ok’ to change the data type, or ‘Cancel’ to go back to the Experimental Data window.

For more information about data types, experimental data, and the Experimental Data window, consult chapter 6 - ‘The Experimental Data Window’.

Setting the range of active data

The Range Select option is used to determine how much of the data in the Experimental Data window will be fit (during any fit) and plotted (in the Graph window). Any data of the selected data type(s) which lies with the selected ranges of angles of incidence and wavelength will be active for fitting and plotting. To set the ranges and data types which are active, use the following procedure.

- Activate the Experimental Data window.
- Select ‘Range Select’ from the menubar.
- Specify the desired range of angles of incidence.
- Specify the desired range of wavelengths.
- Select one or more data types from the displayed list. Note that all data types are included by default.
- Select ‘Ok’

See chapter 6 - ‘The Experimental Data window’ for complete information regarding the use of the Range Select option.

Defining layer thicknesses as fit variables

In most cases, parameters which may be varied during a fit will be displayed with a check box which may be enabled to declare the given parameter as a variable parameter. The check box may also then be cleared (disabled) to fix the given parameter such that it is not varied during a fit. There are several types of fit parameters which may be declared.

First, layer thicknesses in the model may be varied. This is accomplished in the following manner.

- Activate the Model window.
- Select the layer whose thickness you wish to vary by clicking on the layer or by using the up and down arrow keys to position the current
layer arrow (‘>’, to the left of the model) next to the appropriate layer and pressing <Enter>. The layer dialog box will be displayed.

- Select the box labeled ‘Fit’, which appears next to the thickness of the layer. The box should display an ‘x’ when the thickness is defined as a fit parameter. If the check box is empty, the layer thickness is not defined as a fit parameter.

Fitting for the optical constants of a layer

The optical constants of any layer or the substrate may also be directly varied. When the optical constants are defined as fit parameters, the value of the optical constants will be fit at each wavelength (photon energy) for which data is present in the Experimental Data window (within the selected range, if applicable). Use the following procedure to define the optical constants of a layer (or the substrate) as fit parameters. Note that the real and/or imaginary parts of the optical constants (complex index of refraction or complex dielectric function) may be varied separately or together.

- Activate the Model window.
- Select the layer whose optical constants you wish to vary by clicking on the layer or by using the up and down arrow keys to position the current layer arrow (‘>’, to the left of the model) next to the appropriate layer and pressing <Enter>. The layer dialog box will be displayed.
- Locate the two check boxes which are labeled ‘n’ and ‘k’. These are the optical constant fit boxes, and they will appear in every layer dialog box, regardless of the layer type (exceptions are the specialty surface roughness and Kramers-Kronig layers).
- Click on the appropriate boxes to define the real and/or imaginary part of the optical constants as fit parameters. If the optical constants are chosen to be displayed as the index of refraction and extinction coefficient (selected from the ‘Defaults’ dialog box, from the ‘Global’ menu which is always present on the menubar), enabling the ‘n’ check box will cause the index of refraction to be fit and enabling the ‘k’ check box will cause the extinction coefficient to be fit. If the optical constants are chosen to be displayed as the real and imaginary parts of the complex dielectric function, enabling the ‘n’ check box will cause the real part of the dielectric function to be fit, while enabling the ‘k’ check box will cause the imaginary part of the dielectric function to be fit.
- Click on ‘Ok’ when you are done to close the layer dialog box.
- The name of the layer in the Model window should now appear in blue, denoting the presence of optical constant fit parameters in that layer.
- Note: When using function-based layers (Cauchy, Lorentz, user-defined, alloy, EMA, parametric semiconductor), make sure you have switched off all fit parameters in the functional optical constant model if you define the optical constants of the layer directly as fit parameters. Attempting to fit for functional model parameters and the optical constants of the layer will usually produce a singular matrix error.
Fitting for parameters in a function-based layer dispersion model

There are many function-based layers supported within WVASE™ (Cauchy, Lorentz, user-defined, alloy, EMA, alloy-temp, parametric semiconductor). To vary parameters within the dispersion models contained in these layers, enable the fit check box next to the parameter you wish to vary in the layer dialog box. Consult chapter 7 - ‘The Model Window’ for specific details about each of the layer types.

Setting the fit weighting

The following procedure is used to specify how the experimental data are weighted during a fit.

- Activate the Fit window.
- Select ‘Defaults’ from the menubar. The Fit Defaults dialog box will be displayed.
- Choose the weighting type for the ellipsometric data from the list at the upper left of the dialog box. You should not use any weighting other than ‘Experimental Standard Deviations’ unless you have thoroughly read the section in chapter 10 - ‘The Fit Window’ dealing with fit weighting and you have a compelling reason to do so.
- Choose the relative weighting for reflectance and transmittance data. The default values of 100 will nearly exclude any reflectance and transmittance data when fit with ellipsometric data. For combined ellipsometric / reflectance or ellipsometric / transmittance fits, set the reflectance and/or transmittance weighting to 500 or 1000 to weight the ellipsometric and reflectance (transmittance) data roughly equally.
- Do not alter the default values for the rest of the parameters in the Fit Defaults dialog box.
- Click on ‘Ok’ to close the Fit Defaults dialog box.

For further information consult chapter 10 - ‘The Fit Window’.

Performing a normal fit

A normal fit consists of varying all of the defined fit parameters simultaneously to obtain model-calculated data which matches the data in the Experimental Data window (within the selected range) as closely as possible. To perform a normal fit, use the following procedure.

- Activate the Fit window.
- Select ‘Normal Fit’ from the menubar.
- A normal fit will begin. The iterations will be shown in the Fit window, and if the ‘Graph Fit Iterations’ option is enabled (in the Fit Defaults dialog box,) the experimental and calculated data will be updated in the Graph window after each iteration.
- During the fit, the hourglass cursor will be displayed instead of the normal arrow, and you will not be able to perform any other actions until the fit terminates.
- To stop the fit prematurely, press the <Esc> key.
When the fit converges or reaches the maximum number of iterations, the arrow pointer will return, and you will be returned to the Fit window.

For more information about normal fits, consult chapter 10 - ‘The Fit Window’.

Performing a point-by-point fit

A point-by-point fit consists of fitting the experimental data one wavelength at a time rather than all at once. The data at each wavelength is fit by varying all of the currently defined fit parameters (maximum of six). This type of fit is most commonly used to fit for optical constants of a layer or the substrate with all other parameters in the model fixed. To perform a point-by-point fit, use the following procedure.

- Activate the Fit window.
- Select ‘Pt-by-Pt’ from the menubar.
- A dialog box will appear displaying the initial values of the fit parameters at the first wavelength, and allowing you to start the fit at the shortest or longest wavelength. You may modify the initial parameter values if you wish. Click on ‘Ok’ when done.
- The first wavelength will be fit, the results will be displayed in the Fit window, and you will be asked if you wish to ‘Change Starting Parameters?’. If you reply ‘Yes’, you will be returned to the previous step where you may change the values of the initial parameters (you should do this if the results of the first wavelength fit are obviously incorrect). If you reply ‘No’, the data at the rest of the wavelengths will be fit, one wavelength at a time. If you reply ‘Cancel’, the point-by-point fit will be aborted and you will be returned to the Fit window.

For more information about point-by-point fits, consult chapter 10 - ‘The Fit Window’.

Viewing the fit statistics after a fit

To view the final MSE, correlation matrix, and 90% confidence limits from the most recent fit, use the following procedure. Note that the final results of a fit must be displayed in the Fit window for the statistical calculations to be performed.

- Activate the Fit window.
- Select ‘Stats’ from the menubar.
- The Fit Statistics dialog box will be displayed. You may view the final MSE, correlation matrix, final parameter values, and 90% confidence limits on the final parameter values in this dialog box.
- Click on ‘Ok’ when you are finished to close the Fit Statistics dialog box and return to the Fit window.

For more information about fit statistics, consult chapter 10 - ‘The Fit Window’.
Generating data from the model

To calculate data from the model shown in the Model window, use the following procedure. Note that, by default, data will be calculated of the same type and at the same wavelengths and angles of incidence as the data (within the currently selected range) in the Experimental Data window.

- Activate the Generated Data window.
- Select ‘Generate Data’ from the menubar.
- Data will be generated, and you may view the new generated data from the Graph window, or in tabular form in the Generated Data window.

For more information about generating data from the optical model in the Model window, consult chapter 8 - ‘The Generated Data Window’.

Choosing the set of data to be graphed

To choose which data will be graphed in the Graph window, use the following procedure.

- Activate the Graph window.
- Select ‘Data’ from the menubar.
- Select the data to be plotted from the list which is displayed.
- The chosen data will be plotted in the Graph window.

For more information on graphing data, consult chapter 9 - ‘The Graph Window’.

Choosing the type of data to be graphed

To choose the form in which the data are to be plotted in the Graph window (psi, delta, pseudo-optical constants, etc.), use the following procedure.

- Activate the Graph window.
- Select ‘Type’ from the menubar.
- Select the desired data type from the list which is displayed.
- The chosen data type will be displayed in the Graph window.

For more information on graphing data, consult chapter 9 - ‘The Graph Window’.

Comparing different sets of optical constants

To compare two or more sets of optical constants, use the following procedure.

- Make sure that each set of optical constants you wish to view have been saved as a material file (.mat).
- Activate the Model window.
- Delete any existing model from the Model window by selecting the ‘DeleteMod’ option from the menubar.
Add each layer whose optical constants you wish to view to the model. The layer thicknesses do not matter, as we are only going to graph the optical constants of the layers.

Once all of the layers you wish to compare have been added to the model, activate the Graph window.

With the Graph window active, select ‘Data’ from the menubar.

Select ‘All Layers (Opt. Const.)’ from the list which appears.

A dialog box will be displayed allowing you to plot either n & k together, n only, k only, or the absorption coefficient (calculated from the extinction coefficient spectrum). Note that if you have chosen to display optical constants as the real and imaginary parts of the dielectric function (from the ‘Defaults’ option in the ‘Global’ menu), the real and imaginary parts of the dielectric function will be displayed instead of n and k.

Choose the set of optical constants you wish to view, and click on ‘Ok’, the spectra for all of the layers in the model will be plotted together in the Graph window, with the layer names given as the legends for the curves.

For more information on graphing optical constants, consult chapter 9 - ‘The Graph Window’.

Deleting all existing fit parameters

To delete all existing fit parameters such that there will be no variable parameters defined anywhere in the model, use the following procedure.

- Activate the Fit window.
- Select ‘Edit Parms’ from the menubar. The ‘Edit Fit Parameters’ dialog box will be displayed.
- Select the ‘Delete All Parms’ button from the ‘Edit Fit Parameters’ dialog box.
- The ‘Edit Fit Parameters’ dialog box will close, and there are now no fit parameters defined in the model.

14.3 Troubleshooting

There are many common problems which occur during data analysis, a number of which will explicitly cause error messages to appear. In this section we describe how to detect and diagnose analysis problems, and provide means for solving or avoiding each problem.

When all else fails, exit WVASE™, exit Windows™, and reboot the computer. This will clear the computer memory, and will sometimes cure unexplainable problems within Windows™.

Singular matrix error

This is a very commonly encountered error message, which occurs when WVASE™ tries to invert the curvature matrix (see chapter 2 - ‘A Short Course in Ellipsometry) as part of the fitting algorithm. This will occur when the derivative of
the calculated data with respect to some fit parameter is zero for all of the data points. In other words, if a fit parameter has no effect on the calculated data, the derivatives of the calculated data with respect to that parameter will be zero, and a row of zeros will appear in the curvature matrix, causing it to be singular (non-invertible).

This is usually a simple error to fix, as you simply need to find the fit parameter which is not effecting the data. The most common cause of this error is defining the optical constants of a function-based layer directly as fit parameters while some of the functional dispersion model parameters are also defined as fit parameters (for example, having ‘n’ and ‘k’ defined as fit parameters in a Cauchy layer, with ‘An’ also defined as a fit parameter).

Another common cause of this error occurs when a parametric optical constant model is used and one or more of the parameters fits to an unphysical value (zero, or a very large number, for example). This occurs quite often with the Lorentz and parametric semiconductor layers. Try to find the offending parameter and switch it off as a fit parameter.

If all else fails, delete all of the fit parameters and start adding them one by one (and performing a fit) until you locate the parameter which is causing the singular matrix error. To delete all of the currently defined fit parameters, activate the Fit window, select ‘Edit Parms’ from the menubar, and click on the ‘Delete All Parms’ button in the dialog box which is displayed.

**Obviously incorrect layer thicknesses**

If you get layer thicknesses which are obviously incorrect, try manually changing the layer thickness(es) and restarting the fit. Usually incorrect layer thicknesses are accompanied by unphysical optical constants, so you may need to reset any optical constant (or parametric model) variables as well. Try manually adjusting the model parameters and generating data to get a feel for how the model parameters effect the data, and try to get the initial model fairly close to the experimental data before you initiate a fit.

**Unphysical optical constants**

The determination of unphysical optical constant spectra will occur in two cases. First, if the optical model is simply incorrect, the optical constants of a layer in the model which are being fit (directly or parametrically) may become unphysical in order to compensate for other deficiencies in the model. Second, if the experimental data are not sensitive to the optical constants being varied (directly or parametrically) the fit is likely to produce very strange optical constants for the given layer.

Try fixing the optical constants of the layer at some reasonable values (easiest with parametric models, particularly the Cauchy model) and fitting for the rest of the model parameters. If you get a very good fit, it is likely the experimental data are not very sensitive to the particular set of optical constants you were trying to vary.

If the data are sensitive to the optical constants of the given layer, but you continually get unphysical optical constants, try adding complexity to the model by introducing roughness, grading, film non-uniformity, etc. You should have some reasonable justification for adding these features, but often times you may stumble on the right addition to the model by simply trying them all and looking for the single model type which provides a good fit and physical optical constants for the layer under study.
Tiny MSE values

Very tiny final MSE values (<1) may occur in several cases. First, when fitting data from bulk samples to determine substrate optical constants, the final MSE will typically be very small. In general, any time there are exactly as many fit parameters as there are data points, you will obtain a vanishingly small MSE from the fit.

Also, if the Fit Weighting (from the ‘Defaults’ menu in the Fit window) is set to something other than ‘Experimental Standard Deviations’, the MSE will tend to be quite small, as the squared differences between the experimental and calculated data will not be divided by the square of the standard deviation of the experimental data point. Make sure that the fit weighting is set to ‘Experimental Standard Deviations’ if you obtain MSE values which seem too small.

Huge MSE values

Huge MSE values (several thousand, 1e99 in the worst case) may be obtained under a number of circumstances. First, if transmission and/or reflectance data are being fit and the reflectance or transmittance weighting is set to a very large number (1e4, for example), the MSE may be very large.

This also commonly occurs when using parametric optical constant models which exhibit strong internal correlations between the parameters in the dispersion model (most often the Lorentz and parametric semiconductor layers). When this is the case, one or more of the parameters may be adjusted to a wildly unphysical value during the fit, and the subsequent calculated data will be nowhere close to the experimental data, yielding a huge MSE. If this occurs, try switching off one or more of the fit parameters in the parametric layer to reduce the parameter correlations.

Huge 90% confidence limits

Three things can cause the 90% confidence limits on the final values of the fit parameters to be large (same order of magnitude as the fit parameter itself). First, if the experimental data are not sensitive to that fit parameter, the 90% confidence limit will be very large. Second, if the final MSE from the fit was very large, the 90% confidence limits on all of the variable parameters will be correspondingly large. Finally, if two (or more) parameters are very strongly correlated, their 90% confidence limits will be very large.

Try reducing the number of fit parameters to reduce the confidence limits. In particular, fix the parameters which seem to exhibit the largest 90% confidence limits, as these parameters probably are either correlated or do not effect the model-calculated data very strongly.

‘NAN’ displayed for correlation matrix element

The symbol ‘NAN’ will sometimes be displayed for correlation matrix elements, and in the worst case may be displayed for 90% confidence limits as well. This symbol stands for ‘Not A Number’, and can be taken as an almost certain indicator of very strong parameter correlations in the model. Try reducing the number of fit parameters and fitting again.
Can’t reproduce example analysis results

Make sure that the fit defaults and global settings of WVASE™ are set exactly as shown in the next section. If you still cannot reproduce the example results, record the results that you get and contact the J. A. Woollam Co., Inc., or its nearest representative.

Abrupt discontinuity in optical constants

An abrupt discontinuity may be observed in the optical constant spectra obtained when fitting directly for the optical constants of a given layer. This commonly occurs due to problems. First, if the experimental data spectra were acquired in parts (i.e. UV data in one scan and VIS-IR data in another scan), but were fit as a whole, a discontinuity may exist in the experimental data which is then mapped into the optical constants being fit for. Examine the experimental data closely to see if a discontinuity exists, and if so try to repeat the data acquisition, being very precise about the calibration of the instrument and the alignment of the sample. Also, it is very important when splitting scans in this manner that all scans from a given sample be performed on exactly the same location on the sample, as film non-uniformity may lead to discontinuities in the data as well.

A discontinuity in the best-fit optical constants will also occur quite often at ‘handedness changes’ in the experimental data. This is most commonly observed at wavelengths where delta exhibits a sharp peak near 180° or a sharp valley near 0°. The data near the handedness changes are very sensitive to surface roughness and index grading in the film, and omission of these features for a sample which is rough and/or graded will nearly always yield a ‘glitch’ in the optical constants at the handedness changes. Also, the delta data near the handedness changes tends to be noisier than the data elsewhere, and this noise can be mapped into the optical constants as well.

To get rid of the glitches in the optical constants at the handedness changes, try adding roughness and/or grading to the model. If you are fitting data from a sample with a roughened glass substrate, try including back surface reflections, starting at a very small value (0.001, for example). If all else fails, use a parametric (function-based) dispersion model for the optical constants, as these models cannot exhibit an abrupt discontinuity in the optical constants.

Abrupt discontinuity in EMA optical constants

You may note occasionally when using EMA models that the optical constants predicted by the EMA model exhibit abrupt (unphysical) discontinuities. This will only occur when using three constituent Bruggeman EMA models, and is a consequence of the fact that the Bruggeman EMA equation (a complex equation) must be self-consistently solved to obtain the effective dielectric function of the layer. There are an infinite number of solutions to this equation, and WVASE™ will sometimes have difficulty obtaining the correct solution, particularly when the three constituents have radically different optical constants.

To alleviate this problem, first make sure that the constituent with the largest volume fraction is given first. If you still have problems, try using the Maxwell-Garnett EMA model instead of the Bruggeman EMA.
Strange behavior using anisotropic Cauchy layer

Don’t forget that if you declare the Cauchy ‘Cn’ parameter for the ‘E-field parallel to optical axis’ index as a fit parameter, you must go to the Fit window, select ‘Edit Parms’ from the menubar, and change the lower bound for this parameter from 1000 to some negative number (-1, for example). Otherwise, as soon as you perform a fit this Cn parameter will be forced equal to 1000 (the default lower bound), and very strange results will be obtained for the calculated data from the model.

Very large roughness thickness

If you obtain a very large thickness for a surface or interfacial roughness layer, this layer thickness is almost certainly correlated to another thickness (or optical constant parameter) in the model. Delete the roughness layer and see if you get about the same final MSE. If so, the roughness is not helping the model and is causing extreme correlations.

If you must leave the roughness layer in the model to obtain a good fit, make sure that your final solution is unique, and is reproducible from a fairly wide range of initial parameter values. Also, keep in mind that the EMA approximation for roughness is expected to fail when the roughness scale (in any direction) reaches approximately 1/10 of the wavelength of the light used for the measurement, such that roughness layer thicknesses greater than a few tens of nm must be viewed with caution.

14.4 WVASE™ settings for the examples

Throughout the examples we will assume that WVASE™ is configured according as described below. Make sure that this is the case before trying the examples.

Memory allocation

The memory allocation for WVASE™ is set by selecting ‘Global’ from the menubar and then selecting ‘Defaults’ from the menu which appears. The Global Defaults dialog box will appear. Select the ‘Memory Allocation’ button in the Global Defaults dialog box, and the Memory Allocation dialog box will appear. Set the ‘Maximum # of Layers’ to 50, the ‘Maximum # of Fit Parameters’ to 500, the ‘Maximum # of Wavelengths’ to 500, and the ‘Maximum # of Data Points’ to 3000. The Memory Allocation dialog box should look like the following.
Fit defaults

The Fit Defaults dialog box is accessed by activating the Fit window and selecting ‘Defaults’ from the menubar. Set the fit weighting to ‘Experimental Standard Deviations’, leave the ‘R’ and ‘T’ weighting factors at the default values of 100, and make sure that the remaining parameters are set at their default values as shown in the dialog box below.

Figure 14-2. Fit Defaults dialog box, with default settings. These settings should be used (unless otherwise specified) for all of the examples in this chapter.

If you change any of these settings while working an example (changes are required for a few of the examples), make sure to set them back to their default values before trying another example or fitting other data.
Global units

The dimensions which WVASE™ will use to specify thicknesses, optical constants, and the light wavelength are set using the Global Defaults dialog box, accessed by selecting ‘Global’ from the menubar, then selecting ‘Defaults’ from the menu which appears. We will use units of nm for film thicknesses and light wavelength, and specify optical constants as the index of refraction (n) and extinction coefficient (k). The Global Defaults dialog box with these settings is shown below.

![Global Defaults dialog box](image)

Figure 14-3. Global Defaults dialog box, with settings used for the examples in this chapter.

There are a few cases where we will use photon energy for the light specification, and these will be noted and explained when they occur.

Example 1: Bare silicon wafer (●)

VASE® data from a bare silicon wafer are stored in the file si_bare.dat. These data are shown below.

![Ellipsometric psi data from a bare silicon wafer](image)

Figure 14-4. Ellipsometric psi data from a bare silicon wafer.
There a number of ways that we can approach the analysis of these data, and the choice of analysis type will generally depend on our purpose for having characterized a bulk silicon wafer. In most cases we simply wish to determine the thickness of the native oxide on the surface of the silicon wafer, but we may also wish to determine the optical constants of the silicon wafer, and this determination may be performed either with or without a native oxide present on the wafer surface.

**Determination of native oxide thickness**

This is the simplest possible analysis we can perform for a bare silicon wafer. In this case, we will use literature optical constants for both the silicon wafer and the native oxide, and simply fit for the thickness of the native oxide. To perform this analysis, delete any existing model, add silicon as the substrate material, add silicon dioxide as a single film, specify the thickness of the silicon dioxide layer to be 2 nm, and declare the silicon dioxide thickness as a fit parameter. Use the silicon optical constants contained in the `examples` directory in the file `silicon.mat` and the silicon dioxide optical constants in the default materials directory (`c:/wvase/mat`), such that the model appears as follows.

![Model for determination of native oxide thickness on a silicon wafer.](image)

Now, execute a normal fit in order to determine the best-fit native oxide thickness. For the experimental data in `si_bare.dat`, this yields a film thickness of 2.29 ± 0.02 nm, and the following fits to the experimental data.
Figure 14-8. Fit to the ellipsometric delta data from a bare silicon wafer, varying only the thickness of the native oxide.

Note that this analysis is very sensitive to the choice of optical constants for the silicon substrate. If we repeat the analysis using the silicon optical constants of Aspnes, as contained in si.mat, we find a native oxide thickness of 2.09 ± 0.02 nm, with the following fits to the experimental data.

Figure 14-9. Fit to the ellipsometric psi data from a bare silicon wafer, varying only the native oxide thickness. Aspnes’ silicon optical constants were employed for the silicon wafer substrate.

Figure 14-10. Fits to the ellipsometric delta data from a bare silicon wafer, varying only the native oxide thickness. Aspnes’ silicon optical constants were employed for the silicon wafer substrate.

Note the poor fit to psi and delta at wavelengths longer than ~500 nm when using the Aspnes Si optical constants. These constants are not as accurate as those of
Jellison (si_jell.mat) used for the first analysis, and we see much poorer fits and a shift of 0.2 nm in the determined native oxide thickness due solely to errors in the substrate optical constants. This is a very good example of how systematic errors in the optical model can induce systematic errors in the best-fit values of the variable parameters in the model.

**Optical constant determination with no native oxide**

A very simple analysis of the above data may be obtained by simply calculating the silicon optical constants from the experimental data, assuming that there is no native oxide or surface roughness on the silicon wafer. To do this, add any silicon material file to the model as the substrate and declare the optical constants n and k of this layer as fit parameters (the silicon layer should be the only layer in the model). Then execute either a normal or point-by-point fit to obtain the optical constants (it is a good idea to try both for educational purposes). This will yield the following results.

![Figure 14-11. Fit to the ellipsometric psi data from a bare silicon wafer, obtained by fitting for the silicon optical constants with no native oxide.](image1)

![Figure 14-12. Fit to the ellipsometric delta data for a bare silicon wafer, obtained by fitting for the silicon optical constants with no native oxide.](image2)
Optical constant determination with native oxide

While the fit performed in the previous section was very simple, we do not expect the resulting silicon optical constants to be very accurate, as there is certainly some native oxide on the surface of the wafer. It is not possible to fit for the native oxide thickness in addition to the silicon optical constants due to strong parameter correlations (although it is quite educational to try). It is possible, however, to make an educated guess as to the native oxide thickness, fix the native oxide thickness, and then fit for the silicon optical constants. Try adding a 2 nm silicon dioxide layer on top of the silicon substrate and fitting again (either normally or point-by-point) for the silicon optical constants. A perfect fit to the experimental data is obtained again, with somewhat different optical constants.

Note that the inclusion of the native oxide in the model makes a huge difference in terms of the silicon optical constant values obtained from the fit. Ellipsometric measurements are very sensitive to the surface quality of the sample, and it is important to make the optical model as accurate as possible in order to achieve accurate best-fit values for the variable model parameters.
Further experiments

1. Try fitting the data from 600 - 1000 nm with a Cauchy dispersion relation, varying all parameters for the index and extinction coefficient except the ‘Band Edge’ parameter, which should be fixed at 6000.

2. Try using surface roughness instead of native oxide.

3. Try fitting for the silicon optical constants with the parametric semiconductor model (advanced).

4. Try fitting for the silicon optical constants with Lorentz oscillators (advanced).

5. Try fitting for the silicon optical constants (directly, or with Lorentz oscillators or the parametric semiconductor model) and the native oxide (or roughness) thickness. Is your best-fit solution unique?

Example 2: Optically thick chromium film (∙)

In this example we will determine the optical constants of a thick chromium film sputtered onto a polished aluminum disk. The chromium film is thick enough that we may treat it as a bulk sample, as light cannot propagate through the film to the bottom interface of the film and back out of the top of the film.

Load the chrome.dat data file into the Experimental Data window. This data was taken on a chromium coated computer disk, but as previously mentioned the chromium coating is optically thick such that it can be modeled as a bulk system.

Determination of optical constants with no native oxide

To determine the chromium film optical constants, begin by building the following nominal model.

![Figure 14-15. Model to be used to fit for the optical constants of the chromium film.](image)

Since the default materials library does not contain chromium, we will use the optical constants for gold (au.mat) to provide initial values of the optical constants. Next, define the optical constants of the substrate (au) as fitting parameters by clicking on the 'n' and 'k' Opt Const Fit boxes in the au.mat layer dialog box.

Having defined the chromium optical constants as fit parameters, we may now use the ‘Pt by Pt’ menu option from the Fit window to fit the data. This option will fit for the optical constants one wavelength at a time, as opposed to the ‘Normal fit’ option, in which the optical constants are fit simultaneously at all wavelengths. A dialog box will appear allowing you to enter starting parameters for the fit. The fit can proceed from either the longest wavelength to the shortest, or from the shortest wavelength to the longest. In most cases (particularly for metals) the choice of which direction the point-by-point fit will be performed in is not critical.

After the data at the first wavelength is fit, a dialog box will appear displaying the final MSE from the first wavelength fit and the resulting optical constants at the first wavelength. This dialog box also provides you with several options. You may choose to change the starting optical constants and repeat the fit at the first wavelength by selecting ‘Yes’. You may also proceed with the fit by answering ‘No’, or cancel the fit. The point-by-point fit is the preferred method for fitting optical constants (when there are no other fit parameters defined) for two
reasons. First, the fit proceeds much more quickly than a normal fit, as fitting for all of the optical constants at once (a normal fit) requires \textit{WVASE} to invert very large matrices. Second, use of the point-by-point fit option helps to keep the optical constants on the correct branch, as the 'n' and 'k' determined at the current wavelength are used as the starting values for the next wavelength. This can be critical when point-by-point fitting for the optical constants of thick transparent or semi-transparent films which exhibit interference oscillations in the experimental data.

Fitting for the optical constants 'n' and 'k' of a bulk sample at each wavelength will almost always yield a nearly perfect fit to the experimental data. Exceptions are cases where there is a coating on the sample (unbeknownst to the user!), the sample is very rough or significantly oxidized, or the surface of the sample is textured or patterned such that the sample surface depolarizes the light beam. Here are the fits you should obtain for the chromium data in \textit{chrome.dat}.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{psi_data_fit.png}
\caption{Fit to the ellipsometric psi data from an optically thick chromium film, obtained by fitting for the chromium optical constants, assuming no overlayers.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{delta_data_fit.png}
\caption{Fit to the ellipsometric delta data from an optically thick chromium film, obtained by fitting for the chromium optical constants, assuming no overlayers.}
\end{figure}

Note that in the above fits the model calculated data are nearly indistinguishable from the experimental data. A good means of gauging the quality of a given fit is to view the difference between the experimental and calculated data, rather than viewing these data directly. To do this, activate the Graph window, select ‘Data’ from the menubar, and select ‘Difference between Gen and Exp’. \textit{WVASE} will subtract the data in the Experimental data window from the data in the Generated Data window and display the result in the Graph window. The ‘Type’ menu from the Graph window may then be used to select which experimental data quantity (psi, delta, pseudo-optical constants, reflectance, transmission, etc.) will be
displayed. Here are the differences between the experimental and calculated data in the previous two figures.

Figure 14-18. Difference between the experimental and best-fit calculated ellipsometric psi data from an optically thick chromium film.

Figure 14-19. Difference between the experimental and best-fit calculated ellipsometric delta data from an optically thick chromium film.

For an ideal fit, the differences plotted above should show random noise distributed around zero. Actually, these plots are dominated by random noise, but show a roughly constant offset from zero for each angle of incidence. There are a number of different possible causes of this constant offset. Errors in the calibration of the VASE° or the alignment of the sample and roughness or oxidation of the chromium film surface are the most likely causes, although this effect may also be observed if the chromium film is not actually optically thick.

The best-fit optical constants for the chromium film obtained from the point-by-point fit are shown below, along with reference chromium spectra from the literature for comparison.
We see in the above figure that our best-fit optical constants for the chromium film are qualitatively similar to those from the literature, but, as is usually the case for deposited metal films, there are significant differences between the actual optical constant spectra of the film and the literature constants.

**Determination of optical constants with native oxide**

While our best-fit optical constants will probably work reasonably well for the analysis of samples consisting of other films deposited on similar chromium films, they are not necessarily the true optical constants of the chromium film. The chromium surface has almost certainly oxidized, and this was not taken into account in our previous model. Unfortunately, we are already fitting for as many parameters as we possibly can, and attempting to vary the oxide thickness in addition to the chromium optical constants will lead to total correlation amongst these parameters.

We can, however, make a reasonable guess as to the oxide thickness and fit for the chromium optical constants with a fixed oxide at the surface of the chromium film. The material file *chromeox.mat* contains the optical constants of $\text{Cr}_2\text{O}_3$ obtained from the analysis of a spray coated chromium oxide film, and should provide a reasonable approximation for the optical constants of the oxide on the chromium film under study. Add the layer *chromeox.mat* to the model above the chromium substrate and specify 2 nm for the *chromeox* thickness, but do not declare the oxide thickness as a fit parameter. The model should now appear as follows.

```
1 chromeox 2 nm
0 cr 1 mm
```

Figure 14-21. Model for determination of chromium film optical constants, with a 2 nm native oxide included at the surface of the chromium film.

Make sure the chromium optical constants ($n$ and $k$) are still defined as fit parameters, and perform the point-by-point fit again. You should obtain a nearly perfect fit again. The new chromium optical constants are shown below, with the constants obtained with no oxide and the literature constants shown for comparison.
So, not only do our film optical constants not match the literature constants exactly, but we can obtain different spectra depending on whether we include a surface oxide in the model or not. At this point it is up to the user to make an educated decision as to the best choice of optical model, i.e. to decide whether the native oxide exists and how thick it is.

**Further experiments**

1. Try fitting for the thickness of the oxide and the optical constants of the chromium. This fit is completely correlated.

2. Try a three constituent EMA for the surface layer, consisting of chromium, chromium oxide, and voids (33% of each).

3. Try fitting for the volume fractions of the surface roughness, with two or three constituents.

4. Try using Palik’s constants for chromium (cr.mat in the default materials directory) and fitting for the surface overlayer thickness and optical properties. Model the surface layer as any one of the following - EMA layer (2 or 3 constituents), Cauchy layer, chromeox.mat.

5. Try Lorentz oscillators to model the chromium optical constants (advanced).

6. Try fitting for the chromium optical constants (directly or with Lorentz oscillators) and the native oxide (or surface roughness) thickness. Is your solution unique?

**Example 3: Bulk HgCdTe (●●)**

In this example we will determine the composition of a bulk HgCdTe (Mercury Cadmium Telluride, or MCT for short) film, as well as the effective thickness of an EMA layer approximating the surface roughness. HgCdTe is a very low bandgap semiconductor which is commonly used for infrared detectors.

**Determination of alloy fraction and surface roughness**

Load the data file mct_bulk.dat into the Experimental Data window. Limit the spectral range of the experimental data from 250 to 730 nm with the
‘Experimental Data Range Select’ command. We must limit the spectral range because the fit will be performed with the HgCdTe alloy interpolation material file, which only contains optical constants within this range.

Next, build the following nominal model for the sample.

```
1 EMA (MCT)/50% VOID  5 Å
0 MCT x=0.200
```

**Figure 14-23. Nominal model for bulk HgCdTe sample.**

When defining the two material constituents for the EMA layer, it is important to 'couple' the optical constants of the bulk MCT (layer #0) to the MCT optical constants in the EMA layer by answering 'Yes' to the 'Couple to existing layer' prompt. Surface roughness is typically modeled as a mixture of the bulk with 50% void. The void fraction should be fixed at 50% and not defined as a fitting parameter to avoid parameter correlation problems. Use the default settings for the EMA layer, i.e. the Bruggeman EMA type and a depolarization factor of 0.333.

Define the EMA layer thickness (which represents the surface roughness) and the MCT alloy fraction (composition) as fit parameters (in the Model window) and perform a normal fit. This should yield the model and data fits shown below. Note that if the data analysis is performed without the surface roughness layer (a useful exercise), the MSE is larger by an order of magnitude.

```
1 EMA (MCT)/50% VOID  18.998 Å
0 MCT x=0.222
```

**Figure 14-24. Best-fit model for the bulk HgCdTe sample.**

**Figure 14-25. Fit to the ellipsometric psi data for the bulk HgCdTe sample.**

**Figure 14-26. Fit to the ellipsometric delta data for the bulk HgCdTe sample.**
Further experiments

1. Try the further experiments listed at the end of the first example (bare silicon).

Example 4: Uncoated glass cover slip (●●●)

This is a very important example, as we will demonstrate several important concepts and analysis techniques through the characterization of a simple bare glass cover slip, approximately 0.1 mm thick.

General principles

There are two data files in the examples subdirectory which were acquired from the same location on the bare glass cover slip. The file glass.dat contains ellipsometric data acquired from the cover slip, while the second file, glass_t.dat, contains normal incidence intensity transmission data acquired from the cover slip with a VASE® instrument. We will fit the ellipsometric psi data in glass.dat in order to determine the glass index of refraction, and then fix the glass index and fit the transmission data in glass_t.dat to determine the glass extinction coefficient.

The ellipsometric data contained in the file glass.dat are shown in the following two figures.

![Ellipsometric psi data acquired from a thin glass cover slip.](image1)

![Ellipsometric delta data acquired from a thin glass cover slip.](image2)

There are three characteristics of the experimental data shown in these figures which indicate that back-surface reflections were collected during the
acquisition of the data, namely the jump in the psi spectra at \( \sim 320 \) nm, the constant offset of the delta spectra for wavelengths greater than \( \sim 320 \) nm, and the lack of strong dependence of this constant offset on the angle of incidence. The first two features are related to the fact that the glass is non-absorbing for wavelengths greater than \( \sim 320 \) nm and begins to absorb below this wavelength, while the third feature is due to the relatively weak dependence on the angle of incidence (for this very thin sample) of the number of back surface reflections which enter the detector.

For wavelengths less than \( \sim 320 \) nm, the absorption in the glass prevents the light beam from propagating to the back surface and back out the top surface of the cover slip, as the intensity of the beam decays exponentially as it propagates. As a result, only the reflection from the top surface of the sample was collected at the shorter wavelengths. This is a very weak reflection, and to make matters worse, the intensity of the arc lamp light source is rather low in the UV region as well, leading to a large random noise component on the data measured in this spectral region.

For wavelengths greater than \( \sim 320 \) nm, the cover slip is transparent and both the front and back surface reflections are collected by the detector. Also, the output of the arc lamp is much greater in the visible part of the spectrum, such that the random noise component of the measured data is much smaller in this spectral region. Also, the back and front surface reflected beams exhibit different polarization states, leading to the discontinuity in the data when the back-surface reflections begin to be collected at \( \sim 320 \) nm. Also, delta should always be either 0° (for angles of incidence greater than the Brewster angle) or 180° (for angles of incidence less than the Brewster angle) for a transparent bulk sample, as the light beam entering the detector (in the absence of back-surface reflections) will always be linearly polarized. When the back surface reflection is collected, however, two (or more) beams enter the detector, each of which exhibits a different linear polarization. As a result, the delta value measured by the ellipsometer will not be zero, as seen in the above data.

Fitting ellipsometric data with back-surface reflections (such as the spectra shown above) can be somewhat tricky due to the discontinuity in the data at the onset of the back-surface reflections. To circumvent this difficulty, we will split the analysis into three stages. First, we will fit the data at the longer wavelengths to determine the index of refraction of the glass, via a Cauchy dispersion model. Then, we will fix the index of the glass and fit the transmission data over the entire spectral range in order to determine the extinction coefficient spectrum for the cover slip.

### Analysis of psi to obtain the glass index

Load the experimental data file `glass.dat` into the Experimental Data window. The back surface of the cover slip was not roughened prior to measurement of the experimental data, so we must change the definition of the experimental data type in order to tell WVASE™ that the data contain back-surface reflection effects. To do this, select ‘Change Data Type’ from the menubar (with the Experimental Data window active) and select ‘Eb: Ellipsometric with Backside correction’ from the list of supported data types. The experimental data in the Experimental Data window is now defined as ellipsometric data with back-surface reflections, and the letters ‘Eb’ should now appear on every line of numbers in the Experimental Data window. Activate the Graph window, select ‘Generated and Experimental Data’ from the ‘Data’ menu, and use the ‘Type’ menu to view the psi delta spectra in the Graph window.

Create the optical model for the cover slip by deleting any model currently present in the Model window and adding the layer `cauchy.mat`. Do not change any of the parameter values in the Cauchy layer dialog box, but click on the ‘Fit’ boxes"
next to the ‘An’ and ‘Bn’ parameters to declare these parameters as fit variables, thus effectively varying the index of refraction. Close the Cauchy layer dialog box (click on ‘Ok’) and select ‘Options’ from the menubar. The model options dialog box will appear. Specify 0.5 for the # of back-surface reflections and click on the ‘Fit’ to the right to define the # of back-surface reflections as a fit parameter. This is the complete optical model we will use to fit the ellipsometric psi data in the long wavelength region where the glass is transparent. We are fitting for the glass index of refraction by varying the two Cauchy parameters ‘An’ and ‘Bn’ and varying a single additional parameter to account for the back-surface reflection effects. The model should appear as follows.

\[
\text{Fit Statistics}
\]

Figure 14-29. Model for analysis of psi data from a bare glass cover slip to determine the glass index of refraction.

Activate the Fit window, and select the ‘Defaults’ option from the menubar, causing the fit defaults dialog box to be displayed. This option is used to tell WVASE™ to fit the ellipsometric psi data and ignore the delta data. To do this, select ‘Psi only’ in the list under ‘Fit weighting’, then click on ‘Ok’. This tells WVASE™ to calculate the MSE from the psi data only.

Next, we need to tell WVASE™ to only fit the data at wavelengths above the discontinuity in psi. To do this, activate the Experimental Data window and select the ‘Range Select’ option from the menubar, causing the static experimental data range select dialog box to be displayed. Specify the lower wavelength bound to be 350 nm (arbitrarily chosen to lie above the discontinuity in psi), set the upper wavelength bound to be 1000 nm, and click on ‘Ok’. This tells WVASE™ to use only the data between 350 nm and 1000 nm when plotting in the Graph window or fitting from the Fit window.

We are now ready to perform the fit. First, generate data from the current model (go to the Generated Data window and select ‘Generate Data’ from the menubar) and compare the generated and experimental data (in the Graph window) to establish that the initial model-generated data is reasonably close to the experimental data. Next perform a normal fit by selecting ‘Normal fit’ from the Fit window menubar. After a few iterations, and a message box will appear stating that the change in the MSE is less than the convergence limit.

Go to the Fit window, and examine the final MSE and best-fit values of the fit parameters. You should see a final MSE of 2.988e-002, while the final fit parameter values are 0.96154 for the # of back reflections, 1.5043 for An, and 6.9047e-003 for Bn. Select ‘Stats’ from the menubar to view the statistical information calculated from the fit. The following dialog box will be displayed.

Figure 14-30. Statistics dialog box, showing results of fit for the index of the glass cover slip.
Note that the confidence limits on the variable parameters are very small and there are no off-diagonal elements in the correlation matrix whose magnitude approaches one (the largest is 0.570). This indicates that the fit parameters are not strongly correlated and the solution is unique.

Go to the Graph window, and compare the experimental and (best-fit) generated psi data. You should see a very close match, as shown below.

![Figure 14-31. Fit to the psi data only for a glass cover slip, using a back-surface reflection corrected Cauchy model.](image)

The fit looks very good in the previous figure, but to truly evaluate the quality of the fit we should look at the difference between the experimental and generated data. Select ‘Data’ from the menubar, then select ‘Difference between Gen. and Exp’ from the options list which is displayed. The experimental data will be subtracted from the generated data, and the difference is plotted in the Graph window, as shown below.

![Figure 14-32. Difference between the experimental and best-fit calculated psi data (shown in the previous figure) from a glass cover slip.](image)

The differences shown above are dominated by random noise, but do show a slight systematic dispersion, indicative of a slight inability of the simple two-parameter Cauchy model to reproduce the index spectrum of the cover slide over the selected spectral range. We could possibly alleviate this by restricting the spectral range further, however we will use the Cauchy model to extrapolate the index below 350 nm for the determination of the extinction coefficient, so we should make sure it is accurate at least down to 350 nm. We might also improve the fit by using a more flexible parameterization than the two parameter Cauchy model. Try defining the third Cauchy parameter ‘Cn’ as a fit parameter and repeating the normal fit. This will yield a final MSE of 2.663e-002 and the following differences between the generated and experimental psi data.
The MSE did not improve much, but the systematic dispersion of the differences has been almost completely eliminated, indicating that the fit to the experimental data is nearly perfect. Our determination of the index of refraction of the glass is now complete (at least from 350-1000 nm), and we will now fit the transmission data to determine the glass extinction coefficient.

Analysis of transmission to obtain the extinction coefficient

Load the experimental data file glass_t.dat into the Experimental Data window. This file contains normal angle of incidence transmission data acquired through the cover slip with a J. A. Woollam Co., Inc. VASE®. Go to the Graph window and select ‘Transmission’ from the ‘Type’ menu to view the transmission data. You will need to select ‘Generated and Experimental’ from the ‘Data’ menu as well so that the differences are not plotted. Generate data, and compare the generated and experimental transmission in the Graph window. Note that the selected data range was been automatically reset to include all of the transmission data when the file was loaded, such that data are plotted from 250 - 1000 nm, as shown below.

Note that the data are in reasonable agreement above 350 nm, but the glass absorption causes the transmission to decrease very sharply below ~ 350 nm.

Go to the Fit window and select ‘Edit Parms’ from the menubar. The fit parameter editing dialog box will be displayed. Click on the ‘Delete All Parms’ button in the lower right portion of this dialog box. All fit parameters will be
switched off and the dialog box will close. Next go to the Model window, and click on the Cauchy layer, and click on the box next to ‘k’ to define the extinction coefficient as a fit parameter to be varied at each measured wavelength. We are now ready to fit the transmission data to determine the extinction coefficient of the cover slip. First, make sure that the thickness of the Cauchy layer is set to 0.1 mm (the thickness of the cover slip), as the substrate thickness is used for the calculation of the transmission.

Go to the Fit window and perform a point-by-point fit. This will yield an exact match between the experimental and generated transmission data, as we are varying one parameter at each wavelength to fit one data value. Go to the Graph window and select ‘Current layer (Opt. Const.)’ from the ‘Data’ menu. The Cauchy layer optical constants will be displayed, as shown below.

![Figure 14-35. Glass cover slip optical constants, after having fit the transmission data to determine the extinction coefficient (dashed line).](image)

Note the sharp increase in the extinction coefficient as the wavelength decreases below ~ 320 nm, which is the absorption edge we expected to see. Notice also that the extinction coefficient exhibits an abrupt change of slope above ~300 nm. This feature is unphysical, and is a common artifact which occurs when the transmission goes to zero. When this happens, fitting for the extinction coefficient will produce a number which is large enough to cause the transmission to be zero, but may not necessarily be accurate.

Save the optical constants of the cover slip by opening the Cauchy layer dialog box, clicking on the ‘Optical Constants’ button, then clicking on the ‘Save’ button. Do not save the dispersion model parameters, as this will save the exponential absorption tail parameters in the Cauchy layer rather than the wavelength-by-wavelength extinction coefficient values we determined from the fit.

Finally, load glass.dat back into the Experimental Data window and change its type to ‘Eb’. Generate data, and view the psi data in the Graph window (shown below).
The discontinuity in psi can indeed be modeled well by the back-surface correction algorithm. View delta from the Graph window, as shown below.

The model qualitatively reproduces the measured delta data, but the fit is not as good as the fit to the psi data. This may be due to the approximate nature of the back-surface correction algorithm, surface roughness on the glass, or errors in the calibration of the ellipsometer. Nevertheless, we conclude from the fit to psi that our results for the glass optical constants are reasonably accurate.

Very Important!

Be sure to set the Fit Weighting (from ‘Defaults’, in the Fit window menubar) back to ‘Experimental Standard Deviations’ before fitting other ellipsometric data.

Further experiments

1. Try fitting both psi and delta.
2. Try adding surface roughness and fitting both psi and delta.
3. Try fitting the Cauchy layer exponential absorption model to the transmission data. Set the ‘Band Edge’ parameter to 3000 and do not vary it.
4. Try calculating the normal and/or oblique angle of incidence reflectance of the cover slide using the ‘Range’ menu option from the Generated Data window to specify reflectance data.

5. Compare the cover slide optical constants with those of fused silica by adding sio2.mat to the model and viewing ‘All Layer Opt. Const.’, from the ‘Data’ menu in the Graph window.

6. Try a four term user-defined dispersion layer rather than the Cauchy layer for the glass index. See if you can construct a function for the extinction coefficient which fits the transmission data well (advanced).

7. Try fitting a Lorentz oscillator to the glass absorption edge (advanced).

8. Try fitting the psi and transmission data simultaneously for the Cauchy parameters and extinction coefficient (advanced).

---

**Example 5: Organic film on silicon (●●)**

In this example we will determine the thickness and optical constants of an organic film deposited on a silicon wafer. The film is nominally 180 nm thick. Ellipsometric data from this sample were acquired at 65°, 70°, and 75° angle of incidence over the spectral range 250 1000 nm, by 10 nm steps.

**General information**

Load organic.dat into the Experimental Data window. The psi and delta data are shown below.

![Experimental Data](image)

*Figure 14-38. Ellipsometric psi data from a 180 nm organic coating on a silicon wafer.*
Figure 14-39. Ellipsometric delta data from a 180 nm organic coating on a silicon wafer.

Note the peak in delta at ~550 nm. This is a ‘handedness change’, and the fact that delta peaks at 180° indicates that the film is probably transparent at that wavelength.

It is rarely possible (but an instructive exercise) due to parameter correlations to fit directly for the thickness and optical constants (n and k) of a film. As a result, to obtain the thickness and optical constants of the organic film, we must find a spectral region where the film is transparent (k = 0) such that we can fix k at zero and fit only for the thickness and index of refraction of the film. This is an uncorrelated fit which will yield a unique solution unless the film is very thin (< 10 nm, very approximately) or very thick (>2 microns, very approximately).

**Cauchy fit for thickness and index**

Go to the Model window and add silicon (silicon.mat) as the substrate. Add a Cauchy layer (cauchy.mat), specify An to be 1.7, specify Bn to be 0.001, specify Cn to be 0.0001, and define An, Bn, and Cn as fit parameters, thereby varying the index of refraction through the Cauchy. Specify the thickness of the Cauchy layer to be 180 nm, and define the thickness as a fit parameter. The model should appear as shown below.

```
1  cauchy  180 nm
0  silicon  1 mm
```

Figure 14-40. Model for analysis of ellipsometric data from an organic film on a silicon wafer.

Generate data from the model and compare the generated and experimental data (shown below).
Note that the data match qualitatively at wavelengths longer than ~700 nm, but are not very similar at the shorter wavelengths. This is a very good time to experiment with the Cauchy layer thickness and parameter values to see how these parameters effect the calculated data. Note that increasing (decreasing) the thickness or the An Cauchy parameter causes the spectra to be shifted to longer (shorter) wavelengths, while changing the Cauchy Bn or Cn parameter (which changes the dispersion of the organic film index of refraction) will cause changes in the shape of calculated spectra.

We will now locate a region of the measured spectrum where the film is transparent. We assume that the film is transparent at the longest measured wavelength (1000 nm), and we want to fit as much of the measured data as possible, provided the film is transparent at each wavelength we are fitting. Start by restricting the experimental data range to 500 - 1000 nm (arbitrarily chosen). Perform a normal fit to determine the An, Bn, and Cn Cauchy parameters and the organic film thickness. This yields an MSE of 28.75 and a rather poor fit. Restrict the data range to 550 - 1000 nm and perform a normal fit again. This time we get an MSE of 7.178 and a somewhat better fit. Restrict the data range to 600 - 1000 nm and perform a normal fit. This yields an MSE of 5.834 and a pretty good fit to the experimental data, as shown below.
Further reduction of the spectral range yields slight improvement in the MSE, so we will stop at this point and consider the film to be transparent over the range 600 - 1000 nm. This being the case, we have now determined the thickness of the film from the last fit, yielding 184.27 nm. The best-fit values of the Cauchy parameters were An = 1.662, Bn = 1.3838e-002, and Cn = 4.9007e-003. All three Cauchy parameters are positive, therefore the dispersion of the film index is physically reasonable (view the film index in the Graph window to convince yourself of this).

**Determination of optical constants with thickness fixed**

We will now determine the film optical constants over the entire measured spectral range 250 - 1000 nm. Open the Cauchy layer dialog box and turn off the thickness and all three Cauchy parameters (An, Bn, and Cn) as fit parameters. Define the optical constants ‘n’ and ‘k’ of the Cauchy layer as fit parameters, and expand the selected data range from the Experimental Data window to 250 - 1000 nm. The model should now appear as follows.

```
<table>
<thead>
<tr>
<th>Layer</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>cauchy</td>
<td>154.27</td>
</tr>
<tr>
<td>silicon</td>
<td>1.00</td>
</tr>
</tbody>
</table>
```

*Figure 14-45. Model for determination of the organic film optical constants over the entire spectral range. The film thickness is fixed, and was determined from the Cauchy fit in the previous step.*
Perform a point-by-point fit starting from the long wavelength end. The resulting fit should look like the following.

Figure 14-46. Generated and experimental psi data for an organic film on silicon, from point-by-point fit with the film thickness fixed.

Figure 14-47. Generated and experimental delta data for an organic film on silicon, from point-by-point fit with the film thickness fixed.

Here are the resulting optical constants of the organic film (stored in organic.mat).

Figure 14-48. Organic film optical constants.
Further experiments

1. Try the Cauchy fit from 800 - 1000 nm, then point-by-point fit and see how the resulting optical constants compare to those in the previous figure.
2. Try adding surface roughness during the Cauchy fit.
3. Try the anisotropic Cauchy model instead of the Cauchy model. Is the fit improved?
4. Try a Lorentz oscillator model for the organic film (advanced).
5. Try the parametric semiconductor model for the organic film (very advanced).
6. Try calculating the reflectance of this sample.

Example 6: Anisotropic organic film on silicon (●●●)

The data file *anisotr.dat* contains ellipsometric data acquired from a one micron thick polymer film deposited on a silicon wafer. These data are shown in the following figures.

\[ 	ext{Figure 14-49. Ellipsometric psi data from a 1 micron thick polymer film on silicon.} \]

\[ 	ext{Figure 14-50. Ellipsometric delta data from a 1 micron thick polymer film on silicon.} \]

The ellipsometric spectra shown above may be divided into two distinct spectral regions. For wavelengths less than ~380 nm the film is opaque, and the experimental data change relatively slowly with changing wavelength. For
wavelengths longer than ~400 nm, the film is transparent, and the experimental data exhibits strong interference oscillations. We will follow the procedure given in the previous section to determine the thickness and optical constants of this film.

**Biaxial layer fit for thickness and index**

First we will fit the data at the longer wavelengths where the film is transparent in order to determine the thickness and index of refraction of the film. Load the experimental data file *anisotr.dat* into the Experimental Data window, and restrict the spectral range (‘Range Select’ menu from the Experimental Data window) to 500 - 1000 nm. Create an optical model consisting of a 1000 nm Cauchy layer (*cauchy.mat*) on top of crystalline silicon (*silicon.mat*). Specify initial guesses of 1.7 for ‘An’ and .03 for ‘Bn’ in the Cauchy layer, and declare the film thickness and both ‘An’ and ‘Bn’ as fit parameters. The model should appear as follows.

![Figure 14-51](image)

*Figure 14-51. Isotropic Cauchy model for initial analysis of thick anisotropic organic film on silicon.*

Go to the Generated Data window and generate data. You should get the following for psi and delta.

![Figure 14-52](image)

*Figure 14-52. Experimental and generated ellipsometric psi data for a 1 micron polymer film on silicon. Generated data were calculated from the nominal optical model.*

![Figure 14-53](image)

*Figure 14-53. Experimental and generated ellipsometric delta data for a 1 micron polymer film on silicon. Generated data were calculated from the nominal optical model.*
Now, even though the generated delta data match the experimental delta data qualitatively, the generated and experimental psi data are not very close. Perform a normal fit. You should get a final MSE of 319.2 and the following fits.

![Generated and Experimental Data](image1)

*Figure 14-54. Generated and experimental ellipsometric psi data from a 1 micron polymer film on silicon. Generated data were calculated from the best-fit Cauchy model.*

![Generated and Experimental Data](image2)

*Figure 14-55. Generated and experimental ellipsometric delta data from a 1 micron polymer film on silicon. Generated data were calculated from the best-fit Cauchy model.*

These fits are very poor, and no matter how much we adjust the Cauchy model (experiment at will) it is not possible to obtain a better fit. The polymer molecules in this film are actually oriented such that the film exhibits optical anisotropy, with one axis (along the film normal) exhibiting a different index of refraction than the other two (both of which lie in the film plane).

Right-click on the Cauchy layer and select ‘Add Uniaxial Anisotropy’ in the context-specific pull-down menu. This converts the Cauchy layer into a uniaxial-type biaxial.mat layer coupled with several “dummy” layers (zero-thickness layers that “hold” optical constants used in the biaxial.mat). See next figure.
On top of the silicon, there are the following layers (bottom to top):

- **Cauchy.mat** is the original Cauchy layer, but its thickness now equals zero. It now represents the in-plane optical constants $N_x = N_y$ that are coupled into the biaxial.mat layer at the Mat#1 position (see figure above).

- **$dN_z$** is a user.mat layer that parameterizes the difference in optical constant dispersion between the out-of-plane optical constants ($N_z$), and the in-plane optical constants (cauchy.mat here). That is, $dN_z = cauchy.mat - N_z$. See figure below. The index difference is described by the dispersion equation $n = A*(1 + B*wvl^2 + C*wvl^4 + D*wvl^6 + E/wvl^2)$. The wavelength units are eV.

- **$N_z$** is a refractive index additive layer (same as sum_nk.mat) which sums the in-plane optical constants, cauchy.mat, and the index-difference layer, $dN_z$ (i.e., $N_z = cauchy.mat + dN_z$). The dialog box is shown in the figure below. $N_z$ provides out-of-plane optical constants to the Uniaxial layer at the Mat#2 position (see Figure 14.56).

Figure 14-56. Left: Context-specific pop-menu. Top-left arrow points to location of ‘Add Uniaxial Anisotropy’ item. Top-right: Uniaxial anisotropic model after ‘Add Uniaxial Anisotropy’ pop-menu item has been selected. Bottom-right: Biaxial layer set to uniaxial mode (bottom-right arrow).

Figure 14-57. $dN_z$ layer. Note that it is a user.mat layer.
Ex Situ Data Analysis Examples

Figure 14-58. Nz layer. It is a refractive index additive layer.

- **Uniaxial** is a biaxial.mat layer set to uniaxial mode into which $N_z$, the out-of-plane optical constants, and the in-plane optical constants (cauchy.mat in this example) are coupled to the starting layer used when established.

This seems like a very complicated way to create a uniaxial anisotropic layer. In fact, to achieve the same effect one could simply couple two different and independent cauchy.mat layers into the Mat#1 and Mat#2 positions of the Biaxial layer. However, the advantage of this more complicated approach is that it forces the out-of-plane $N_z$ layer is always linked to be in-plane Cauchy layer, the only difference being the very small offset contained in the dNz layer. This forced linkage between in-plane and out-of-plane more closely matches the dispersion seen in most anisotropic materials, which typically have very similar in-plane and out-of-plane indices separated by only a small, slightly dispersive offset.

For transparent films, anisotropy will often cause characteristic asymmetries or “bulges” in Psi vs. wavelength oscillations. To view these effects, first reset the model as follows. Set the thickness of the Uniaxial layer (layer 4) to 1000nm. In the Cauchy layer, Set $A_n = 1.8$, $B_n = 0.01$, and activate both as fit parameters. In the dNz layer, activate the A parameter as a fit parameter (see Figure 14.57 above), but leave all parameters equal to zero for now – this effectively makes layer isotropic, as there is no difference between the Cauchy and Nz indices.

Range Select the 70 degree angle of incidence, 500 to 1000nm data only. Finally, generate data and select the Psi data type. The resulting Graph window should look like the following figure.

![Generated and Experimental Graph](image)

Figure 14-59. Generated and experimental ellipsometric psi data from a 1 micron polymer film on silicon. Generated data were calculated from a nominal isotropic model. Note the “Psi bulge” that is sometimes evident in the Psi values of transparent anisotropic films.
In the figure above, note that the Psi curves for the isotropic model are more symmetric than the anisotropic film data. The anisotropic model has a “bulge” in Psi. Psi will bulge in one direction for positive $dN_z$ values, and in the other for negative $dN_z$ values. To a varying extent, this asymmetric “bulge” can be seen in Psi for all three incident angles.

Now open the $dN_z$ layer and set $A = -0.2$ and generate data (now $N_z - N_x = -0.2$ at all wavelengths). The result Psi plot should look like the figure below. Note that the generated data now also has the Psi bulge.

![Psi plot](image)

Figure 14-60. Generated and experimental ellipsometric psi data from a 1 micron polymer film on silicon. Generated data were calculated from a uniaxial isotropic model with $N_z - N_x$ equal to -0.2. Note that both the model and experimental data now has the “Psi bulge”.

Range select all angles and wavelengths from 500 to 1000nm then perform a normal fit. This should produce an MSE = 58.03, which is considerably better than the isotropic model best MSE of 319.

We can improve this fit by activating the $C_n$ parameter in the Cauchy layer, and the $B$ and $C$ parameters in $dN_z$ layer. This allows more flexibility in both the in-plane Cauchy layer and the $dN_z$ difference parameterization. With these parameters activated, another normal fit produces an MSE = 11.1, with Psi and Delta curves shown below.

![Psi plot](image)

Figure 14-61. Best-fit generated and experimental ellipsometric Psi data from a 1 micron polymer film on silicon.
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Figure 14-62. Best-fit generated and experimental ellipsometric delta data from a 1 micron polymer film on silicon, using anisotropic Cauchy model.

This fit yields a film thickness of 998.691 nm, and the following index spectra for the Uniaxial layer (viewed by activating the Graph window, selecting ‘Current layer optical constants’ from the ‘Data’ menu).

![Figure 14-63. Anisotropic index spectra for 1 micron polymer film.](image)

The best-fit Cauchy parameters for the index with the ‘E-field perpendicular to optical axis’ were $A_n = 1.8041$, $B_n = 1.5781e-002$, and $C_n = 3.7295e-003$. The best-fit Cauchy parameters for the index with the ‘E-field parallel to optical axis’ were $A_n = 1.5851$, $B_n = 9.8633e-003$, and $C_n = 5.9119e-004$.

Direct fit for isotropic optical constants in the UV

The next logical step would be to fix the film thickness and fit for the film optical constants over the entire measured spectral range. Activate the Experimental Data window, choose ‘Range Select’ from the menubar, and set the wavelength range to 250 - 1000 nm to include all of the data in the active data range.

Next, delete all of the existing fit parameters. To do this, go to the Fit window and select ‘Edit Parms’ from the menubar. Click on the ‘Delete all Parms’ button in the ‘Edit Parms’ dialog box to fix all of the fit parameters.

Now go to the Model window and define the optical constants (‘n’ and ‘k’) of the Cauchy layer and the Nz layer as fit parameters. Perform a point-by-point fit, starting at the longer wavelengths, and watch what happens. The fit will proceed without a problem as long as the extinction coefficient (k) values are very small, but as soon as k becomes appreciable the optical constant values will begin to wander.
The net result for the in-plane and out-of-plane $n$ and $k$ values are shown in the figure below.

This occurs because the ellipsometric data only contains enough information to determine two optical constant parameters. When $k$ is very small, we are effectively fitting for the two index values only, as $k$ is zero. However, when $k$ becomes significant, we are now fitting for four parameters, and this is a totally correlated fit, hence the singular matrix error occurs. Our only option in this case is to assume the film is isotropic in the region where it is opaque and fit for the ‘effective’ optical constants of the film.

To do this, select the Experimental Data window and restrict the data range to 250 - 370 nm. Select the Model window. Note that the layer thickness is 998.7 nm (you can also open the layer and use Ctrl+‘c’ to copy the thickness, then later use Ctrl+‘v’ to paste the thickness). Delete the Uniaxial, Nz and dNz layers (in that order), until the only layers remaining are the Cauchy layer and the silicon substrate layer. Enter the layer thickness of 998.7nm in the Cauchy layer. Define the optical constants ‘$n$’ and ‘$k$’ of the Cauchy layer as fit parameters. The model should appear as shown below.

```
1 cauchy 998.691 nm
0 si_jaw 1 mm
```

Perform a point-by-point fit, starting at the shortest wavelength and specifying $n = 1.8$ and $k = 0.2$ for the initial values at the first wavelength. You should get the following results.
Figure 14-66. Best-fit generated and experimental ellipsometric psi data from a 1 micron polymer film on silicon, using isotropic model to fit for n and k in the spectral region where the film is opaque.

Figure 14-67. Best-fit generated and experimental ellipsometric delta data from a 1 micron polymer film on silicon, using isotropic model to fit for n and k in the spectral region where the film is opaque.

Figure 14-68. Effective optical constants of 1 micron polymer film, assuming film is isotropic.

Unfortunately there is nothing we can do to fit the data in the spectral range 380 - 500 nm, as the film is partially transparent in this region. Fitting with the anisotropic Cauchy model (in the region 380 - 500 nm) will produce poor fits, while fitting with the isotropic model (as we did at the short wavelengths) will yield interference oscillations in the resulting optical constants.

Further experiments

1. Try fitting the Uniaxial (biaxial.mat) layer over a wider spectral range.
2. Try adding roughness to the Uniaxial layer.
3. Try thickness non-uniformity correction instead of light bandwidth correction.

Example 7: Silver film on fused silica (●●)

In this example we will simultaneously fit ellipsometric and transmission data from a 30 nm silver film deposited on a fused silica substrate in order to determine the silver film thickness and optical constants.

Determination of film thickness and optical constants

Load the data file silver.dat into the Experimental Data window. Note that this file contains both ellipsometric and transmission data, as shown below. The back-surface of the sample was roughened prior to the acquisition of the ellipsometric data, such that there are no back-surface reflection effects in the experimental ellipsometric data.

Figure 14-69. Ellipsometric psi data acquired from a 30 nm silver film deposited on fused silica.

Figure 14-70. Ellipsometric delta data acquired from a 30 nm silver film deposited on fused silica.
First, create the optical model by adding sio2.mat (fused silica) as the substrate and adding ag.mat (literature optical constants for silver) as a film. Specify the film thickness to be 30 nm, such that the model should appear as follows.

Figure 14-72. Initial model for analysis of silver film on fused silica.

Specify the silver film thickness as a fit parameter, and perform a normal fit. This should yield an MSE of 26.28, a silver film thickness of 38.571 nm, and the following fits.

Figure 14-73. Fit to the ellipsometric psi data from a 30 nm silver film on fused silica, obtained using literature silver optical constants and fitting for the silver film thickness.
Figure 14-74. Fit to the ellipsometric delta data from a 30 nm silver film on fused silica, obtained using literature silver optical constants and fitting for the silver film thickness.

Figure 14-75. Fit to the normal incidence transmission data from a 30 nm silver film on fused silica, obtained using literature silver optical constants and fitting for the silver film thickness.

While the use of literature optical constants for the silver film produces a reasonable qualitative fit, we can get a much better fit by varying the silver optical constants directly, in addition to the silver film thickness. Open the silver film dialog box and declare the optical constants 'n' and 'k' as fit parameters. The film thickness should still be defined as a fit parameter. Perform a normal fit. You should get a final MSE of 2.592, a silver film thickness of 35.915 nm, and the following fits to the experimental data.
Figure 14-76. Fit to the ellipsometric psi data for a 30 nm silver film on fused silica, obtained by varying the thickness and optical constants of the silver film.

Figure 14-77. Fit to the ellipsometric delta data for a 30 nm silver film on fused silica, obtained by varying the thickness and optical constants of the silver film.

Figure 14-78. Fit to the normal incidence transmission data for a 30 nm silver film on fused silica, obtained by varying the thickness and optical constants of the silver film.

We can get a slight improvement to this fit (particularly the transmission from 300-400 nm) by adding surface roughness atop the silver film. Add an EMA layer above the silver, and specify it to consist of 50% silver (ag.mat, coupled to the existing layer in the model) and 50% voids (void.mat). Specify the thickness of the EMA layer to by 0.1 nm and declare the EMA layer thickness as a fit parameter (in addition to the silver layer thickness and optical constants, which are already declared as fit parameters). Perform a normal fit. You should get a final MSE of 2.427, a silver film thickness of 34.171 nm, a roughness layer thickness of 0.74006 nm, and the following fits. The best-fit model is also shown.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>EMA (ag)/50% void</td>
<td>0.74522</td>
</tr>
<tr>
<td>Ag</td>
<td>34.158</td>
</tr>
<tr>
<td>SiO2</td>
<td>1</td>
</tr>
</tbody>
</table>

Figure 14-79. Best-fit model for silver film on fused silica, with surface roughness.
Figure 14-80. Fit to the ellipsometric psi data from a 30 nm silver film on fused silica, fitting for the silver thickness and optical constants and the surface roughness layer thickness.

Figure 14-81. Fit to the ellipsometric delta data from a 30 nm silver film on fused silica, fitting for the silver thickness and optical constants and the surface roughness layer thickness.

Figure 14-82. Fit to the normal incidence transmission data from a 30 nm silver film on fused silica, fitting for the silver thickness and optical constants and the surface roughness layer thickness.

This fit yields the following optical constants for the silver film (stored in the examples subdirectory as silver.mat).
Further experiments

1. Experiment with the transmission weighting (from the ‘Defaults’ menu in the Fit window). Set it very large and note the excellent fit to the transmission data, accompanied by a much larger MSE. How does the transmission weighting effect the correlations in the model?

2. Try using Lorentz oscillators for the silver film optical constants.

3. Try a surface oxide instead of surface roughness for the silver layer.

4. Try fitting the ellipsometric data only to determine the silver film thickness and optical constants. Is your solution unique?

5. Try fitting the transmission data only to determine the silver film thickness and optical constants. There are commercially available instruments which claim to be able to do this and yield a unique solution! What do you think?

Example 8: Indium tin oxide (ITO) on glass (●●●●●)

This is a very difficult example, and can be frustrating. Novice users should try the first section only.

In this example we will determine the thickness, surface roughness, index grading profile, and optical constants of an inhomogeneous indium tin oxide (ITO) film on glass, as well as the index of the glass substrate. We will obtain this information by fitting ellipsometric data alone, using a user-defined parameterization for the glass substrate and the Drude model for free electron optical absorption (via Lorentz oscillators) for the ITO layer.

Uniform Lorentz oscillator layer model

Load the experimental data file ito.mat into the Experimental Data window. The data should appear as below. Note that data were acquired at a very large number of angles of incidence. This was done to ensure that at least one angle of incidence was used for which delta was near 90° at every measured wavelength.
Figure 14-84. Ellipsometric psi data acquired from an ITO film on glass. The back surface of the substrate was roughened prior to data acquisition.

Figure 14-85. Ellipsometric delta data acquired from an ITO film on glass. The back surface of the substrate was roughened prior to data acquisition.

Note the sharp increase in psi at ~ 1300 nm - a sure indicator that this is a transparent conducting oxide film with reasonably low resistivity. This feature occurs at the onset of the optical absorption due to the free electrons (conduction electrons) in the ITO film.

We will fit these data by using parametric dispersion models for the optical constants of the glass substrate and the ITO film. For the glass substrate, we will use a user-defined 7-term power series dispersion relation to model the index of refraction and assume the extinction coefficient to be zero over the measured spectral range. We will model the ITO film optical constants with a single Lorentz oscillator, with the center energy of the oscillator fixed at zero eV. In this limit the Lorentz oscillator model reduces to the Drude model for optical absorption by free carriers.

Create the optical model by first adding the layer sio2_usr.mat as the substrate, then adding a 100 nm film of lorentz.mat. Define the thickness of the film (lorentz.mat) as a fit parameter. Do not change the default initial values for the parameters in the user-defined dispersion model layer for the substrate, and define the first parameter (‘A’) in the user-defined model as a fit parameter. This model assumes that the dispersion of the substrate index of refraction is the same as that of fused silica, and allows the magnitude of the index to vary.

For the Lorentz oscillator layer, specify the number of oscillators to be one, specify the value of $\varepsilon_r(\infty)$ to be 4.0, set the amplitude of the oscillator to 2.8 eV$^2$, set
the broadening of the oscillator to 0.1 eV, and fix the center energy of the oscillator to zero eV. Define the thickness, $e_1(\infty)$, and the oscillator amplitude and broadening as fit parameters. At this point, the model should appear as shown below. We have also shown the user layer and Lorentz layer dialog boxes as they should appear in the model.

![Figure 14-86. Lorentz oscillator model for analysis of ITO film on glass.](image)

![Figure 14-87. User-defined dispersion model for fused silica (sio2_usr.mat), with the constant term ('A') defined as a fit parameter.](image)

![Figure 14-88. Lorentz oscillator dispersion model layer (lorentz.mat), with initial values as given above for the analysis of an ITO film on glass. The thickness and three other parameters ($e_1(\infty)$, amplitude, and broadening) are defined as fit parameters.](image)

Here are the optical constants of the ITO layer with the parameter values shown above.
Figure 14-89. ITO layer optical constants, calculated from Lorentz oscillator parameterization specified in the text.

We are now fitting for a single index parameter for the substrate, the film thickness, and three parameters in the Lorentz model for the ITO optical constants. Go to the Generated Data window and generate data to see how close the initial model is to the experimental data. The generated and experimental data should look like the following (we will suppress the legends for clarity).

Figure 14-90. Generated and experimental ellipsometric psi data for 100 nm ITO film on glass. Generated data are calculated from the initial optical model.

Figure 14-91. Generated and experimental ellipsometric delta data for 100 nm ITO film on glass. Generated data are calculated from the initial optical model.
At this point, it is a very good idea to try specifying different values for the Lorentz oscillator parameters and regenerating the data to get a feel for how the Lorentz oscillator parameters affect the ITO optical constants and the generated data. In many cases our initial guesses will not be very good and it will be necessary to guess at the Lorentz oscillator parameters to get initial generated data which are reasonably close to the experimental data.

Perform a normal fit. This will yield a final MSE of 14.23, an ITO layer thickness of 84.048 nm, and the following fits to the experimental data. From here to the end of this example we will suppress the display of the legends on plots of the experimental data to preserve clarity.

![Figure 14-92](image1)

*Figure 14-92. Fit to the ellipsometric psi data for an ITO film on glass, using a single Lorentz oscillator model for the ITO layer optical constants.*

![Figure 14-93](image2)

*Figure 14-93. Fit to the ellipsometric delta data for an ITO film on glass, using a single Lorentz oscillator model for the ITO layer optical constants.*

Note that the fits for this model are not very good. To obtain better fits for this sample it is necessary to allow variation of the ITO optical constants along the direction of the film normal (through the film). ITO films are usually amorphous (and insulating) after deposition, and are then annealed in oxygen to produce conducting films. Unfortunately, this annealing process usually produces a film which has differing conductivity (and hence differing optical properties) through the film.
Graded Lorentz oscillator layer model

The ‘standard’ grading model involves mixing the layer optical constants with the void optical constant spectra to produce an effective shift of the layer optical constants, and then allowing the effective percentage of voids in the film to vary with position through the film. To try this for the ITO film, add the layer graded.mat above the lorentz layer in the model. Specify the graded layer thickness to be 85 nm (roughly the best-fit value from the previous fit), specify material #1 to be lorentz.mat, coupled to the existing layer in the model, and specify material #2 to be void.mat. Specify a two node grading, with the value at the bottom node equal to zero and the value at the top node equal to 1. Finally, define the thickness of the graded layer and the void percentage of the top node (currently set to 1%) to be a fit parameters, such that the graded layer dialog box looks like the following.

Figure 14-94. Graded layer dialog box, set up for standard grading of ITO using voids.

Next, set the thickness of the Lorentz oscillator layer underneath the graded layer to be zero, and turn this thickness off as a fit parameter (we have replaced this layer with the graded layer, and are only using it to generate optical constants for the graded layer). The model should now appear as shown below.

Figure 14-95. Initial graded model for ITO on glass. Note that the first constituent of the graded layer is coupled to the Lorentz layer just below the graded layer.

We are now fitting for two dispersion model parameters for the substrate, three Lorentz oscillator parameters for the ITO, the thickness of the graded ITO layer, and a single grading parameter (the effective void percentage at the top of the film). Note that we would encounter a 100% parameter correlation if we were to try to vary both of the effective void percentages in the graded layer.

Perform a normal fit. This yields a much better fit, but still yields unphysical optical constants for the substrate. The reason this model does not work is that the grading of the ITO optical constants cannot be accurately modeled by simply mixing the ITO optical constant spectra with voids. Changing the conductivity of the ITO changes the dispersion of the optical constants significantly, not just the magnitude of the optical constants.
We can construct a much better graded model by defining two Lorentz oscillator layers - one which models the ITO optical constants at the top of the film and one which models the ITO optical constants at the bottom of the film. We will then grade linearly between these two sets of optical constants. To implement this model, delete the existing graded layer from the model and repeat the fit for a single Lorentz layer on the user-defined substrate. Save the optical constants of the ITO layer (save the dispersion model parameters) as temp.mat. Add another Lorentz oscillator layer (lorentz.mat) above the existing Lorentz oscillator layer (temp) in the model, and set all of the oscillator parameters in the new layer equal to those of the existing layer. Set the thickness of both Lorentz oscillator layers (temp and lorentz) to be zero, and make sure neither thickness is declared as a fit parameter. Define \( \varepsilon_i(\infty) \) and the oscillator amplitude and broadening of both Lorentz layers as fit parameters.

Next, add a graded layer at the top of the model, specify the thickness of the graded layer to be 85.0 nm, and specify temp.mat for material #1 and lorentz.mat for material #2, with both coupled to the existing layer in the model. Your model should now look like this.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>3 graded(temp)/(lorentz)</td>
<td>85 nm</td>
</tr>
<tr>
<td>2 lorentz</td>
<td>0 nm</td>
</tr>
<tr>
<td>1 temp</td>
<td>0 nm</td>
</tr>
<tr>
<td>0 sio2 usr</td>
<td>1 mm</td>
</tr>
</tbody>
</table>

Figure 14-96. Initial graded model with two Lorentz oscillator layers for ITO film on glass.

Specify the grading to have two nodes, fix the bottom node value to zero and the top node value to 100, but do not define either node value as a fit parameter. We are now fitting for the graded layer thickness, three Lorentz oscillator parameters in each Lorentz layer (six total parameters), and two Cauchy parameters for the substrate.

Perform a normal fit. This will yield a final MSE of 5.91, a graded layer thickness of 77.511 nm, and somewhat better fits to the experimental data. There are two additions to the model which improve the fits considerably. The first is the addition of surface roughness. Add the layer ema.mat above the graded layer in the model, specify one constituent to be lorentz.mat (as the graded layer is 100% lorentz.mat at the top of the film) and the other constituent to be voids. Set the void fraction to 50%, and the EMA layer thickness to 0.1 nm. Define the EMA layer thickness as a fit parameter.

The second addition is to include a pole to model the dispersion of the index of refraction due to the interband absorption in the ITO film. Specify the number of Lorentz oscillators in each Lorentz oscillator layer (lorentz and temp) to be two, and specify the amplitude of the second oscillator (in each layer) to be 0.1, the broadening to be zero, and the center energy to be 4.5 eV. Define the amplitude and center energy of the second oscillator to be a fit parameter in each Lorentz layer.

Now, we expect the interband absorption contribution to be relatively independent of the conductivity of the ITO, so we will couple these parameters together for the two layers.

To do this, go to the Fit window and select ‘Edit Parms’ from the menubar. Locate En1.2 and En1.1 in the parameter list. Both should have the value 4.5, as we just specified. Highlight En1.2, click on ‘Coupled parameters’ on the right side of the ‘Edit Parms’ dialog box, and specify that this parameter is coupled to ‘En1.1’ with a coupling constant of one. The appropriate parameter number for ‘En1.1’ will be given in the parameter list in the furthest left column. Then ‘Am1.1’ to ‘Am1.2’
with a coupling constant of one. When you are done, the ‘Edit Parms’ dialog box should look similar to the following.

Figure 14-97. ‘Edit Parms’ dialog box, with two Lorentz oscillator center energies coupled together and two Lorentz oscillator amplitudes coupled together.

Now perform a normal fit. This will yield a final MSE of 4.209, and the following results.

Figure 14-98. Best-fit model for ITO film on glass.

Figure 14-99. Best-fit parameter values and correlation matrix from analysis of ITO film on glass. This dialog box is displayed by selecting ‘Stats’ from the Fit window menubar after the fit.
Figure 14-100. Fit to the ellipsometric psi data from an ITO film on glass.

Figure 14-101. Fit to the ellipsometric delta data from an ITO film on glass.

Figure 14-102. ITO optical constants at the bottom of the ITO film (temp.mat).
Figure 14-103. ITO optical constants at the top of the film (lorentz.mat).

Figure 14-104. Substrate optical constants, from analysis of ITO film on glass.

The fit is still not perfect, however we must keep in mind that the grading model employed for the ITO is at best an approximation, as the conductivity (and hence the dispersion of the optical constants) is changing continuously through the film.

Further experiments

1. Try fitting for the substrate dispersion with the complete graded model with surface roughness.
2. Try adding more nodes to the grading. Is your solution unique?
3. Try implementing the grading by splitting the film into multiple Lorentz oscillator layers. Start with one layer, divide it into two layers (varying both layer thicknesses and all Lorentz oscillator parameters), then divide the thickest layer in two and repeat the procedure. How far can you go with this and still obtain a unique solution?
4. Try adding thickness non-uniformity to the model and see if the fits are improved.
5. Try implementing continuous grading rather than the piecewise linear grading used in the example.
Example 9: Diamond-like carbon (DLC) on glass (●●)

In this example we will fit ellipsometric, reflectance, and transmittance data simultaneously to obtain the optical constants and thickness of an absorbing diamondlike carbon film.

**Determination of film thickness and optical constants**

Load the experimental data file *dlc.dat* into the Experimental Data window. This file contains ellipsometric, reflection, and transmission data that were previously appended together and stored as a single file. The reflectance and transmittance data were acquired on a Perkin-Elmer Lambda-9 spectrophotometer and converted into the file format required by WVASE™ (see Appendix B). The ellipsometric data were acquired on a J.A. Woollam Co., Inc. VASE® instrument with the IR extension option installed.

Build the following nominal model.

![Figure 14-105. Initial model for DLC on glass.](Image)

As we do not have optical constants for DLC in the default materials library, we will use the dielectric Al₂O₃ for a starting material. In order to get the optical constants of the film reasonably close to those of DLC, we will first fit for the optical constants of the film with the film thickness fixed. Define ‘n’ and ‘k’ of the Al₂O₃ layer as fit parameters and perform a point-by-point fit (with the layer thickness fixed). For these data, choose the 'Shortest Wvl' as the starting position (if you choose the 'Longest Wvl', the algorithm wanders into the wrong branch for n & k around 600 nm).

Next, add a 10Å surface roughness layer to the model, as shown below.

![Figure 14-106. Model for DLC on glass, with surface roughness.](Image)

The fit iterations will take a long time, as there are 284 fitting parameters, ellipsometric data at 3 angles, and reflectance and transmittance data. However, the fit does converge to the results shown below after a few iterations. The surface roughness layer is not absolutely necessary, but it does reduce the MSE slightly and noticeably improves the transmission data fit (try fixing the roughness thickness at zero and repeating the fit, and compare the results). The discrepancy in the reflection data fit is probably due to measurement inaccuracies, as good reflection standards are difficult to maintain.

![Figure 14-107. Best-fit model for DLC film on glass.](Image)
Figure 14-108. Fit to the ellipsometric psi data for DLC film on glass.

Figure 14-109. Fit to the ellipsometric delta data for DLC film on glass.

Figure 14-110. Fit to the reflectance data for DLC film on glass.
Further experiments

1. Try using the 7-term power series model for fused silica (sio2_usr.mat) for the substrate and fitting for the constant term in the power series in addition to the film thickness and optical constants and the roughness thickness. Is the result unique?

2. Try using the alloy interpolation file dlccvd.mat for the DLC layer and fitting for the ‘alloy fraction’ (related to the optical bandgap of the DLC film).

3. Try using the parametric semiconductor layer for the DLC layer (advanced).

4. Try excluding the reflectance and/or transmittance data from the fit and see what you get. Is your result unique?

5. Experiment with the weighting of the reflectance and transmission data (via the ‘Defaults’ option from the menubar of the Fit window). How does the weighting effect the results (fit parameter values, correlations, confidence limits).

6. Try fitting the reflectance and transmittance only. Is your result unique?

Example 10: GaAs / AlGaAs / GaAs (●)

In this example we will determine multiple film thicknesses and film composition of an AlGaAs layer using the AlGaAs alloy interpolation file.
Determination of AlGaAs alloy fraction and thickness

Load the experimental data file algaas.dat into the Experimental Data window. Build the following nominal model, which includes a 20 Angstrom native oxide on top of the 200 Angstrom GaAs cap layer.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>GAASOX</td>
<td>20 Å</td>
</tr>
<tr>
<td>GAAS</td>
<td>200 Å</td>
</tr>
<tr>
<td>ALX_GAAS x=0.500</td>
<td>200 Å</td>
</tr>
<tr>
<td>GAAS</td>
<td></td>
</tr>
</tbody>
</table>

Figure 14-113. Initial model for the two layer GaAs / AlGaAs structure on GaAs.

Note that when the alx_gaas.mat layer is added, WVASE™ displays a message stating that the optical constant data for alx_gaas do not cover the spectral range of the experimental data. As a result, we must restrict the range of experimental data which will be fit such that no wavelengths longer than 826 nm are included in the fit. Do this using the ‘Range Select’ option from the Experimental Data window menu bar.

Next, define all three layer thicknesses and the alx_gaas alloy fraction (composition) as fit parameters and perform a normal fit. Upon completion of the fit, the WVASE™ screen should look like the following.

Figure 14-114. Final results of fit for GaAs / AlGaAs / GaAs structure.

Further experiments

1. Try using the parametric semiconductor model for the AlGaAs layer. This would be the method of choice if we did not have an alloy interpolation file for AlGaAs. Can you obtain a unique solution? (advanced)
Example 11: Polycrystalline silicon / SiO₂ / silicon (•••)

In this example we will determine the thickness and optical constants of a polycrystalline silicon (poly-Si) film deposited on a thin thermal silicon dioxide layer. We will also determine the thicknesses of the underlying silicon dioxide film and the native oxide at the surface of the poly-Si film.

There are two sets of data in the examples directory which were acquired from this sample. The first file, poly_ox.dat, contains ellipsometric data acquired from the sample, while the second file, poly_r.dat, contains p-polarized reflectance data acquired at near-normal incidence (15°) with the VASE™ instrument from the same location on the sample.

EMA model for poly-Si

Load the experimental data file poly_ox.dat into the Experimental Data window. To create the optical model, add crystalline silicon (silicon.mat) as the substrate, then add sio2.mat as the first layer. Specify this oxide to be 50 nm thick and define the thickness of this oxide film as a fit parameter.

To model the poly-Si layer, we will use a 3-constituent EMA layer, consisting of a mixture of crystalline silicon (c-Si), amorphous silicon (a-Si), and voids. Add the layer ema.mat to the model above the oxide layer, specify the thickness of the EMA layer to be 450 nm and define the EMA layer thickness as a fit parameter, and select material #1 to be c-Si (silicon.mat), material #2 to be a-Si (asi.mat), and material #3 to be voids (void.mat). You will be asked whether to couple the crystalline silicon constituent to the existing layer in the model. You may select either ‘Yes’ or ‘No’, as this coupling will not effect the results. Set the a-Si fraction at 10% and the void fraction at 10%, and declare both the a-Si and void fractions as fit parameters. The EMA layer dialog box should look like this when you are finished.

Figure 14-115. EMA layer dialog box (ema.mat) set up to model a poly-Si film.

Note that we do not claim there are actually voids in the poly-Si film, rather we are using the mathematical artifice of mixing with voids to allow more flexibility in the optical constant spectra which may be produced by the EMA layer.

To complete the optical model, add the native oxide layer by adding sio2.mat above the EMA layer. It does not matter whether you couple this layer to
the lower silicon dioxide layer. Specify 3 nm for the native oxide thickness and declare this thickness as a fit parameter. The model should now appear as follows.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>silicon</td>
</tr>
<tr>
<td>1</td>
<td>sio2</td>
</tr>
<tr>
<td>2</td>
<td>ema silicon/10% asi/10% void</td>
</tr>
<tr>
<td>3</td>
<td>sio2</td>
</tr>
</tbody>
</table>

**Figure 14-116. Initial model for analysis of poly-Si on oxide on silicon sample.**

Go to the Generated Data window and generate data to see how close the initial model is to the experimental data. The initial generated data and the experimental data are shown below.

**Figure 14-117. Generated and experimental ellipsometric psi data for a poly-Si film on a thin thermal oxide film on silicon. Generated data are calculated from the initial model.**

**Figure 14-118. Generated and experimental ellipsometric delta data for a poly-Si film on a thin thermal oxide film on silicon. Generated data are calculated from the initial model.**

The calculated data from the initial model matches up with the experimental data fairly well, and we are ready to perform a fit. It is a very good idea at this point, however, to experiment with changing the layer thicknesses and volume fractions in the model and regenerating data to see how these parameters effect the calculated data. In particular, it will usually be necessary when fitting data from thick transparent films which exhibit strong interference oscillations (as this film does) to systematically adjust the film thickness in order to get the period of the interference
oscillations (most conveniently viewed in delta) to match up reasonably well before attempting a fit.

Perform a normal fit. You should get a final MSE of 103.6, and the following results.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Description</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>SiO₂</td>
<td>5.5803 nm</td>
</tr>
<tr>
<td>2</td>
<td>EMA silicon/8.8% a-Si/10.6% void</td>
<td>446.12 nm</td>
</tr>
<tr>
<td>1</td>
<td>SiO₂</td>
<td>44.573 nm</td>
</tr>
<tr>
<td>0</td>
<td>Silicon</td>
<td>1 mm</td>
</tr>
</tbody>
</table>

Figure 14-119. Best-fit model for poly-Si on oxide on silicon.

Figure 14-120. Fit to the ellipsometric psi data for poly-Si on oxide on silicon.

Figure 14-121. Fit to the ellipsometric delta data for poly-Si on oxide on silicon.

Note that while the fits are qualitatively in agreement, there are significant discrepancies between the generated and experimental data, particularly in psi in the short wavelength end of the spectrum. The most probable reason for this is that the poly-Si film is not homogeneous (uniform) along the film normal, rather the a-Si and void fractions at the surface of the film are not the same as those at the bottom of the film. It is also possible, however, that the EMA model is simply not capable of reproducing the optical constant spectra of the poly-Si film. We find that the EMA model works best if the film is only a few percent crystalline or a few percent amorphous, and tends to fail if the film is more mixed in nature.
Parametric semiconductor model for poly-Si

We can improve our results considerably by using the parametric semiconductor layer to model the poly-Si film. Rebuild the nominal optical model, and replace the EMA layer with the layer p-si.mat, which is the parametric semiconductor model for crystalline silicon. Specify the poly-Si layer thickness to be 450 nm. The model should now appear as follows.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 silicon</td>
<td>1 mm</td>
</tr>
<tr>
<td>1 silica</td>
<td>44.573 nm</td>
</tr>
<tr>
<td>2 p-silicon</td>
<td>450 nm</td>
</tr>
<tr>
<td>3 silica</td>
<td>5.5803 nm</td>
</tr>
</tbody>
</table>

Figure 14-122. Initial parametric semiconductor model for poly-Si on oxide on silicon sample.

Delete all of the fit parameters from the model, and generate data from the nominal model with the parametric semiconductor layer for the poly-Si film. This will take a while, as the lookup tables for the parametric semiconductor layer must be calculated. Here are the data generated from the nominal model (50 nm bottom oxide, 450 nm poly-Si, 3 nm native oxide at surface).

Figure 14-123. Experimental and generated ellipsometric psi data for poly-Si on oxide on silicon. Generated data were calculated from nominal model with a parametric semiconductor layer for the poly-Si film.

Figure 14-124. Experimental and generated ellipsometric delta data for poly-Si on oxide on silicon. Generated data were calculated from nominal model with a parametric semiconductor layer for the poly-Si film.
Ouch! The generated data are not even close to the experimental data, which we should have expected since we now have crystalline silicon in the model for the poly-Si layer, which we know from the previous analysis contains a significant a-Si fraction. To fit these data, we will start with the short wavelength end of the spectrum and work towards the longer wavelengths.

First, the parametric semiconductor model is set up to work in terms of photon energy, rather than wavelength, so select the ‘Defaults’ option from the ‘Global’ menu and change the default light units to photon energy (eV). Next go to the Experimental Data window and limit the spectral range to 3.0 - 5.5 eV. Then, go back to the Generated Data window and regenerate data. You should see the following.

![Generated and experimental ellipsometric psi data from poly-Si on oxide on silicon sample. Generated data were calculated from the nominal model with a parametric semiconductor layer for the poly-Si. Data are shown as a function of photon energy, over the restricted range 3.0 - 5.0 eV.](image1)

![Generated and experimental ellipsometric delta data from poly-Si on oxide on silicon sample. Generated data were calculated from the nominal model with a parametric semiconductor layer for the poly-Si. Data are shown as a function of photon energy, over the restricted range 3.0 - 5.0 eV.](image2)

Now, in this spectral region the poly-Si film is opaque (as evidenced by the lack of interference oscillations in the previous two figures) and the light beam does not sense anything below the poly-Si film. As a result, we can fix the poly-Si and bottom oxide thicknesses and fit the data in this spectral range to determine the top oxide thickness and adjust the parameters in the poly-Silicon layer.

Open the p-si dialog box in the model, and declare the amplitudes, and center energies of all of the active oscillators, as well as the broadenings of the first
two active oscillators as fit parameters. To define a fit parameter, highlight the appropriate oscillator, click on the fit box next to the desired parameter, then click on the ‘Change’ button. If you do not click on the ‘Change’ button none of the changes or fit parameter definitions will be registered. Also, declare the magnitude of pole #1 as a fit parameter by clicking on the appropriate check box. When you are done the parametric semiconductor layer dialog box should look like this.

![Parametric semiconductor layer dialog box](image)

You should get a final MSE of ~ 20.44, and good fits to the experimental data (over the limited range 3.0 - 5.5 eV). Now, go to the Experimental Data window and expand the spectral range to 1.0 - 5.5 eV. Go to the Generated Data window and generate data to see how our model looks over the entire spectral range. The generated and experimental data from this generation are shown below.

![Generated and experimental ellipsometric psi data](image)

You should get a final MSE of ~ 20.44, and good fits to the experimental data (over the limited range 3.0 - 5.5 eV). Now, go to the Experimental Data window and expand the spectral range to 1.0 - 5.5 eV. Go to the Generated Data window and generate data to see how our model looks over the entire spectral range. The generated and experimental data from this generation are shown below.

![Generated and experimental ellipsometric psi data](image)
Figure 14-129. Generated and experimental ellipsometric delta data for poly-Si on oxide on silicon. Generated data calculated from model fit to data above 3.0 eV only.

The psi data does not look good, but the oscillations in delta match up fairly well, which is the most important in terms of whether a fit started from this point will succeed. Now add the poly-Si and bottom oxide thicknesses as fit parameters and perform a normal fit. This fit will take many iterations (you may need to fit several times to get to the minimum), as there are fairly strong correlations between the parameters within the poly-Si layer. You should get a final MSE of 55.3, and the following results.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>3 sio2</td>
<td>6.0686 nm</td>
</tr>
<tr>
<td>2 psi</td>
<td>436.22 nm</td>
</tr>
<tr>
<td>1 sio2</td>
<td>41.214 nm</td>
</tr>
<tr>
<td>0 silicon</td>
<td>1 mm</td>
</tr>
</tbody>
</table>

Figure 14-130. Best-fit model for poly-Si on oxide on silicon, using parametric semiconductor layer for the poly-Si film.

Figure 14-131. Fit to the ellipsometric psi data for poly-Si on oxide on silicon, using parametric semiconductor layer for the poly-Si film.
Figure 14-132. Fit to the ellipsometric delta data for poly-Si on oxide on silicon, using parametric semiconductor layer for the poly-Si film.

It is possible to improve this fit somewhat by varying some of the shape parameters for the poly-Si layer. It is very highly recommended that the user experiment with varying parameters in the poly-Si layer to gain experience at judging which parameters have the strongest effect on the fit. As a general rule, try varying a given parameter, and if it fits to either its upper or lower bound (as viewed in the ‘Edit Parms’ dialog box from the Fit window) then fix the parameter at the appropriate bound and do not vary it.

By varying most of the shape parameters in the poly-Si layer, we can get a final MSE from this model of 38.12. Here is what the final poly-Si parametric semiconductor model dialog box looks like (stored as poly prm.mat in the examples directory).

![Final parametric semiconductor layer dialog box for poly-Si film.](image)

Note the shape parameters which are being varied. Also, note that the magnitude and position of pole #1 are being varied, and the center energy of the ‘0’ oscillator is being varied. The ‘0’ oscillator is not active, however the first oscillator connects to the ‘0’ oscillator, hence the position of the zero oscillator will effect the shape of the poly-Si absorption tail, and the data are sensitive to this parameter. Here are the results of the fit using the above set of fit parameters for the poly-Si
layer in addition to the thicknesses of all three layers in the model (final MSE was 38.12.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>3 sio2</td>
<td>6.1447 nm</td>
</tr>
<tr>
<td>2 poly_prm</td>
<td>438.32 nm</td>
</tr>
<tr>
<td>1 sio2</td>
<td>47.601 nm</td>
</tr>
<tr>
<td>0 silicon</td>
<td>1 mm</td>
</tr>
</tbody>
</table>

Figure 14-134. Best-fit model for poly-Si on oxide on silicon, using parametric semiconductor model for poly-Si layer.

Figure 14-135. Fit to the ellipsometric psi data for poly-Si on oxide on silicon, using parametric semiconductor model for the poly-Si layer.

Figure 14-136. Fit to the ellipsometric delta data for poly-Si on oxide on silicon, using parametric semiconductor model for the poly-Si layer.
Finally, we sometimes check our optical models by measuring reflectance from the sample under study and comparing the reflectance calculated from the best-fit model (from fitting the ellipsometric data). With the best-fit model still in the Model window, load the file poly_r.dat into the Experimental Data window, then go to the Generated Data window and generate data. Go to the Graph window, and select ‘Reflection’ from the ‘Type’ menu to view the experimental and generated reflectance, shown below.

![Graph](image)

**Figure 14-138.** Experimental and calculated near-normal incidence reflectance for poly-Si on oxide on silicon. The solid curve was calculated from the best-fit model obtained from fitting ellipsometric data.

### Further experiments

1. Fine tune the poly-Si optical constants by taking the final best-fit model (above), and fitting directly for the poly-Si optical constants with all of the layer thicknesses fixed. Experiment with the optical constant smoothing function to try and eliminate glitches in the optical constants which occur at the handedness changes in the delta spectra.

2. Try a two layer EMA model for the poly-Si layer. Is this model unique?

3. Try a two layer parametric semiconductor model for the poly-Si layer. Is this model unique?
4. Try graded layers (either grading the EMA model or the parametric semiconductor model) for the poly-Si layer.

5. Try coupling some of the parameters for the two poly-Si layers in the double parametric semiconductor layer model together.

6. Try fitting the reflectance and ellipsometric data simultaneously. Does this decorrelate the double layer model?

---

**Example 12: TiN / SiO₂ / silicon (●)***

In this example we will determine the thickness and optical constants of a thin metal film deposited on top of a thick dielectric film (thermal silicon dioxide) on silicon. We will also obtain the thickness of the underlying dielectric film. This is one of the very rare cases in which it is possible to obtain the thickness and optical constants of an absorbing film on an opaque substrate from the analysis of ellipsometric data alone. This analysis is possible because the thick dielectric film sets up interference oscillations in the data, and the thin metal film dampens and phase shifts these oscillations. The analysis of data from at least two widely separated angles of incidence from this type of structure will usually yield a unique solution for both layer thicknesses and the optical constants of the top (metal) film.

**Determination of both film thicknesses and the TiN optical constants**

Load the experimental data file *tin.dat* into the Experimental Data window. Create the following nominal model by adding *silicon.mat* as the substrate, *sio2.mat* as the first layer, and *ag.mat* as the top layer. We are using the silver optical constants as an initial guess at the TiN film optical constants. Specify the thickness of the silver layer as 50 nm and the silicon dioxide thickness as 600 nm. The initial optical model should look like the following.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>silicon</td>
</tr>
<tr>
<td>1</td>
<td>sio2</td>
</tr>
<tr>
<td>2</td>
<td>ag</td>
</tr>
</tbody>
</table>

Figure 14-139. Initial optical model for TiN / silicon dioxide / silicon sample.

Again, since we do not have TiN optical constants in the default materials library, will use another material (silver) as the starting material. To get the optical constants of the silver layer closer to the optical constants of the TiN film, define the optical constants (‘n’ and ‘k’) of the silver layer as fit parameters and perform a point-by-point fit (the silver layer thickness and the silicon dioxide thickness should be fixed). The data fits will not be very good after this procedure, as only the nominal thickness values were used. However, these optical constants will provide a good enough starting point for the next fit.

Next, define the silver and silicon dioxide layer thicknesses as fit parameters in addition to the silver layer optical constants (‘n’ and ‘k’) which were previously defined as fit parameters. Perform a normal fit. When the fit converges, the results should be identical to those shown below.

Although it is not always possible to solve for ‘n’, ‘k’, and ‘t’ simultaneously, there are two main reasons why this structure was directly solvable: 1) the TiN layer was thin enough that light could penetrate it, and 2) the thick transparent layer (SiO₂) created pronounced interference effects in the ellipsometric data (data at multiple angles was absolutely necessary to obtain this direct solution).
Figure 14-140. Best-fit model for TiN / silicon dioxide / silicon sample, obtained by varying both layer thicknesses and the TiN film optical constants.

Figure 14-141. Fit to the ellipsometric psi data for TiN / silicon dioxide / silicon, obtained by varying both layer thicknesses and the TiN film optical constants.

Figure 14-142. Fit to the ellipsometric delta data for TiN / silicon dioxide / silicon, obtained by varying both layer thicknesses and the TiN film optical constants.

Figure 14-143. TiN film optical constants, from the previous fit.

Further experiments

1. Try using a Lorentz oscillator parameterization for the TiN optical constants.
2. Try varying the silicon dioxide index, via a Cauchy or user-defined dispersion relation. Is the resulting fit unique?

3. Try adding a native oxide layer atop the TiN film. Try using TiO$_2$ optical constants for the oxide (Cauchy layer with An = 2.0, Bn = 0.01, approximately) and fixing the oxide thickness at 2 nm. Do you get better results? Try varying the oxide thickness as well as all of the other fit parameters. Is your resulting fit unique?

Example 13: Five layer high-low stack on silicon (●●●)

In this example we will fit ellipsometric data from a five layer high-low stack deposited on a silicon wafer to determine all five layer thicknesses, the indices of refraction of the high- and low-index dielectric films, and the thickness of the surface roughness layer.

Determination of layer thicknesses and index spectra

Load the experimental data file hi-lo.dat into the Experimental Data window. The low index material is silicon dioxide, so we will use the 4-term user-defined modified Cauchy model for these layers, with only the constant term varying (initially). The high index material is unknown, so we will use a 3-term Cauchy model for this layer.

To create the optical model for this sample, first add silicon.mat as the substrate. Next, add cauchy.mat, set the thickness of the Cauchy layer to 125 nm, and set the Cauchy parameters to An = 2.3, Bn = 0.03, and Cn = 0.004. Define the thickness and all three Cauchy parameters as fit parameters. Next add the layer sio2_us4.mat to the model above the Cauchy layer. Set the thickness of this layer to 200 nm, and declare the thickness and the ‘A’ parameter in this layer as fit parameters.

Now add the other three layers to the model, coupling them to the existing layers already in the model. First add cauchy.mat, couple it to the existing layer, specify the thickness to be 125 nm, and declare the thickness as a fit parameter. Then add sio2_us4.mat, couple it to the existing layer, specify the thickness of this layer to be 200 nm, and define the thickness as a fit parameter. Finally, add cauchy.mat again, couple it to the existing layer, specify the thickness of this layer to be 125 nm, and declare the thickness of the layer as a fit parameter. The optical model should now look like this.

```
5 (cauchy) Coupled to #1 125 nm
4 (sio2_us4) Coupled to #2 200 nm
3 (cauchy) Coupled to #1 125 nm
2 sio2_us4 200 nm
1 cauchy 125 nm
0 silicon 1 mm
```

*Figure 14-144. Initial optical model for five layer high-low index stack.*

Now go to the Generated Data window and generate data from this model. The generated and experimental data are shown below.
Our initial model is reasonably close, and we may now perform a normal fit. This will not always be the case, and usually you will find it necessary to manually adjust thicknesses (and perhaps Cauchy parameters) in the model until the generated data are close enough to the experimental data for a fit to succeed in reaching the proper minimum.

Perform a normal fit. This will yield a final MSE of 11.23 and a good fit to both the ellipsometric psi and delta data. We can improve this fit somewhat and still obtain a unique solution by adding a surface roughness layer at the top of the stack. Add the layer ema.mat at the top of the model. Use a 2-constituent EMA, consisting of 50% cauchy.mat (coupled to the existing layer) and 50% voids. Set the EMA thickness to 0.1 nm and declare this thickness as a fit parameter (in addition to all of the other previously defined fit parameters). Perform a normal fit again.

This fit yields a best-fit MSE of 8.807, and is our final result. The results of the fit are as follows. Note that the Cauchy parameterization for the high index material is stored in the examples directory as high_c.mat, while the user-defined dispersion layer parameterization for the low index layer is stored as low_usr.mat.
Figure 14-147. Best-fit model for five layer high-low index stack on silicon.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Material</th>
<th>Thickness (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>silicon</td>
<td>1 mm</td>
</tr>
<tr>
<td>1</td>
<td>high_c</td>
<td>124.95</td>
</tr>
<tr>
<td>2</td>
<td>low_usr</td>
<td>205.21</td>
</tr>
<tr>
<td>3</td>
<td>(high_c) Coupled to #1</td>
<td>123.19</td>
</tr>
<tr>
<td>4</td>
<td>(low_usr) Coupled to #2</td>
<td>188.09</td>
</tr>
<tr>
<td>5</td>
<td>(high_c) Coupled to #1</td>
<td>122.3</td>
</tr>
<tr>
<td>6</td>
<td>ema (high_c)/50% void</td>
<td>2.1155</td>
</tr>
</tbody>
</table>

Figure 14-148. Fit to the ellipsometric psi data for the five layer high-low index stack on silicon.

Figure 14-149. Fit to the ellipsometric delta data for the five layer high-low index stack on silicon.
Figure 14-150. Index of refraction of the high-index layer, from a three term Cauchy parameterization with $A_n = 2.3338$, $B_n = 0.034981$, and $C_n = 0.002363$.

Figure 14-151. Index of refraction of the low-index layer, from a 4-term user-defined modified Cauchy parameterization, with $n(\lambda) = 1.4889 + 0.00765/\lambda + 0.001/\lambda^2 + 7.5e-5/\lambda^4$.

Further experiments

1. Try including a native oxide of 2 nm of silicon dioxide at the surface of the silicon substrate. Does this effect the results of the fit?
2. Try a 4-term user-defined dispersion layer for the high-index material.
3. Try grading the high index layers (advanced).
4. Try fitting for the index spectra of all of the layers, without coupling the layers together. Is this fit unique?

Example 14: SiO$_2$ / Si$_3$N$_4$ / SiO$_2$ / poly-Si / SiO$_2$ / Si (●●●)

In this example we will use the previously discussed EMA model for poly-Si film optical constants to obtain five layer thicknesses and the poly-Si film optical constants for a five layer stack on silicon.
EMA model for poly-Si

Load the experimental data file poly-si.dat into the Experimental Data window. Build the nominal model shown below.

<table>
<thead>
<tr>
<th></th>
<th>Layer Type</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>silicon</td>
<td>1 mm</td>
</tr>
<tr>
<td>1</td>
<td>SiO2</td>
<td>8.8778 nm</td>
</tr>
<tr>
<td>2</td>
<td>EMA Si/5% asi/5% void</td>
<td>262.03 nm</td>
</tr>
<tr>
<td>3</td>
<td>SiO2</td>
<td>17.123 nm</td>
</tr>
<tr>
<td>4</td>
<td>Si3N4</td>
<td>10.591 nm</td>
</tr>
<tr>
<td>5</td>
<td>SiO2</td>
<td>13.108 nm</td>
</tr>
</tbody>
</table>

*Figure 14-152. Nominal optical model for five layer stack on silicon.*

The EMA layer is used to determine the composition of a poly-silicon layer. A 3- constituent mixture of crystalline silicon, voids, and amorphous silicon, along with the Bruggeman theory, is used in this model. Define all layer thicknesses and the 2 EMA fractions as fitting parameters.

Perform a normal fit. You should get a final MSE of 8.968, and the following results.

<table>
<thead>
<tr>
<th></th>
<th>Layer Type</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>silicon</td>
<td>1 mm</td>
</tr>
<tr>
<td>1</td>
<td>SiO2</td>
<td>8.8778 nm</td>
</tr>
<tr>
<td>2</td>
<td>EMA Si/4.86% asi/4.7% void</td>
<td>262.03 nm</td>
</tr>
<tr>
<td>3</td>
<td>SiO2</td>
<td>17.123 nm</td>
</tr>
<tr>
<td>4</td>
<td>Si3N4</td>
<td>10.591 nm</td>
</tr>
<tr>
<td>5</td>
<td>SiO2</td>
<td>13.108 nm</td>
</tr>
</tbody>
</table>

*Figure 14-153. Best-fit model for five layer structure on silicon.*

*Figure 14-154. Fit to the ellipsometric psi data for five layer structure on silicon.*
Figure 14-155. Fit to the ellipsometric delta data for five layer structure on silicon.

Check the fit statistics to make sure that this best-fit model is unique!

Further experiments

1. Try using a parametric semiconductor layer for the poly-Si layer in this analysis. Is your result unique?
2. Try using the bandwidth or thickness non-uniformity corrections. Does either make a significant difference.

Example 15: Thermal oxides on silicon - multiple sample analysis (•••••)

There are five experimental data files in the examples directory which were acquired from five different samples consisting of thermally oxidized silicon wafers. Each wafer was oxidized for a different length of time, such that the thermal oxide films on the five wafers are of differing thicknesses. The silicon wafers used for the oxidation were identical, so these samples are a natural candidate for a multiple sample analysis. Also, the oxide films are extremely uniform, and these samples are nearly structurally ideal.

Direct fit for silicon optical constants

The five data sets are (nominal oxide thicknesses are given in parentheses) thermal1.dat (10 nm), thermal2.dat (35 nm), thermal3.dat (50 nm), thermal4.dat (100 nm), and thermal5.dat (350 nm). It is an instructive exercise to fit each of these data sets separately to determine the thickness and (for all but the 10 nm film) the silicon dioxide index (via a Cauchy or user-defined dispersion model). Note that the experimental data in these files were acquired over the spectral range 1.24 - 5.5 eV (225.5 - 1000 nm) using a VASE® instrument. Data were acquired below 250 nm (photon energies greater than 5.0 eV) by optimizing the ellipsometer for UV data acquisition, as discussed in chapter 12 - “VASE® Data Acquisition - Procedures and Strategies”.

We will perform a simultaneous analysis of all five data sets in order to determine the silicon (substrate) optical constants, the thermal oxide index of refraction (we assume the oxide to be transparent over the entire measured spectral range).
range), and the thickness of each of the thermal oxide films. To do this, we must first load each experimental data file into a separate Experimental Data window.

Start by loading the file thermal1.dat into the Experimental Data window. Next, select sample #2 by either pressing and holding <alt> and then pressing ‘2’, or by selecting ‘Select’ from the Model window and choosing #2 for the ‘Current Model’. When sample #2 is selected, an entirely new set of windows will be displayed by WVASE³⁹, and the title bars on the Model, Experimental Data, and Generated Data windows will all display the designation ‘#2’, signifying that the experimental and generated data and the optical model in the given windows ‘belong’ to sample #2. Go to the Experimental Data window and load the data file thermal2.dat.

Using the same procedure, load thermal3.dat into the Experimental Data window for sample #3, load thermal4.dat into the Experimental Data window for sample #4, and finally load thermal5.dat into the Experimental Data window for sample #5. Now, go back to the first sample set by pressing <alt>-1. Go to the Model window and select ‘Select’ from the menu bar. The following dialog box will be displayed.

![Select Model Dialog Box](image)

Figure 14-156. The ‘Model Select’ dialog box, showing five sets of experimental data present, no models defined, and only data set #1 active in any fit which may be performed.

Note the ‘x’s on the right side of this dialog box, which denote the presence of experimental data in the Experimental Data window for that sample set. We will now define the optical models for each of the five samples. First, make sure that the Model window is active and that you have the first sample set of windows displayed (there will be no numbers displayed on the title bars of the Experimental and Generated Data and Model windows when the first data set is active). If the first data set is not displayed, press <alt>-1 to make it active.

Now, define the optical model for the first sample (thermal1.dat) by adding the parametric semiconductor model layer for crystalline silicon (p-si.mat) as the substrate and then adding the 4-term user-defined dispersion layer for silicon dioxide (sio2_us4.mat). Specify the thickness of the silicon dioxide layer to be 10 nm, and declare this thickness as a fit parameter. The first model should look like the following.

![Optical Model](image)

Figure 14-157. Nominal optical model for the first data set.
Activate the second data set by pressing <alt>-2. Go to the Model window (which should display ‘Model #2’ on the title bar), and add p-si.mat as the substrate. You will be asked if you wish to couple to the existing layer, to which you should reply ‘Yes’. Whenever you add a layer to any model other than #1, WVASE™ will check the first model to see if that layer is present in model #1. If so, you will have the option of coupling to the layer in the first model. Any layer that you wish to couple across samples must be present in the first model, as WVASE™ only checks the first model for layer coupling. The p-si.mat layer will appear in the Model window, with the message that it is ‘coupled to #0’, meaning that it is coupled to layer ‘0’ in the first model. Now add the user-layer for silicon dioxide (sio2_us4.mat), specify that it is coupled to the first model, set the thickness of this layer to 35 nm, and declare the thickness as a fit parameter. The second model should now look like the following.

```
1 (sio2_us4) Coupled to #1 35 nm
0 (p-si) Coupled to #0 1 mm
```

Figure 14-158. Nominal optical model for the second data set.

Next go to models #3, #4, and #5 and specify the nominal optical models in the same manner. All of the silicon substrates should be coupled back to the first model, and all of the silicon dioxide user-defined dispersion model layers should also be coupled back to the first model. Also, the oxide film thickness in each model should be declared as a fit parameter.

Activate the first data set (press <alt>-1), go to the Model window, and select ‘Select’ from the menubar. The following dialog box will appear.

```
0   (p-si) Coupled to #0
1   (sio2_us4) Coupled to #1 35 nm
```

Figure 14-159. ‘Model Select’ dialog box, with five experimental data sets and five models present. Only the first data set is selected for fitting.

To activate all five data sets to be fit simultaneously, click on the check boxes for data sets #2 - #5 under the column heading ‘Active in Fit’ in the above dialog box, which will now appear as follows.
We are now ready to perform a fit, however (as always), it would be a good idea to check that our nominal optical models yield generated data which are reasonably close to the experimental data for each sample. To do this, activate each data set in turn (#1 - #5), go to the Generated Data window, generate data, and compare the experimental and generated data in the Graph window. In this case the nominal generated data matches the experimental data very nicely for all five samples, but if necessary we could manually adjust the oxide thickness for any sample to bring the generated data into better agreement with the experimental data for that sample prior to a fit (particularly important for the thicker films which exhibit interference oscillations).

Activate the first data set (press <alt>-1), go to the Fit window, and perform a normal fit. This will yield a final MSE of 11.75, and the five oxide film thicknesses will be listed in the Fit window (11.552, 34.701, 50.664, 100.91, and 352.61 nm, for models #1 - #5, respectively). Activate each data set in turn and check the match between the experimental and generated data for that sample in the Graph window. The fits are quite good at this point, but we can improve them considerably.

Activate the first data set (press <alt>-1), go to the Model window, and define all four of the parameters in the silicon dioxide user-defined dispersion layer (A, B, C, and E) as fit parameters. This effectively varies the index of refraction of the oxide layer on all five samples, as we have coupled the silicon dioxide layers together for all of the samples. Perform a normal fit again. This will yield a final MSE of 9.407, oxide thicknesses of 11.479, 34.469, 50.275, 100.29, and 350.22 nm for models #1 - #5, respectively, and the following parameter values in the user-defined model for silicon dioxide: A = 1.4527, B = 0.0017026, C = 0.0026175, and E = 5.6177e-005. Verify the fit quality by viewing the experimental and calculated psi and delta data for each model.

We are now ready to perform the complete fit. We can do this in two ways - either by varying the optical constants (n and k) of the silicon substrate explicitly or by varying parameters in the parametric semiconductor model representation for crystalline silicon. The parametric semiconductor model approach may reduce parameter correlations in the model and is guaranteed to produce silicon optical constant spectra which are Kramers-Kronig consistent, hence this is probably the better choice. The parametric semiconductor model is somewhat complicated, however, so we have left this approach as an exercise for the interested user (refer to

Figure 14-160. 'Model Select' dialog box, with five experimental data sets and five models present, and with all five data sets selected for simultaneous fitting.
the previous example of poly-Si / oxide / silicon for procedures useful for fitting the parametric semiconductor model parameters for silicon).

Activate the first model, open the silicon layer dialog box, and click on the ‘n’ and ‘k’ check boxes to define the silicon optical constant values at each measured wavelength as fit parameters. We are now fitting for the optical constants of the silicon substrate, the index of refraction of the oxide films (via a 4-term user-defined dispersion model), and the thickness of each of the five oxide films.

Perform a normal fit. This may take quite a while, as there is a large amount of experimental data present and a considerable number of fit parameters (two for each wavelength at which data were measured, plus four user-defined dispersion model parameters, plus five layer thicknesses). You should get a final MSE of 3.94, and the following results.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 (sio2_us4)</td>
<td>10.749 nm</td>
</tr>
<tr>
<td>0 p-si</td>
<td>1 mm</td>
</tr>
</tbody>
</table>

Figure 14-161. Best-fit model for 10 nm oxide on silicon, from multiple sample analysis.

![Psi Data](image1.png)

Figure 14-162. Fit to the ellipsometric psi data for 10 nm thermal oxide on silicon, from multiple sample analysis.

![Delta Data](image2.png)

Figure 14-163. Fit to the ellipsometric delta data for 10 nm thermal oxide on silicon, from multiple sample analysis.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 (sio2_us4)</td>
<td>33.833 nm</td>
</tr>
<tr>
<td>0 (p-si)</td>
<td>1 mm</td>
</tr>
</tbody>
</table>

Figure 14-164. Best-fit model for 35 nm oxide on silicon, from multiple sample analysis.
Figure 14-165. Fit to the ellipsometric psi data for 35 nm thermal oxide on silicon, from multiple sample analysis.

Figure 14-166. Fit to the ellipsometric delta data for 35 nm thermal oxide on silicon, from multiple sample analysis.

Figure 14-167. Best-fit model for 50 nm oxide on silicon, from multiple sample analysis.

Figure 14-168. Fit to the ellipsometric psi data for 50 nm thermal oxide on silicon, from multiple sample analysis.
Figure 14-169. Fit to the ellipsometric delta data for 50 nm thermal oxide on silicon, from multiple sample analysis.

Figure 14-170. Best-fit model for 100 nm oxide on silicon, from multiple sample analysis.

Figure 14-171. Fit to the ellipsometric psi data for 100 nm thermal oxide on silicon, from multiple sample analysis.

Figure 14-172. Fit to the ellipsometric delta data for 100 nm thermal oxide on silicon, from multiple sample analysis.

Figure 14-173. Best-fit model for 350 nm oxide on silicon, from multiple sample analysis.
**Figure 14-174.** Fit to the ellipsometric psi data for 350 nm thermal oxide on silicon, from multiple sample analysis.

**Figure 14-175.** Fit to the ellipsometric delta data for 350 nm thermal oxide on silicon, from multiple sample analysis.

Here is the silicon dioxide index spectrum you should get from this fit, generated from the best-fit user-defined dispersion model parameters $A = 1.4532$, $B = 0.0017129$, $C = 0.0027806$, and $E = 3.7888\times10^{-5}$ (stored in the examples directory as sio2_msm.mat).

**Figure 14-176.** Thermal silicon dioxide index of refraction, from multiple sample analysis of five thermal oxide films.

Here are the silicon optical constants obtained from the fit, shown with the literature constants for crystalline silicon for comparison. These constants are stored in the examples directory as si_msm.mat.
There are obviously problems with this result, as we should have obtained silicon optical constant spectra which were very close to the literature spectra. Try to repeat this fit from different starting values, and you will find that the fit is very strongly correlated. This problem can be alleviated by using the parametric semiconductor model for the silicon substrate and varying parameters in this model rather than varying the optical constants of the silicon substrate directly.

**Parametric semiconductor model for silicon**

To demonstrate this, we will perform the same fit using the parametric semiconductor model for the silicon substrate. Activate the first model and turn the optical constants ‘n’ and ‘k’ of the silicon substrate off as fit parameters. When these check boxes are not selected, the parametric model is active, and we can fit for parameters in the model. First perform a normal fit with no variables in the silicon parametric model to fine tune the silicon dioxide index and thicknesses.

Open the dialog box for the substrate in the first model, click on the ‘Replace Layer’ button, and select the file si_pr_ms.mat from the examples directory. Define fit parameters in this layer as shown in the dialog box below.
Note that we have fixed a number of the parameters in this model. Make sure you get the dialog box to appear exactly as it appears above. This parameter set has been carefully optimized to yield minimal parameter correlations with maximum flexibility, and it is an instructive exercise to try to obtain this parameter set starting from the parameterization in \( p\text{-si} \).mat.

Make sure that the four user-defined dispersion layer parameters for the silicon dioxide layer are still defined as fit parameters, and that all five oxide layer thicknesses are still defined as fit parameters. We are now fitting for the five oxide layer thicknesses, four user-defined dispersion model parameters for the silicon dioxide layer(s), and all of the fit parameters defined above for the parametric semiconductor model for the silicon substrate.

Perform a normal fit. This will take considerable time, but will yield a final MSE of 5.212, and good fits to all of the data sets. We can improve the analysis still further, however, by the addition of an interfacial oxide layer between the silicon and oxide regions.

**Inclusion of thin interfacial layer**

We will add a thin region (fixed arbitrarily at 2 nm thickness) of material at the bottom of each oxide layer which is forced to exhibit the same dispersion of the index of refraction as the bulk oxide, but which may have a slightly higher index than the bulk oxide. Not only does this provide a better analysis of the data for the five oxide samples, but it provides a very useful tutorial on coupling fit parameters between layers and across models as well.

Activate the first model, and add the layer \( \text{sio2\_int} \).mat between the silicon substrate and the oxide layer. This file is identical to \( \text{sio\_us4} \).mat, but has a different filename such that we may couple to it independently. Specify the thickness of this layer to be 2 nm, and declare all four parameters in the dispersion model (A, B, C, and E) to be fit parameters. Go to each of the other four models and add the same layer in the same location, specifying that it is coupled back to the existing layer in the first model. Once you have added this layer to each model, go through all five models again and subtract 2 nm from each of the top oxide thicknesses (to compensate the model for the addition of the interfacial layer). Do not alter the previously defined fit parameters for the silicon substrate, the top oxide layer, or the five oxide thicknesses.

At this point we have included the 2 nm interfacial oxide region in each model, and forced the index spectrum of all five interfacial oxide layers to be identical. Now we need to couple the dispersion of the index of refraction of the interfacial oxide layer to that of the bulk oxide, while leaving the magnitude of the index as an independent variable. To do this, activate the first model, go to the Fit window, and select ‘Edit Parms’ from the menubar. The following dialog box will be displayed.
To couple the dispersion of the index of the interfacial layer to that of the bulk oxide, we need to find the B, C, and E parameters for the dispersion model describing the interfacial layer in the above list of parameters and couple them to the B, C, and E parameters for the dispersion model describing the bulk oxide. The bulk oxide dispersion model parameters will be labeled A.2, B.2, C.2, and E.2 in the above list (parameters for layer #2 of the first model), while the interfacial oxide dispersion model parameters are labeled A.1, B.1, C.1, and E.1 in the above list (parameters for layer #1 of the first model). The interfacial layer parameters will be at the bottom of the list, as they were the last fit parameters to be defined. Highlight the row containing parameter B.1, click on the round target next to ‘Coupled Parameter’, and specify parameter #6 as the parameter to be coupled to, with a coupling constant of 1. Note that parameter #6 in the above list is B.2, which is the parameter we wish to couple parameter B.1 to. If B.2 is not parameter #6 in this dialog box, make sure to specify the correct parameter number for B.2. Couple parameter C.1 to parameter C.2 and couple parameter E.1 to parameter E.2 in similar fashion.

We are now fitting for all five oxide thicknesses, four user-defined dispersion model parameters for the bulk oxide, one dispersion model parameter for the interfacial oxide (with the other three tied to the corresponding parameters in the bulk oxide dispersion model), and the previously defined fit parameters in the parametric semiconductor model for the silicon substrate.

Perform a normal fit. This will yield a final MSE of 5.039, and even better fits to the five experimental data sets. Note that the A parameter for the interfacial oxide fits to 1.6152, such that the index of the interfacial region is about 0.16 greater than that of the bulk oxide.

We will make one final addition to the model (primarily for educational purposes) which will improve the analysis somewhat. We will now allow the thickness of the interfacial oxide region in each model to vary, but we will couple all five interfacial region thicknesses together such that they are identical. In this way we can vary the interfacial oxide thickness on all five samples and only add a single parameter to the model.

To do this, define the interfacial oxide layer thickness as a fit parameter in each of the five models. Next, go to the first model, activate the Fit window, and...
select ‘EditParms’ from the menubar. This time, find the five interfacial layer thicknesses (they will be easy to spot as they should all have the value 2) in the list of fit parameters. Couple four of the interfacial layer thicknesses to the remaining one, such that the dialog box looks similar to the following.

![Edit Fit Parameters dialog box](image)

**Figure 14-180. ‘EditParms’ dialog box, with four interfacial oxide thicknesses coupled to the first interfacial oxide thickness.**

Perform a normal fit. This will yield a final MSE of 5.039, exactly the same as we obtained with the interfacial oxide thickness fixed. This is almost certainly due to very strong correlation between the interfacial oxide thickness and other parameters in the model, and we should use the results obtained with the interfacial oxide layer thickness fixed.

Thus, our best-fit model was obtained by varying all five oxide thicknesses, four dispersion model parameters for the bulk oxide index of refraction, one dispersion model parameter for the interfacial oxide index of refraction (with the other three parameters coupled to the corresponding parameters in the bulk oxide model), and all of the fit parameters defined for the parametric semiconductor model for the silicon substrate. This model yielded a best-fit MSE of 5.039, and silicon dioxide layer thicknesses of 9.125, 32.162, 48.108, 98.121, and 347.45 nm for models #1-#5, respectively.

Here are the index spectra obtained for the bulk and interfacial oxide layers from this analysis. The bulk oxide spectrum (stored as sio2_blk.mat) is described by the following parameter values: A = 1.4547, B = 0.0010039, C = 0.0030496, and E = 3.0576e-005. The interfacial oxide (stored as sio2_nt) is described by the same parameter values, except A = 1.6152.
Figure 14-181. Silicon dioxide index spectra from multiple sample analysis, shown for the bulk oxide (sio2_blk) and the interfacial oxide (sio2_nt).

Here are the best-fit parameter values for the silicon parametric semiconductor model (stored as si_msam.mat).

Figure 14-182. Best-fit parameter values for the silicon parametric semiconductor model, from multiple sample analysis of five thermal oxide films.

These parameter values yield the following optical constant spectra for the silicon substrates, shown with the literature spectra for comparison.

Figure 14-183. Silicon optical constants from multiple sample analysis (si_msam) and from the literature (p-si).

Note that our results are much closer to the literature values, as the use of the parametric semiconductor model (and the restriction that the silicon optical
constants be Kramers-Kronig consistent) has suppressed the parameter correlations sufficiently that we are able to obtain a unique solution.

To fine tune our solution, we can now bypass the parametric semiconductor model now that we have determined the oxide index spectra (bulk and interfacial) and all of the oxide thicknesses. Select ‘Edit Parm’s’ from the Fit window menubar, and click on the ‘Delete all Parm’s’ button to delete all of the currently defined fit parameters. Go to the first model, open the silicon substrate dialog box and define the optical constants ‘n’ and ‘k’ as fit parameters. We are now fitting directly for the silicon optical constants at each measured wavelength, with all other parameters in the model held fixed. Execute either a normal (slow) or point-by-point (much faster) fit. You should obtain the following optical constants (stored as si_msnk.mat), shown with the literature silicon optical constant spectra for comparison.

![Graph showing optical constants](image)

**Figure 14-184.** Silicon optical constant spectra from direct fit for fine tuning after the multiple sample analysis (si_msnk) and the literature (p-si).

**Further experiments**

1. Try fitting for all four interfacial oxide dispersion model parameters without coupling them to the bulk oxide and see what happens.
2. Try a Cauchy model rather than the 4-term user-defined dispersion model for the oxide layers. Do you get as good of results?
3. Try repeating the analysis with only the first four or first three films. Do you still get a unique solution?
4. Go through the five data sets and examine the difference between the best-fit calculated and experimental data. Do random errors dominate the differences, or are there still systematic trends in the difference plots. What physical effects in these samples could be lacking in our model?
Chapter 15 In Situ Dynamic Data Analysis and Examples

[Revised January 1, 2001 (version 3.343)]

This chapter describes how to analyze dynamic SE data acquired with an M-XX instrument. Although the principle is the same, the software will appear different for other instruments.

The WVASE® software incorporates all of the tools necessary to analyze in situ data and simultaneously determine average layer growth rates, film thicknesses, and optical constants. However, the analysis of in situ real-time data can be somewhat complex. Thus, one must carefully plan the experiment and break the analysis into smaller parts. Once a correct procedure is obtained, in situ SE can be a very simple and powerful technique.

This chapter is divided into six sections that cover all of the important details of using WVASE® for dynamic data analysis. The sections are as follows:

- Viewing The 'Raw' Data … How to select and interpret sections of the data that pertain to different aspects of the process.
- Basic Analysis Strategies … Guidelines of different basic analysis strategies. Covers analysis with known optical constants, linear growth modeling and multiple time-slice modeling.
- Creating Optical Constant Libraries … An important consideration for studying new materials or processes is the extraction and creation of new optical constant libraries.
- Special Data Acquisition Considerations … How to deal with the often encountered non-idealities of window effects and substrate wobble.
- In Situ Data Analysis Examples … Step through real examples of in situ analysis to develop the procedures and strategies.

15.1 Viewing The ‘Raw’ Data

To illustrate the immense amount of in situ SE data which can be acquired while monitoring a process in real-time, consider the 3D plot of the ellipsometric Psi
data vs. time and wavelength for a HgCdTe growth run shown in Figure 15.1. This plot shows only a 15 minute subset (out of a 4 hour growth run) of in situ SE data. To visualize how the spectroscopic ellipsometric data evolves throughout the growth run, it is useful to plot 2D ‘slices’ of the data set either as a function of time (at a few selected wavelengths) or wavelength (at a few selected times). The WVASE® software provides powerful capabilities for selecting and viewing the in situ SE data. Before proceeding with the analysis of real-time in situ SE data, it is necessary to discuss the techniques to select, manage, and display specific portions of the large ellipsometric data set.

Figure 15.1. 3D plot of in situ SE data during HgCdTe growth initiation.

The ‘Range Select’ command

Use the ‘Range Select’ command from the Experimental Data window to select data for graphing and fitting.

After the ellipsometric data from a growth run has been saved (the filename ‘extension’ for in situ ellipsometric data files is ‘.BDT’), it can be read into the ‘Experimental Data’ window of the WVASE® program using the File | Open Exp. File menu option. The Range Select command, which is found from the ‘Experimental Data’ window of the WVASE® program, is the basis for the manipulation and display of in situ SE data. Selecting the Range Select menu brings up the dialog box shown in Figure 15.2.
The Dynamic Data mode

The most important element of the dialog box in Figure 15.2 is the 'Spectroscopic mode enabled' checkbox which is found in the upper right-hand corner of the screen. When this box is not selected, the Dynamic Data mode is used to display the SE data. In the Dynamic mode, the data is plotted as a function of time. The time range (in minutes) of the data that will be plotted is specified in the 'Time:' section of the dialog box. When this box is selected, the Spectroscopic Data mode is used to display the data. Spectroscopic Data mode will be discussed in the next section.

To reduce the number of data points (time slices) to use for graphing and fitting, the user can specify the '# of data points to Skip'; that is, instead of plotting or fitting each data point within the specified time range (which corresponds to the default 'Skip' value of zero), every n\(^{th}\) data point can be displayed by setting the 'Skip' value equal to 'n' (for example, to select every other data point, set the 'Skip'=1).

The 'Selected Wavelengths' section of the 'Range Select' dialog allows the user to select the wavelengths to use for graphing and fitting the data. The 'For Data Fitting' and 'For Graphing Only' buttons allow for choosing the wavelengths used for fitting separately from those for graphing to allow easier viewing of the data.

The wavelengths for fitting or graphing can be chosen in one of two ways. The first way is to enter a range of wavelengths in the two text boxes (above the wavelength list) and then click on the Select Range button. The second way is to use the list of wavelengths displayed at the bottom of the 'Selected Wavelengths' section. To select wavelengths, click on the first desired wavelength, and then hold down the 'Ctrl' key while clicking the mouse on additional wavelengths. A range of wavelengths can be selected by holding down the mouse button and dragging the cursor over the desired wavelength range, or by holding down the 'Shift' key and clicking on the first and last wavelength in the desired range.

When graphing dynamic data, it is usually desirable to select only a handful of wavelengths (3-5) evenly distributed across the spectral range of interest. While
more wavelengths can certainly be selected (it is possible to select all measured wavelengths), this makes for a very cluttered graph which is difficult to read and interpret.

Clicking the ‘OK’ button on the ‘Range Select’ dialog box causes WVASE® to select the specified subset of ellipsometric data, and update the WVASE® ‘Graph’ window accordingly. Figure 15.3 shows a graph of the ellipsometric Psi data which resulted from the ‘Range Select’ specifications shown in Figure 15.2.

![Figure 15.3. SE Psi data at 3 wavelengths displayed in the ‘Dynamic’ mode.](image)

The Spectroscopic Data mode

The other display mode for SE data is the ‘Spectroscopic’ mode. In this mode, a spectrum of ellipsometric data vs. wavelength is displayed at a selected time (or times) during the growth run. Figure 15.4 shows a ‘Range Select’ dialog box which is set to the ‘Spectroscopic’ mode, by clicking the corresponding checkbox in the upper right corner of the screen.

![Figure 15.4. ‘Range Select’ dialog box with the ‘Spectroscopic’ mode selected.](image)

In this dialog box, the spectroscopic ‘timeslices’ to graph can be specified by entering a value in the ‘Time Slice (min.):’ box, and clicking on the ‘Add to list’ button. To remove timeslices from the list, simply highlight the desired timeslice.
and click on the ‘Delete’ button. All the defined timeslices can be removed by selecting the ‘Delete All’ button.

In Spectroscopic Data mode, the wavelengths specified for graphing are ignored. The wavelengths selected for fitting will be the wavelengths that are plotted. To specify which wavelengths will be plotted, click on the ‘For Data Fitting’ radio button, and highlight the desired wavelengths in the ‘Selected Wavelengths’ list box. In Figure 15.4, the 2 - 4 eV spectral range is specified. Clicking on the ‘OK’ button accepts the range select specifications and displays a ‘Spectroscopic’ mode plot in the WVASE® ‘Graph’ window (Figure 15.5). In this graph, spectroscopic data at two times (t=13.72 min. and t=24.94 min.) are displayed.

![Figure 15.5. 'Spectroscopic' mode graph with two timeslices of SE data.](image)

**Data Selection Shortcuts**

There is another very useful way to define spectroscopic timeslices. Start by selecting a time range of data, using the ‘Dynamic’ mode. To define a timeslice, go to the WVASE® ‘Graph’ window, and right-click the mouse button at the desired ‘x’ position in time. A vertical line will appear on the graph to represent the location of the timeslice, as shown in Figure 15.6. To specify additional timeslices, hold down the ‘Shift’ key while right-clicking the mouse at the desired times. To quickly toggle between Dynamic and Spectroscopic modes without bringing up the Range Select dialog box, simply double click the mouse anywhere inside the ‘Experimental Data’ window.

![Figure 15.6. Defining Spectroscopic timeslices in the Dynamic Data mode.](image)
Which parameters to plot?

Using the techniques described thus far, different time and wavelength ranges can be selected and plotted in both Dynamic and Spectroscopic modes. The next question is: for a given time/wavelength range which parameter type is most useful to plot? The ‘Type’ menu option from the WVASE® Graph window is used to select the ellipsometric parameter (or derived quantity) to plot. The choices include: Psi, Delta, Tan(Psi), Cos(Delta), <e1>, <e2>, <n>, <k>, Re(rho), and Im(rho). The ‘< >’ Pseudo dielectric and optical constants and the complex ‘rho' parameters are defined in the short course chapter.

Which data type to plot is largely a matter of personal preference, but the general guideline is to plot the parameter which appears to have the most sensitivity to the current sample property of interest. For example, it may be useful to monitor the ellipsometric Delta parameter during oxide desorption (as this parameter is more sensitive to the existence of thin overlayers), and the ellipsometric Psi parameter during sample heating. During growth of thick semiconductor layers, it may be useful to view the Pseudo dielectric function parameters (for example, <e2>), as the composition of the layer is directly related to shifts in the critical point structure of its dielectric function. During most of the growth, the layer is optically thick and can be considered as a bulk material, such that the Pseudo dielectric function parameters derived from the ellipsometric Psi and Delta data are equal to the dielectric function of the growing layer.

When viewing the SE data, it may be helpful to switch between the different data types, especially when a data analysis is being performed. It is important that an analysis model fit both the ellipsometric Psi and Delta data (or correspondingly, <e1> and <e2>). The Style | 2D menu option in the WVASE® ‘Graph’ window brings up a dialog box which will allow the user to specify a ‘Double Y axis’ graph. This graph style, which is shown in Figure 15.7, provides a concise way to visualize and present spectroscopic timeslices of SE data along with the model analysis results.

![Figure 15.7. Double Y axis plot of SE data with Model Fit.](image)

Ellipsometric Anatomy of a HgCdTe Growth Run

Now, we will consider data from a HgCdTe growth run as an example of what can be learned by just viewing the raw ellipsometric data. The growth run data is shown in Figure 15.8. For clarity, only two wavelengths are shown on this graph. Each wavelength, 2.83 eV and 1.63 eV, is more sensitive to different aspects of the growth process. The main phases of the process are labeled on the graph:
1. The CdZnTe substrate is heated to 340° C and held at this temperature for 10 minutes to remove the oxide overlayer from the surface. The ellipsometric data is sensitive to both the temperature of the sample and the overlayer thickness. By observing when the raw data near the end of this phase become constant, it is possible to determine when the substrate temperature and surface morphology are stable.

2. The CdZnTe substrate is cooled to 180° C in preparation for the HgCdTe growth. Once again, the raw ellipsometric signal can be used as an excellent indicator of the relative substrate temperature stability.

3. The growth of the HgCdTe layer is initiated at the beginning of this phase. The oscillations which are observed in the data (especially at the longer wavelength) are due to constructive and destructive interference in the light beam reflected from the sample. At the shorter wavelength, which is more optically absorbing, the oscillation is damped out fairly quickly. Once the film reaches a critical thickness, light can no longer penetrate the depth of the film, and the oscillations are no longer observed (within a given spectral range). For that spectral range, the film can be considered ‘optically thick’, and from a data modeling standpoint it can be considered like a bulk substrate. From the constant nature of the raw ellipsometric signals in the optically thick regime, one can imply that the HgCdTe composition must also be relatively constant through the layer growth.

![Experimental Data](image)

*Figure 15.8. Raw real-time in situ ellipsometric data during HgCdTe growth run.*

It is also informative to view a few spectroscopic timeslices of data at different phases of the growth. For example, Figure 15.9 shows the Pseudo <e2> function of the CdZnTe substrate measured during the cool down transition between phases 1 and 2. The critical point structure near 3.2 and 3.8 eV sharpens and shifts to higher energies as the substrate cools. This behavior in the optical constants vs. temperature is typical for most semiconductor materials.
Figure 15.9. Timeslices of Pseudo $e_2$ data for CdZnTe substrate during cool down.

Figure 15.10 shows a number of spectroscopic timeslices chosen at the end of phase 3 where the HgCdTe layer was optically thick. On this scale, all of the data lie on top of each other, indicating that the composition and surface morphology of the HgCdTe layer must be reasonably constant during this 4 hour portion of the growth.

Figure 15.10. Spectroscopic timeslices during optically thick region of HgCdTe growth.

15.2SE Analysis Tools

Specialty Layer Types for In Situ Analysis

This section reviews the main layer types for in situ data analysis with a description of general usage. The layers described include Delay, Virtual, FastDyn, and SemiGrow layers.

Using the Delay Layer

The Delay layer is used with dynamic data to model a period of time when SE data was acquired but nothing happened to the sample.

The Delay layer is used in a model to specify a period of time when nothing is happening in a process. Figure 15.11 shows a view of the Delay layer dialog. This layer has one parameter, a ‘Delay Time’, which specifies the amount of time to delay. This layer can be used when data is acquired for some amount of time before a process starts. When analyzing the data, the delay time is set to match the time that the ellipsometer was taking data before the process began. The delay layer can also be used in the middle of a growth cycle, if there is a delay between the deposition of multiple layers. In this case the delay layer would be introduced on top of the first layer and beneath the second layer.
**The Virtual Interface Approach**

This section describes the Virtual Interface approximation which is used in the Virtual, FastDyn, and SemiGrow layers.

As a sample structure becomes more complicated, it becomes increasingly difficult to accurately model all of the layers. Small errors in the underlying film thicknesses or optical constants can upset the data analysis of the current layer growth on the surface. To simplify the data analysis, the ‘Virtual Interface’ approximation is employed, as is schematically represented in Figure 15.12.

**Actual Sample:**

<table>
<thead>
<tr>
<th>layer #4</th>
<th>‘Virtual Interface’</th>
<th>layer #4</th>
</tr>
</thead>
<tbody>
<tr>
<td>layer #3</td>
<td></td>
<td>layer #3</td>
</tr>
<tr>
<td>layer #2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>layer #1</td>
<td></td>
<td>‘pseudo substrate’</td>
</tr>
<tr>
<td>substrate</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Simplified Optical Model:**

In the ‘Virtual Interface’ (VI) approximation, the previous growth history of a sample is encapsulated into a single ‘pseudo substrate’. This ‘pseudo substrate’ can be defined anywhere within the sample, and does not have to correspond to an actual interface in the structure, hence the term ‘Virtual’ interface. For example, to determine the 21st layer thickness which is being grown on top of a 20 layer stack, a virtual interface could be inserted, or ‘dropped’, after the growth of the 20th layer, and a simple optical model consisting of the ‘pseudo substrate’ defined at the virtual interface with a single layer could be used to extract the top layer thickness. This is certainly much easier than building a 21 layer optical model and fitting only for the top layer thickness. Any errors in the layer thicknesses and/or optical constants of the bottom 20 layers could directly propagate into errors in the top layer thickness.

The optical constants for the ‘pseudo substrate’ are found by directly transforming the Psi and Delta values measured at the growth time corresponding to the position of the virtual interface. For semiconductor structures, the ‘pseudo substrate’ optical constants obtained in this manner can accurately encapsulate the optical behavior of all previously grown layers. The VI approximation is nearly exact when all of the materials in a layer stack have high and relatively similar indices of refraction (such as compound semiconductor structures). However, the approximation completely breaks down for lower index materials (such as multilayer dielectric film stacks). The accuracy of the VI approximation can be numerically verified by performing multi-layer model simulations in the WVASE® software.

In the WVASE® analysis software, there are three ways to define a virtual interface for use in modeling dynamic SE data. The first approach is to build a

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Figure 15.11. The Delay Layer dialog. The delay layer is used to specify a time during a process where nothing is happening.

Figure 15.12. Schematic of the ‘Virtual Interface’ approximation.

The virtual interface method works well for semiconductors and metals but doesn’t work at all for multilayer dielectrics.
model using the ‘VIRTUAL.MAT’ layer as the substrate combined with a ‘DELAY.MAT’ layer to specify when the layer growth begins. This approach, while still supported in WVASE, has been supplanted by the ‘FASTDYN.MAT’ and SEMIGROW.MAT dynamic data analysis layers. In addition to more conveniently implementing the virtual interface approximation, the FastDyn and SemiGrow layers provide highly optimized routines for modeling in real-time the growth of semiconductor layers. They are each described in detail in this section of the manual.

**Using the Virtual Layer**

The Virtual layer can be used as a substrate when fitting dynamic data to greatly simplify the model building process. It uses the virtual interface approximation described above and is only valid when working with high index, absorbing materials such as semiconductors or metals.

Figure 15.13 shows an example of the Virtual layer dialog. The most important aspect of using this layer is specifying the location of the virtual interface. The most common way to use this layer is by specifying a fixed time where the interface occurs. To do this you select the ‘Fixed at time’ option and specify the time the interface is to occur. The ‘# of pts. to average’ text box specifies the number of data points to average (going backward from the fixed time value) when extracting the virtual interface parameters. The other option for indicating the interface location, ‘Running separation’, uses an interface that moves as the data is analyzed. In this mode the interface is always a certain number of points (specified in the dialog box) behind the current point being fit. This is useful for getting information from the ‘near surface’ region of the growing film, although it is probably better to use the FastDyn or SemiGrow layers for extracting near surface information if possible. The ‘Don’t try both branches’ box specifies that the software should try both mathematical branches when extracting the virtual interface parameters. This box should NOT be selected when a rotating compensator instrument is used (M-2000®) but should be selected when a rotating analyzer instrument (M-44® or M-88®) is used since these cannot measure the handedness of the Delta parameter.

![Virtual Interface dialog](image)

**Using the FastDyn Layer**

The FastDyn layer is a specialized layer for analyzing in situ data using the virtual interface approximation. It was designed specifically for semiconductor applications but can be used for any application where the virtual interface...
approximation can be applied. The main advantage of the FastDyn algorithm is that it can extract the optimum composition, temperature, and/or layer growth rate which provides the best fit to all of the available dynamic SE data. To optimize the fit sensitivity to specific parameters such as composition, it is certainly possible to use restricted spectral and time ranges of ellipsometric data in the FastDyn analysis. This can further reduce the calculation time of the algorithm, such that sample parameters with excellent precision can be extracted in less than 1 second. This time is less than the SE data acquisition time in most growth environments, and is completely adequate for real-time monitoring and control in most semiconductor growth applications.

The layer dialog box for the WVASE® ‘FastDyn’ layer is shown in Figure 15.14. To use this layer in WVASE®, build a model where ‘FASTDYN.MAT’ is the substrate, and the layer on top of the substrate specifies the optical constants of the growing film (the top line in the ‘FastDyn’ dialog box displays the name of this file for reference), as shown in Figure 15.15. The thickness of the top layer is not used in the FastDyn analysis algorithm.

Figure 15.14. Dialog box for the WVASE® FastDyn analysis layer.

![Figure 15.14](image)

Figure 15.15. WVASE® model for using the FastDyn analysis layer.

While the appearance of Figure 15.14 is daunting, using the FastDyn layer to analyze dynamic SE data is fairly straightforward. The first step in performing a FastDyn analysis is to specify which data will be used in the fit. This specification is done using a combination of the WVASE® ‘Experimental’ window’s Range Select menu option (see Figure 15.2), and the FastDyn layer dialog box itself. Since the FastDyn analysis is geared exclusively towards dynamic data, it is important to disable the ‘Spectroscopic mode’ checkbox in the Range Select dialog box.

The other important things to specify in the Range Select dialog box are the time range for the selected data, and the wavelength ranges for fitting and graphing the data. When fitting layer optical constants, all of the available wavelengths are usually selected ‘For Data Fitting’. When using an existing optical constant library, it is common to select a wavelength range which has the highest sensitivity to the parameter of interest (for example, the 1.8 - 3.4 eV spectral range is more sensitive to HgCdTe composition). When selecting the ‘For Graphing Only’ wavelengths, it
is best to highlight a few discrete wavelengths evenly spaced across the fitting wavelength range. Next, specify the time range which contains the subset of dynamic data to be analyzed.

When analyzing layer growth, it is important to consider the possibility of non-uniform growth rates and/or composition. Since FastDyn assumes constant layer growth rate and optical constants, any variation in these values during the time period of the analysis will degrade the fit. This is not really a limitation of FastDyn, it simply suggests a smaller time range of data should be selected for the analysis. In fact, performing the analysis with different time ranges is a good way to verify the layer growth uniformity.

NOTE: When selecting a time range for extracting optical constants, it is especially important to stay away from the growth initiation interfaces, as K-cell flux transients, interface mixing, and/or surface roughening, which can occur at these interfaces can degrade the FastDyn fit and corrupt resulting optical constants and growth rates.

The FastDyn analysis layer adds another level of data selection on top of the basic time and spectral ranges specified in the Range Select dialog box; these options are found in the ‘Experimental Data for Fit’ section of the FastDyn dialog box. The most important value in this section is the ‘# of Data Points for Fit’ entry. This number specifies the maximum number of timeslices of SE data that will be used in the analysis (keep in mind that even though the dynamic data is displayed at only a few wavelengths, all of the selected wavelengths are still used for fitting). The distribution of the timeslices with respect to the selected experimental data set is determined by highlighting the appropriate button (Figure 15.16 graphically illustrates the different FastDyn data selection criteria):

- **Entire Layer**: The timeslices are equally distributed across the selected experimental data range. This is useful for modeling the growth of an entire layer (Figure 15.16a).
- **Near Surface**: The timeslices are consecutively chosen at the end of the selected time range. In this manner, the data for the analysis comes only from the ‘Near Surface’ of the growing layer (Figure 15.16b).
- **Layer End Points**: In this mode, half of the data points are consecutively chosen starting at the beginning of the selected time range, and the other half are chosen at the end of the time range. This may be useful when the growth rate is not constant throughout the whole layer (Figure 15.16c).
- **Surface + Layer**: FastDyn will perform two separate data fits in each analysis. In the first fit it uses two data points, one at the layer start and one at the most recent data point, and extracts the film thickness. In the second fit, a Near Surface analysis is performed using the growth rate calculated from the result of the first fit. If the ‘Average Composition’ box is checked, FastDyn will also return the average composition value from the ‘Entire Layer’ fit. This mode is very useful for extracting both the near surface composition and the film thickness.

NOTE: At the first timeslice in the selected data set, a virtual interface is implicitly defined and calculated by the FastDyn analysis algorithm.
Figure 15.16. FastDyn data selection modes, with the ‘# of Data Points for Fit:’ = 10: (a) entire layer mode, (b) near surface mode and (c) layer end points mode.

The ‘Selection Start Time (min):’ entry can override the time range of the dynamic data which is defined using the Range Select command. If this entry is set to a time greater than the starting time of the displayed dynamic data, only data points with times greater than (or equal to) the ‘Selection Start Time’ will be used in the FastDyn fit. If the ‘Selection Start Time’ is less than the starting time of the displayed data, the entry is not used by FastDyn. This allows the user to view a larger portion of the dynamic data set (by setting the Range Select appropriately), while FastDyn analyzes a desired subset of the displayed data.

The ‘Layer Start Time (min):’ and ‘Layer End Time (min):’ specify the starting and ending times for the layer growth. If the layer is growing throughout the duration of the specified experimental time range, leave these entries at their defaults.
values of ‘0’ and ‘9999’ respectively. These options are useful for precisely quantifying the thickness of a grown layer, and should be used with the FastDyn ‘Entire Layer’ mode. The ‘Calculated Thickness (Å)’ entry is calculated by multiplying the FastDyn determined growth rate by the difference between the Start and End layer times (or the last time in the selected experimental data range and the Start time, if the End Time is not within the selected range). This thickness is a parameter which is derived from the growth rate fit; however, for the purposes of reporting this value to the user and/or other external programs, it can also be defined as a pseudo fit parameter by checking the adjacent box. FastDyn assumes that the material interfaces at the beginning and end of the layer growth are abrupt and ideal. Figure 15.14 illustrates the use of these entries on a typical ellipsometric layer growth trajectory. These parameters can also be defined as fit parameters, such that FastDyn can accurately determine the layer growth starting and ending times by fitting to the experimental data.

Figure 15.17. FastDyn settings to describe the growth of a layer.

<table>
<thead>
<tr>
<th>Fit Parameters</th>
<th>Name</th>
<th>Value</th>
<th>Fit min. thick (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Growth Rate</td>
<td>4</td>
<td></td>
<td>0</td>
</tr>
<tr>
<td>Composition</td>
<td></td>
<td></td>
<td>0</td>
</tr>
<tr>
<td>Angle</td>
<td>75.61</td>
<td></td>
<td>0</td>
</tr>
</tbody>
</table>

Figure 15.18. The Fit Parameters section of the FastDyn dialog box.

The ‘Fit Parameters’ section of the FastDyn layer dialog box (Figure 15.18) defines which layer parameters will be fit during the FastDyn analysis. Starting values for the Growth Rate, Composition (if the material file specified for layer #1 is an ALLOY or ALLOY-TEMP file), and Angle (of incidence) can be entered in the corresponding boxes, and fit parameters can be defined by clicking on the adjacent boxes. The ‘min. thick (Å)’ boxes specify the minimum layer thickness which is required before FastDyn will actually fit the parameter. For example, if the layer is too thin, there will not be much sensitivity to the composition of the layer, such that fitting the composition may not provide acceptable accuracy (or even worse, it may cause the composition parameter to wander off to an unphysical value which prevents the fit from converging to the correct value in subsequent fits). If the ‘min. thick (Å)’ value is set to 100, the composition will actually ‘fit’ only when the layer thickness (as calculated by the previous FastDyn analysis) exceeds 100Å.
The ‘Fit Specifications’ section (Figure 15.19) determines how the L-M regression algorithm operates for the FastDyn analysis of the data. The ‘Max # of fit Iterations’ specifies how many iterations the L-M algorithm will perform before returning the fit results. When fitting dynamic data, the starting parameter values are usually close to the final best fit values. This means that a lower number for the ‘Max Iterations’ (in the 4 - 10 range) is usually acceptable. Lower numbers also reduce the FastDyn analysis time. The ‘Min. # of points for fit’ number works in a manner similar to the ‘min. thick’ settings found in the ‘Fit Parameters’ section: FastDyn will not actually perform a fit until the number of selected timeslices equals or exceeds the ‘Min. # of points for fit’ value. This is very helpful when analyzing dynamic data in real-time. An appropriate FastDyn model can be built, and the fit can be started at the same time the layer growth is initiated. The FastDyn analysis will not begin fitting the data until sufficient information exists to robustly extract the desired parameters (i.e., the ‘Min. # of points’ are available, and the ‘min. thick’ has been reached). The ‘Fit Virtual Interface Parm’s checkbox can be used to define the pseudo substrate optical constants as fitting parameters. This slightly increases the FastDyn analysis time, but it can increase the accuracy of the fit somewhat by minimizing the effect of noise in the experimental Psi and Delta data on the virtual interface calculation. When the ‘Fill Gen. Data Window’ box is checked, FastDyn will fill the WVASE® ‘Generated Data’ window with ellipsometric data calculated from the best fit model. This data is subsequently displayed in the ‘Graph’ window, where the quality of the FastDyn fit can be visually inspected. Normally this option is left on, but it can be turned off to slightly reduce the FastDyn analysis time.

**Extracting Optical Constants with FastDyn**

As an demonstration of using FastDyn to extract layer optical constants, the FastDyn analysis algorithm will now be used to extract optical constants of the layers grown in a MCT / HgTe structure. Before proceeding, it is important to verify that the WVASE® software has enough memory allocated to perform the analysis. In the WVASE® Global | Defaults menu option, click on the ‘Memory Allocation’ button. The resulting dialog box in Figure 15.20 shows the appropriate memory allocation values which should be used for the FastDyn analysis of optical constants with data acquired by an M-88® system.

**Figure 15.20. Typical ‘Memory Allocation’ settings for FastDyn optical constant analysis of in situ data taken at 88 wavelengths.**
The general strategy when extracting optical constants for a growing layer is to start with an optical constant file which is fairly similar to the growing material. Fixing the growth rate at its nominal value, the optical constants are first fit over a very limited time range. The time range of dynamic data is then incrementally increased in subsequent fits, and the growth rate is also added as a fit parameter. Finally, the selected time range is set to include most of the dynamic data acquired during the layer growth, and the resulting FastDyn analysis (in which the virtual interface parameters are also fit) returns the best optical constants and growth rate which represent the entire grown layer. This procedure helps the L-M regression algorithm ‘lock on’ to the correct branch for the optical constants. If you try to start the FastDyn optical constant fit using the full layer growth time range with even slightly wrong starting optical constants or growth rate, the L-M algorithm will probably ‘get lost’ and return a poor data fit and unphysical optical constant values.

In this example, the 3rd MCT layer in a multilayer stack is being investigated. A step-by-step procedure for extracting the optical constants of this layer is as follows:

1. **Range Select** a small time range of data near (but not too close to) the beginning of the layer growth, in this example $t = 110 - 112$ minutes. Build a WVASE® model as shown in Figure 15.15, and set up the FastDyn parameters as shown in Figure 15.14. The ‘hgte’ optical constant file is from the standard WVASE® optical constant library, and contains room temperature HgTe optical constants. These will serve as ‘reasonable’ starting values for the growth temperature optical constants of the MCT layer. To define the optical constants of the growing layer as fitting parameters, click on the ‘n’ and ‘k’ boxes in the ‘Opt Const Fit’ section of the ‘hgte’ layer dialog box. In the FastDyn layer, the growth rate is fixed at a nominal value of 4 Å/second. The Angle of incidence is fixed at a value of 75.61° (which was determined by a substrate data fit), and held fixed throughout the subsequent optical constants analysis. Using these settings, perform a Normal Fit in the WVASE® ‘Fit’ window.

2. Next, extend the selected time range to $t = 110 - 115$ minutes. Add the FastDyn Growth Rate as a fit parameter, and again perform a Normal Fit.

3. Finally, select the $t = 110 - 130$ time range. Add the ‘Virtual interface’ parameters to the fit by selecting ‘Fit Virtual Interface Parms’ in the FastDyn dialog box, and perform a Normal Fit. The resulting data fit is shown in Figure 15.21, and the extracted optical constants from the fit are shown in Figure 15.22. The growth rate from this fit was $3.7905 \pm 0.00609$ Å/second.

![Figure 15.21. Data fit from FastDyn analysis of MCT layer growth.](image)
Figure 15.22. MCT optical constants from FastDyn analysis of layer growth.

After successfully completing the above procedure, the optical constants can be saved, and the procedure repeated for another film in the multi-layer MCT / HgTe structure.

A close examination of Figure 15.21 reveals that the fit is not perfect near the starting time. This effect is likely due to non-uniformity in the initial layer growth rate and/or composition.

Using the SemiGrow Layer

The SemiGrow layer implements the virtual interface model and is used to fit data in real time. This layer is easier to setup than the FastDyn layer but can not be used for extracting optical constants.

SemiGrow is the newest layer added to WVASE® for supporting dynamic data analysis. It was developed for use in real-time process monitoring and control, but can also be used to analyze data after all of the data has been acquired. It’s primary purpose is to satisfy the following objectives:

- Provide useful composition values as early as possible during the initial growth of a layer.
- Report accurate thickness values, over the complete range of possible layer thicknesses (10Å – 1µm).
- Constrain the reported SE parameters to always be physical, i.e., near their nominal values during the initial part of growth.
- Make the analysis easier to set up and test.

The SemiGrow layer essentially implements the ‘Surface+Layer’ functionality of the FastDyn layer, but with many of the complex FastDyn settings either eliminated or internally fixed at optimum values. To use the ‘SemiGrow’ analysis in WVASE® build a model with a ‘SemiGrow’ layer as the substrate and add an optical constant file for the growing material as layer #1 in the model. Do not add a surface roughness layer as you would when using FastDyn. The SemiGrow layer dialog is shown in Figure 15.23. There are two main sections on the SemiGrow dialog box: one for Layer Thickness analysis, and the other for Near Surface analysis.
In Situ Dynamic Data Analysis

Figure 15.23. The SemiGrow Layer dialog. The SemiGrow layer implements the virtual interface model and is used to fit data in real time. This layer is easier to setup than the FastDyn layer but cannot be used for extracting optical constants.

For the Layer Thickness Analysis, a virtual interface (VI) is dropped near the layer start time. The ‘Layer Start Time’ entry should contain the exact time (in minutes) that the layer growth was initiated. The most recent SE data time slice is then fit to extract the film thickness which has been grown on the virtual interface.

The ‘Relative VI Location’ entry specifies the location of the VI relative to the layer start time. This accounts for the fact that, in general, the layer start time will not precisely coincide with an SE data acquisition point. For a layer growth which is preceded by a soak, the Relative VI Location should be slightly negative, such that the VI is guaranteed to precede the film growth. For cases in which multiple layers are grown without an intervening soak, or in which interfacial layers degrade the SE data fit, the Relative VI Location should be positive to avoid fitting data which would corrupt the SE analysis. In this case, SemiGrow will automatically ‘fix up’ the thickness to account for the VI not coinciding with the layer start time; this is done by multiplying the average layer growth rate times the difference between the VI time and the layer start time, and adding this value to the thickness determined from the VI fit.

When the current layer thickness exceeds the ‘Max. fittable thickness’ value, no fit to the SE data is performed. Instead, the most recent layer growth rate is used to linearly extrapolate the layer thickness. In this manner, SemiGrow can automatically provide reasonable thickness values to a growth supervisor program over the entire range of film thickness.

The two SemiGrow analysis sections are basically independent. You can fit only for the thickness, only for near surface fit parameters, or fit for both simultaneously. The only coupling that SemiGrow introduces between the fit sections (when fitting for both simultaneously) is that the last ‘n’ thickness values are fit to a line to determine the growth rate for the Near Surface analysis (‘n’ is set by the ‘# of thickness points used to determine rate.’ entry). If the thickness is not fit, then it is important to seed the Growth Rate appropriately, as the Near Surface Analysis uses this value in the fit. The Near Surface Analysis utilizes the most recent four SE timeslices: the ‘n-3’ and ‘n-2’ timeslices are averaged to define the...
VI, and the ‘n-1’ and ‘n-0’ timeslices are averaged and subsequently fit for by the regression analysis. Surface roughness is optically modeled as a 50% Bruggeman EMA mixture of the growing layer optical constants with void.

The ‘Filter Value’ settings in the Near Surface Analysis section are used to constrain the parameter values during the regression fit. This minimizes the correlation in the angle, roughness, and composition parameters which can occur during the initial stages of growth. Resulting in unphysical parameter values. This constraint is implemented by adding terms to the Chi-Square error function which is minimized in the regression analysis. These terms make it unfavorable for a parameter to stray too far from its previous value. The amount by which a fit parameter is ‘constrained’ is determined by the ‘Filter’ values. A smaller Filter value enforces a stronger constraining. Separate Filter values allows for some parameters to be more heavily constrained than others. By carefully tuning the Filter values, an acceptable compromise can be obtained between the stability and time response of the analysis.

## 15.3 Basic Analysis Strategies

In this section basic strategies for analyzing *in situ* data will be discussed. These strategies include using previously determined optical constants as well as extracting optical constants using constant growth rate modeling or multiple time slice modeling. *WVASE* generated data will be used to demonstrate these techniques in a tutorial fashion and then real-world examples can be found in the ‘In situ Data Analysis Examples’ section later in this chapter.

An example of Ni deposition onto Si will be used to demonstrate the strategies. In this example, ~150Å of Ni is deposited onto a ~1000Å SiO2/Si Substrate.

### Determination of Fit Parameters Using Known Optical Constants

The data for this example can be found in the \WVASE\Examples directory under the file name ‘Ni on Si #1.bdt’

In this example the optical constants of all layers are known. The parameters to determine are the thickness of the oxide on the silicon substrate and the thickness of the Ni film as it grows. It is also necessary to determine the angle of incidence since it is difficult to precisely know it in an *in situ* environment. Open the file ‘Ni on Si #1.bdt’ in the \WVASE\Examples subdirectory to follow along. The Psi and Delta data at selected wavelengths versus time are shown in Figures 14.24. The Ni film growth starts at 1.0 minutes after data acquisition is started and ends at approximately 3.48 minutes after acquisition was started.

![Figure 15.24. Ellipsometric (a) psi and (b) delta data acquired during the growth of a Ni film on SiO2/Si. Only data at three selected wavelengths are shown.](image-url)
First, model the substrate before the deposition is started. The substrate for this sample is ~1000 Å SiO₂ on Si. Build the Model shown in Figure 15.25 which represents this sample and set the oxide thickness and angle of incidence as fitting parameters.

![Figure 15.25. Model used to analyze the ellipsometric data acquired before the Ni film growth starts.](image)

Second, select a time slice before the beginning of the deposition (between 0.0 min. and 1.0 min.) and switch the view to spectroscopic mode. The graph window should look similar to Figure 15.26. Perform a normal fit. The results should be 1006Å for the SiO₂ layer thickness and 75° for the angle.

![Figure 15.26. Data fit for the substrate before film growth (spectroscopic mode shown for a timeslice at 0.60 minutes).](image)

Now that the model for the substrate is well defined, it is time to add the nickel layer to the model. The ‘Ni.mat’ material file is located in the Metals material directory which is accessible from the ‘Add Layer’ dialog. The model should now look like Figure 15.27. Set the Ni thickness as a fit parameter bringing the total number of fit parameters to three: SiO₂ thickness, Angle, and Ni thickness. At this time, switch back to the dynamic data mode by double-clicking the left mouse button in the experimental data window. The graph window should again look similar to Figure 15.24.

![Figure 15.27. Model for Ni growth using the fit results (SiO₂ = 1006Å) from the pre-deposition analysis and known Ni optical constants.](image)

Now perform a point-by-point fit to determine the parameters throughout the entire growth run. The fit should be very good since this is generated data. The final thickness for the nickel layer should be near 150Å. Any of the parameters can be viewed versus time in the Graph window by choosing the parameter of interest from the Data|Point by Point Fit Parms’ dialog. For example, the graph of parameter Thick.2 should look like Figure 15.28.
Determination of Fit Parameters and Optical Constants Assuming Linear Growth Rate

The data for this example can be found in the WVASE\textregistered\Examples directory under the file name 'ni on si \#2.bdt'. In this example the parameters of interest are the optical constants of the Ni film and the final thickness of the nickel film. Open the file 'ni on si \#2.bdt'. The structure of the sample for this example is the same as the previous example except the Ni optical constants used to generate the data were modified so the previous approach to fitting will not work. This is an very good technique to learn as many materials (especially metals) often vary with deposition process. Try the approach in the previous section to verify this. The fit results should look similar to Figure 15.29.

![Graph of Fit Parameter Thick.2 vs Time in Minutes](image1)

Figure 15.28. Point-by-point fit results for the Nickel layer thickness.

![Graphs of Psi and Delta data for Nickel film growth](image2)

Figure 15.29. (a) Psi and (b) Delta data for the second example of Nickel film growth along with fit curves from using "known" optical constants.
To start this example, build the model shown in Figure 15.30. Set the SiO$_2$ film thickness, Ni film thickness, n, and k; and angle of incidence as fit parameters. This model is different then in the previous section because of the addition of a delay layer. The delay layer indicates there is a period of time in the data where nothing is happening. In this case it represents the time before the deposition is started.

### Figure 15.30. Model used for constant growth rate analysis of the Nickel deposition for example.

When assuming a linear growth rate, the WVASE$^\text{®}$ software assumes that every layer except the substrate is grown in turn. In this case it expects to first see an SiO$_2$ layer deposited onto the silicon substrate, then a 1.0 minute delay, and then deposition of the ni film. This obviously is not correct since the SiO$_2$ layer is present initially. In order to make this model correct, the growth rate for the SiO$_2$ layer will be set to a very large number. To set the growth rates, activate the Model window and select the ‘Growth’ menu item. Set the SiO$_2$ growth rate to 1000000. Leave the Ni growth rate set to 1 but set it as a fitting parameter. The growth rate dialog should look like figure 15.31.

### Figure 15.31. Growth rate dialog box. The SiO$_2$ growth rate is set to a high number because it is initially thick and not actually deposited during this analysis. This tricks the software into seeing its total thickness immediately.

Close the Layer Growth Rates dialog and generate data. The psi graph should look similar to Figure 15.32.

### Figure 15.32. Initial match to the experimental data before fitting.

Perform a normal fit. When the fit is finished the MSE should be close to 1.16 and the generated and experimental data curves should be nearly identical. The
values of the fit parameters should be the same as in the previous section except that the optical constants are now fit to the modified values used to create this data. Save the new nickel optical constants (with a unique file name).

### Determination of Parameters Using the Multiple Time Slice Model

The data for this example can be found in the WVASE® Examples directory under the file name 'ni on si #2.bdt'.

The multiple time slice model is an advanced modeling feature of the WVASE® software. In principle it is very similar to the multiple sample analysis technique discussed in the ‘VASE Data Analysis’ chapter except it is performed on a set of dynamic data time slices. The time slices are selected just as they were in the ‘Viewing the Raw Data’ section of this chapter. The same data file used in the last example will be used in this one and we will determine the same parameters.

Start by building the model shown in Figure 15.33. Set the nickel thickness, n and k, the SiO₂ thickness, and angle of incidence as fitting parameters. Then select eight time slices at positions similar to those shown in Figure 15.34. As described in a previous section, this is accomplished by clicking the right mouse button on the graph in multiple positions with the shift key held down. Next, switch to spectroscopic mode. The graph should look similar to Figure 15.35, showing the spectroscopic time slices at different points throughout the film growth.

![Figure 15.33. Model for multiple time-slice analysis of the nickel growth example.](image)

![Figure 15.34. Experimental data for Nickel growth shown in dynamic mode with multiple time slices selected (shown as vertical lines).](image)

![Figure 15.35. Experimental data for multiple time slices shown in spectroscopic mode.](image)
Click the right mouse button in the model window. This will bring up the ‘Multi-Model for Dynamic Analysis’ dialog (If this does not work, make sure you are in spectroscopic data mode and try again). This is where the relationships between the fit parameters for each time slice are established. The time slices are represented by rows and the fit parameters (except for the optical constants) are represented in columns. In this example, the angle of incidence and the thickness of the SiO$_2$ layer (Thick.1) are the same for all of the timeslices (see Figure 15.36). Checking the box at the top right of a given fit parameter forces the value of that parameters to be the same for all slices. This was done for Thick.1 and Angle0 to ‘couple’ the parameters for the time slices. The Ni thickness is the only parameter that is different for all time slices. Leaving the box at the right of the Thick.2 parameter unchecked indicates that a separate thickness is to be found for each time slice. The numbers in each box represent initial guesses and the check boxes indicate whether to fit the parameter. Setup the dialog so it looks like the one shown in Figure 15.36.

Right clicking the mouse on the model window when multiple time slices are selected and spectroscopic mode is active will bring up the Multi-Model dialog box.

Perform a normal fit. The fit should be nearly perfect. The resulting MSE for the given time slice selections is 1.19. The parameter values are shown in Table 14.1. Save the optical constants using a unique file name and compare the results with the previous example.

Table 15.1: Results for thickness from each time slice

<table>
<thead>
<tr>
<th>Parameter: Slice #</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thick.2:2</td>
<td>19.006±0.00914</td>
</tr>
<tr>
<td>Thick.2:3</td>
<td>40.002±0.0163</td>
</tr>
<tr>
<td>Thick.2:4</td>
<td>60.008±0.022</td>
</tr>
<tr>
<td>Thick.2:5</td>
<td>80.006±0.0273</td>
</tr>
<tr>
<td>Thick.2:6</td>
<td>100.01±0.0328</td>
</tr>
<tr>
<td>Thick.2:7</td>
<td>116.01±0.0379</td>
</tr>
<tr>
<td>Thick.2:8</td>
<td>133.02±0.0448</td>
</tr>
</tbody>
</table>
Creating Optical Constant Libraries

This section is mostly relevant toward in situ SE monitoring of epitaxial semiconductor growth.

In this section, systematic approaches are outlined for acquiring the optical constant libraries needed to perform real-time analysis of SE data. The methods discussed will show the user how to build a temperature dependant optical constant library for a substrate and composition dependant library for a film. To illustrate these approaches, the building of a temperature dependent library for the CdZnTe substrate is described, and a composition dependent library for HgCdTe under growth conditions is described. However, the methodology which was used to obtain these optical constant libraries is quite general and can be directly applied to the in situ SE monitoring of most epitaxial semiconductor growth applications.

Theoretical Considerations

The term ‘optical constant’ implies that this quantity is an invariant and intrinsic property of a given material. For some material systems, such as TiO$_2$, this statement is far from true: the index of refraction for a TiO$_2$ film can vary from 1.9 to 2.7 depending on the deposition conditions of the film. However, in the case of compound semiconductors, the optical constants of a material system (at a specified composition and temperature) are indeed quite constant, at least to the 1$^{st}$ order, in the ultraviolet and visible spectral regions. (Doping and defect densities may cause some higher order variations in the semiconductor optical constants, but for most epitaxial growth applications, they are not significant.)

Assuming that compound semiconductor material systems do have invariant and intrinsic optical constants, can SE be used to accurately measure these values? While this section describes practical approaches for measuring semiconductor optical constants in an in situ growth environment, it is important to emphasize the difficulty of the optical constant measurement process. To accurately determine the intrinsic optical constants of a material using SE, a number of conditions must be met:

1. The ellipsometer system must acquire perfectly accurate $\Psi$ and $\Delta$ data.
2. The ellipsometer beam angle of incidence must be exactly known.
3. The chamber windows used for optical access to the sample must be completely free of birefringence or the birefringence must be exactly accounted for.
4. The surface quality of the material must be known; an atomically abrupt surface with no overlayer is desired.

Realistically, it is not possible to meet all of these conditions (or even verify that they have been met) in the in situ environment. Of course, one can strive to minimize the possible sources of error in the measurement process, but in the end, the optical constants measured by SE are only an approximation to the intrinsic optical properties of the material.
Just how ‘good’ do the optical constants have to be? This depends on the application. For example, measuring the thickness of an SiO$_2$ layer on a Si substrate does not require perfectly accurate optical constants to achieve an excellent accuracy in the film thickness. Amazingly enough, the intrinsic optical constants of Si, which is the most important and well characterized material in the current semiconductor technology, are still a matter of debate in the literature. Even so, the SiO$_2$ layer thicknesses extracted from the SE data analysis using three different published sets of Si optical constants differed by less than 2Å for films ranging from 100Å - 3500Å [1]. In our experience with in situ SE, we also conclude that the accurate determination of layer thickness does not require perfect fits to the ellipsometric data or extremely ‘perfect’ optical constant libraries.

However, determining layer compositions from in situ SE data to the level of accuracy required for most device applications is a much more difficult problem. For example, being able to measure the change in optical constants induced by a 0.001 change in HgCdTe composition means being able to measure the ellipsometric parameters, Psi and Delta, to ≈0.01° and ≈0.05° respectively. While the current SE technology can easily provide this level of precision, it is very difficult to achieve this level of absolute accuracy in the in situ environment. For example it is very difficult to know the angle of incidence exactly in situ, and an error in the assumed angle translates into errors in the modeled parameters. Extracting accurate compositions from SE data can be a challenging problem which pushes the ellipsometric technique to its limit.

The good news is that it is not necessary to have perfect optical constants to achieve very good systematic reproducibility in the composition extracted from the SE data. Many potential sources of systematic errors (such as windows effects, assumed angle of incidence, systematic instrument errors) do remain fairly constant over time. As long as the measured SE data and the optical constant libraries were acquired under the same conditions, the sample parameters extracted from the data analysis should correlate nicely with the values from the optical constant libraries. Of course, if the optical constant libraries are used under different conditions (another growth chamber and ellipsometer system), there may be some discrepancies in the SE data analysis results. If these discrepancies are fairly small and systematic, it may be possible to ‘tune’ them out by applying a simple correction factor to the results.

The conclusion of this lengthy theoretical discussion is that while it is may be very difficult to measure the true intrinsic optical constants of a given material system, this does not necessarily preclude using ellipsometry to extract systematically accurate parameters, such as composition, from the analysis of the data. Instead of considering the optical constants libraries presented in this chapter as ‘the end result’, one should realize that it is the systematic methodology for measuring (and validating) the optical constant library which is more important.

NOTE: It will probably be necessary for most users to measure and validate their own optical constant libraries for each material system that they wish to monitor with SE. This is especially true in the case of demanding in situ monitoring applications which require very accurate optical constant libraries.

Building a Substrate Optical Constant Library

**Substrate Heat-Clean Procedure**

A standard procedure for most epitaxial semiconductor growth is to heat the substrate to an elevated temperature to remove the oxide and/or any other contaminating overlayer from the surface before initiating the layer growth. This is
an extremely critical part of the growth process, as any imperfections in the crystalline quality of the substrate surface will adversely affect subsequent epitaxial film growth. In the example of HgCdTe growth on CdZnTe substrates, the substrate temperature is typical raised to \( \approx 340°C \) to fully desorb the oxide (a more volatile overlayer component, most likely amorphous Te, comes off at much lower temperatures). After holding at this elevated temperature for \( \approx 10 \) minutes, the temperature is lowered and stabilized at \( \approx 180°C \) before beginning the growth of the HgCdTe layer.

Since this process is so important, it can be very useful to monitor in real-time the substrate temperature and overlayer thickness. Ellipsometry is sensitive to both the oxide overlayer thickness and the substrate temperature. This is dramatically shown in the raw ellipsometric data of Figure 15.37. In this graph, the 1st component of the CdZnTe overlayer (amorphous Te) desorbs from the surface at \( t=5 \) minutes. At about \( t=12 \) minutes, the remainder of the substrate overlayer desorbs. At \( t=18 \) minutes, the substrate cool down is initiated, and the temperature is stabilized for growth (\( t>30 \) minutes). Note that the Psi and Delta curves exhibit differing amounts of sensitivity to the various events in this process. Other wavelengths of the SE data also show different structure throughout the heating process.

![SE Data during CdZnTe Substrate Heat-Clean](image)

**Figure 15.37. SE data at a single wavelength during CdZnTe substrate heating procedure.**

**Problems in Determining Substrate Optical Constants**

While it is useful to qualitatively observe and associate the various events which occur in the substrate heat-clean procedure with changes in the raw SE data, it would be even more useful to quantitatively extract the substrate temperature and overlayer thickness from an analysis of the SE data. To do this, an optical constant library for the CdZnTe substrate as a function of temperature is required.

At first glance, it may seem like building an optical constant library for a substrate is a simple proposition: directly transform the ellipsometric data measured at each wavelength into the substrate dielectric function. However, there are two complications:

1. The *in situ* angle of incidence of the ellipsometric measurement beam with respect to the sample is not known *a priori*.
2. The assumption that the substrate is truly ‘bulk-like’ with no overlayer is questionable. It is not possible to know when the substrate surface is perfectly clean and smooth (even RHEED can not *quantitatively* verify this).

The strategy used to overcome these complications is as follows: 1) an *ex situ* VASE measurement, in which the angle of incidence was accurately known to
0.01°, was performed on a CdZnTe substrate, and 2) it was assumed that the surface before growth (but after the heat-clean process) was perfectly ‘clean’ and could therefore be optically modeled as a bulk material.

**Ex situ VASE Measurement of CdZnTe**

Variable Angle Spectroscopic Ellipsometry (VASE®) data for a CdZnTe sample was acquired at three angles of incidence over a 1.5-4.5 eV spectral range, using a J.A. Woollam Co. *ex situ* VASE® ellipsometer system. The nominal composition of the sample (and all of the CdZnTe substrates used in this work) was Cd_{0.96}Zn_{0.04}Te, which provides a better lattice match to the Hg_{0.80}Cd_{0.20}Te films grown. To extract the resulting CdZnTe optical constants from this data, an optical model consisting of a bulk substrate, with an overlayer was assumed (Figure 15.38). The true character of this overlayer is not known; it could be surface roughness, a native oxide, or possibly a non-stoichiometric overlayer (Te rich, for example). Fortunately, ellipsometry is not highly sensitive to the exact nature of the overlayer, i.e., it can not easily distinguish between a native oxide and surface roughness. Therefore, a surface roughness layer (consisting of a 50% percent EMA mixture of the bulk optical constants with void) was used to model the overlayer.

Figure 15.38. WVASE® model for analysis of *ex situ* VASE data on CdZnTe substrate.

Without prior knowledge of the substrate optical constants, ellipsometry is also not sensitive to the absolute thickness of the overlayer. However, ellipsometry can still accurately determine the relative thickness of the overlayer. For this sample, it was assumed that the overlayer thickness was 25Å. With this assumption, the overlayer thickness of the CdZnTe substrate measured *in situ* before growth was less than a few Å, which is quite reasonable. It was assumed that the overlayer thickness for the *ex situ* sample was 0Å, then the resulting overlayer thickness determined from the *in situ* sample would be about -25Å, which is not physical (although it is still accurate in a relative sense).

The ellipsometric data fits for the CdZnTe substrate are shown in Figure 15.39, and a graph of the resulting optical constants are shown in Figure 15.40. The CdZnTe optical constants are compared with CdTe optical constants which were measured by Aspnes and reported in the literature. The agreement in terms of position and shape of the critical point structures is quite good. The small systematic shift between the curves is easily explained by the 4% Zn which is present in the substrate material.

![Figure 15.39. VASE data fits for the CdZnTe substrate measured ex situ.](image-url)
Determining the in situ Angle of Incidence

Using the ex situ determined CdZnTe optical constants from the preceding section, it was possible to fit for the in situ angle of incidence. The model used for this fit is shown in Figure 15.41; the ‘srough’ layer is simply a shortcut for a 50% EMA mixture of the substrate optical constants with void. The results of the fit are shown in Table 14.2, and a graph comparing the experimentally measured in situ SE data with the model generated data is shown in Figure 15.42.

<table>
<thead>
<tr>
<th>Fit Parameter Name</th>
<th>Value, ‘±’ numbers are the 90% confidence limits</th>
</tr>
</thead>
<tbody>
<tr>
<td>MSE (Mean Squared Error)</td>
<td>0.9197</td>
</tr>
<tr>
<td>Thick.1 (surface roughness in Å)</td>
<td>1.2252±0.571</td>
</tr>
<tr>
<td>Angle0 (angle of incidence)</td>
<td>75.611±0.0123</td>
</tr>
</tbody>
</table>

Table 15.2. Fit parameters from in situ SE data analysis of CdZnTe substrate.

The angle of incidence determined from the preceding data fit was used for all subsequent analysis of the SE data. In WVASE®, this is done by specifying the actual angle of incidence in the WVASE® Experimental Window Angles menu option, as shown in Figure 15.42. This is also where the angle of incidence can be defined as a WVASE® fitting parameter.
While the data fits shown in Figure 15.42 are very good, there are still some potential sources of error in the angle of incidence: 1) the composition of the CdZnTe substrate material, which is assumed to be nominally constant for all substrates, may actually vary slightly from sample to sample, and 2) the temperature of the substrate during the SE measurement may not be exactly at room temperature, as the cryo-shields in the MBE system make it difficult to stabilize the substrate at room temperature (the optical constants used for the model analysis were measured at room temperature). These concerns aside, the maximum error in the fit angle of incidence is still estimated to be less than 0.1°.

### Ramifications of Errors in the Angle of Incidence

Any error in the assumed angle of incident will translate into an error in SE determined layer thicknesses. The magnitude of this error depends on the material structure and optical constants, but for a 1000Å Hg$_{0.8}$Cd$_{0.2}$Te film on a CdZnTe substrate, a 0.01° error in angle of incidence induces a 0.14% error in film thickness. This small systematic thickness error can be ‘tuned’ out of an existing optical constant library, if necessary.

However, angle of incident errors do not affect the SE determined layer compositions, as long as the optical constant spectra within the composition-dependent library were all acquired at the same nominal angle. In this case, the error in the optical constant library due to an inaccurate angle of incidence is systematically incorporated across all of the compositions in the library. When the optical constant library is used to analyze subsequently measured SE data, the fit will return the same ‘inaccurate’ angle of incidence value, but the fit composition will be systematically correct (assuming that the compositions in the library are accurate).

### Extracting In Situ Substrate Optical Constants

Two substrate temperatures were included in the CdZnTe optical constant library: 1) immediately before the layer growth, when the temperature should be stabilized at 180°C (according to the pyrometer), and 2) at the highest temperature of the heat-clean process, which is nominally 340°C (on the substrate thermocouple). In both cases, the oxide overlayer has already been desorbed, such that an ideal substrate optical model (no overlayer) can be used to extract the optical constants (using the previously determined angle of incidence).

The nominal temperature values of 180°C and 340°C may not be perfectly accurate, as the absolute substrate temperature is a very difficult property to measure in situ. However, these nominal values can easily be changed in the optical constant library at a later time to correspond with another more accurate temperature measurement technique. Furthermore, the reproducibility of the SE-based
temperature measurement is not affected by the relative accuracy of the nominal temperature values specified in the optical constant library.

To extract the *in situ* substrate optical constants at the two temperatures, spectroscopic timeslices were chosen at appropriate points in time throughout the substrate heat-clean procedure. Figure 15.44 shows how this was actually done in *WVASE*®, wherein multiple timeslices were selected during the region of constant substrate temperature before growth. *WVASE*® was then switched to the ‘Spectroscopic’ mode, as shown in Figure 15.45. The data for the multiple timeslices lie essentially on top of each other. However, the purpose of selecting the multiple timeslices is to improve the signal-to-noise in the extracted optical constants by averaging the multiple sets of SE data.

![Multiple Timeslices Selected Before Growth](image1)

*Figure 15.44. Selection of multiple timeslices at substrate T=180°C before growth.*

![Spectroscopic Mode, CdZnTe substrate at 180°C](image2)

*Figure 15.45. Spectroscopic SE data on the CdZnTe substrate before growth.*

The next step is to build a simple substrate-only model in *WVASE*®, using the *ex situ* CdZnTe optical constants. The substrate optical constants are defined as fit parameters by clicking on the ‘n’ and ‘k’ boxes shown on the layer dialog (see Figure 15.46). The ‘Normal Fit’ menu option is then selected in the *WVASE*® ‘Fit’ window to extract the best fit optical constants for the selected SE data (the resulting fit is shown in Figure 15.45).
The resulting optical constants are saved to a file (named CZT-180) by clicking on the ‘Optical Constants >>’ button in the substrate layer dialog box (see Figure 15.46). This same process was repeated for the time range when the substrate was nominally at 340°C (time = 14 - 18 minutes, see Figure 15.44) to extract and save another set of CdZnTe optical constants.

**Building an Optical Constant Library**

Three sets of CdZnTe optical constants are now available: the room temperature constants measured *ex situ*, and the two sets of *in situ* constants extracted from SE data at 180°C and 340°C nominal temperatures in the preceding section. To compare these sets of optical constants, the WVASE® model shown in Figure 15.47 was built. By selecting the Data | All Layers (Opt. Const.) menu option in the WVASE® ‘Graph’ window, the plot shown in Figure 15.48 was displayed. From this graph, it is clear that the CdZnTe critical point transitions at 3.3 and 3.8 eV broaden and systematically shift to lower energies as the temperature increases, as expected.
Building a Film Optical Constant Library

To perform real-time monitoring of composition during growth by spectroscopic ellipsometry (SE), a highly accurate and systematic optical constant library which can generate spectra as a function of both composition and temperature is required. The library must encompass the composition and temperature range which would be normally encountered during growth, and it would even be desirable to extrapolate outside this range, in order to detect and diagnose anomalous growth conditions. This section describes a method for acquiring the optical constants for such a library. OC Fitter (A program available from the J.A. Woollam Co. that parameterizes optical constant spectra) would then be used to parameterize the optical constants into a library usable by WVASE®.

Ideally, one would like to determine exact, intrinsic, optical constant spectra for the semiconductor system of interest for the complete range of growth temperatures and compositions, by performing in situ SE measurements during a systematic series of growth runs. The layer compositions and/or temperatures for each run would be known and independently verified by non-ellipsometric means such that accurate values could be associated with each measured optical constant spectra. Unfortunately, this objective is not achievable in a reasonable time frame, as it would typically require a separate growth run and ex situ analysis for each composition. Building an optical constant library across multiple growth runs also tends to introduce some inconsistency into the constituent optical constant spectra, due to potential variations in the ellipsometer angle of incidence, growth temperature, and surface quality.

It is more realistic to determine optical constant spectra for a material system of interest at a few temperatures in the typical growth regime of the system, and at a limited number of representative compositions. Furthermore, only nominal values for temperature and composition need to be assigned to the measured spectra initially. These nominal values may not be accurate in an absolute sense, but they will enable the reproducible in situ determination of temperature and composition at least in a relative sense. The nominal values for temperature and composition can later be replaced by more accurate values when that information becomes available (e.g. through extensive ex situ analysis). Thus, without re-measuring the optical constants, the accuracy can always be fine tuned assuming the precision is good enough. Reproducibility (relative accuracy) is more important and more readily achievable than absolute accuracy, which can still be developed over time.

The following general growth procedure can be used to measure optical constants at nominal temperatures $t_x = t_1 \ldots t_n$ and compositions $c_y = c_1 \ldots c_m$.

1. The wafer temperature is ramped to remove the oxide and a thick buffer layer (ideally a binary material) is grown to provide a smooth, high-quality surface. During the buffer layer growth, the wafer temperature should be stabilized and maintained at $t_1$.

2. The temperature is stabilized at $t_x$ and a layer of composition $c_y$ is grown. A layer thickness greater than the ¼ wave optical thickness of the material should be grown. Because the optical constants are different from the buffer layer, interference effects will be observed in the ellipsometric data. By performing a growth-rate analysis on these data, highly accurate optical constants of the growing layer can be determined, even when the layer is grown on top of a complex multi-layer structure. For many material systems, the growth rates of the test layers can be correlated with the source fluxes to provide a good estimate of the composition after making certain assumptions about the sticking coefficients. By analyzing the measured data at many times (different thicknesses) the data analysis becomes over-determined, and it is possible to
minimize inaccuracies from ellipsometer errors, material interfaces, and surface non-idealities.

(3) A buffer layer is grown (again greater than ¼ wave optical thickness) with the temperature remaining stabilized at \( t_x \). During this growth, the sources setting the composition can be ramped and stabilized for the next composition of interest. Also, optical constants can be extracted from the buffer layer. Comparing the results from the multiple buffer layers provides a good self-consistency check of the temperature stability and potential optical constant accuracy. With the buffer layer grown there is now optical contrast for growing the next layer of interest.

(4) Steps 2 and 3 are repeated ‘m’ times for each composition \( c_y \).

(5) Steps 2 - 4 are repeated ‘n’ times for each temperature \( t_x \). (The total number of temperature and composition dependent optical constant spectra which are acquired in this approach is ‘n x m’.)

There are several advantages of this procedure. It can be used (with some possible modifications) with almost any lattice matched or nearly matched ternary semiconductor system and with different growth techniques (MBE, MOVPE, etc.). The optical constants are determined during a single growth run, eliminating problems with reproducing the angle of incidence and temperatures. The procedure is simple enough that it can be performed on different growth chambers to assess potential differences. The optical constants obtained from observation of the dynamic growing surface may also be more accurate (and useful) than from a static surface.

### The WVASE OC Library File Formats

To use these temperature dependent optical constants in a practical manner, it is necessary to combine them into a ‘library’ file which enables the calculation of optical constant spectra at any arbitrary temperature. This is done by interpolating (or extrapolating) between three discrete sets of optical constants. **WVASE\(^6\)** supports a simple file format to implement such a temperature-dependent optical constant library, which is shown in Table 14.3. This is an ASCII file which can be created by any text editor program (such as the Windows ‘Notepad’). The optical constant values from the discrete files are sequentially ‘pasted’ into this file, separated by blank lines. The syntax of header lines in the file must be exactly as shown in the table. The file must be saved with a ‘.MAT’ extension (for example, CZT-T.MAT), such that **WVASE\(^6\)** can recognize it as a material file.

In a manner similar to the CdZnTe temperature-dependent library shown in Table 15.3, a composition-dependent optical constant library can easily be assembled. The procedure is the same, and the syntax ASCII file format is only slightly different, as shown in Table 15.4.
15.5 Special Data Acquisition Considerations

Window Effects

Since ellipsometry accurately measures the change in polarization state induced by the sample, it is very important that the windows which are used to provide optical access to the sample inside the chamber do not affect the polarization state of the ellipsometric measurement beam. This implies that the windows must be free of strain induced birefringence. One way to satisfy this requirement is to buy...
expensive, specially made windows which are strain-free. Another way is to use the software to account for the effects of the window strain on the light beam.

A patented[2] procedure for accounting for the windows involves separating the effects of the windows into orthogonal 'in-plane' and 'out-of-plane' components. The 'out-of-plane' components can be directly determined by the calibration algorithm. The 'in-plane' window effects combine with the sample's ellipsometric Delta parameter, and therefore cannot be determined directly; a model fit to ellipsometric data acquired on a reference sample is used to extract the 'in-plane' window effects. The WVASE® software automates the process of determining the window parameters, saving the parameters with each data file, and applying the appropriate window corrections in the model calculation during data analysis.

Using WVASE® to Determine Window Effects

It is very easy to model away window effects using the WVASE® software. The process for determining the window effects requires two steps. In the first step the ‘Out-of-Plane’ effects of the windows are accounted for and in the second step the ‘In-Plane’ effects are determined. The standard procedure is as follows:

Determining the Out-of-Plane Window Effects

Mount the standard calibration wafer supplied with the ellipsometer (~250Å SiO₂ / Silicon) and align the sample. Then perform a `Normal Calibration`. When the `Calibration` Dialog appears, make sure the ‘Include Window Effects’ option is checked as shown in Figure 15.49. The number of revolutions should be set to 100 to 200 to acquire very accurate data. Press OK to perform the calibration. If the calibration fit is good then continue to Step 2.

![Figure 15.49. The Calibration Routine dialog with ‘Include Window Effects’ selected](image)

Figure 15.49. The Calibration Routine dialog with ‘Include Window Effects’ selected

Figure 15.50 shows an example calibration with standard fused silica 2-3/4" conflat vacuum windows placed before and after the sample in the beam path of a JAW Co. M-88® ellipsometer system. The calibration graphs show that including window effects in the calibration algorithm dramatically improves the calibration data fit. The corresponding calibration parameters are shown below each graph (which appear in the Hardware Log File). If window effects were not included in the calibration algorithm, the calibration MSE increased from 0.678 to 25.9! The out-of-plane window effect parameters determined in the calibration procedure are internally stored in WVASE®, such that subsequently acquired ellipsometric data will be 'tagged' with these values and applied in the model calculation.
NOTE: If zone-averaged (or 'High Accuracy') ellipsometric measurements are performed, the effects of out-of-plane window retardance on the ellipsometric data are cancelled out, at least to 1st order.

**Including Window Effects in the Calibration**

**Without Window Effects in the Calibration**

Figure 15.50. Calibration results with and without including window effects.

**Determining the In-Plane Window Effects**

Since the in-plane window effects (of both the entrance and exit windows) combine indistinguishably with the sample's Delta values, it is not possible to determine them in the calibration algorithm. Instead, a model fit to ellipsometric data acquired on a reference sample is required to determine the in-plane window effects (which are also called the 'Delta offsets'). A good reference sample for this purpose is the 'standard' wafer shipped with each JAW Co. ellipsometer system, which consists of a ~250Å SiO₂ film on a Si wafer. The best optical model for this sample is stored in the C:\WVASE\MAT\SEMICOND subdirectory, and is named 'TOX_JAW.MOD'. The 10Å interface layer should be fixed for most applications, and only the top SiO₂ thickness and angle of incidence should be defined as fit parameters.

In Figure 15.51, ellipsometric data were acquired on the reference sample through windows, and a model fit was attempted. The Psi data fits OK, but due to the in-plane window effects, the Delta data does not fit well.
Model Fit, **Without** Delta Offsets

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness</th>
<th>Material</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>sin2_jaw</td>
<td>265.98 Å</td>
</tr>
<tr>
<td>1</td>
<td>intr_jaw</td>
<td>10 Å</td>
</tr>
<tr>
<td>0</td>
<td>si_jaw</td>
<td>1 mm</td>
</tr>
</tbody>
</table>

MSE=72.27

Thick.2 265.98±2.29

Angle0 75.78±0.0549

Figure 15.51. Fit results of measurement taken through windows show good agreement for Psi, but not for Delta.

To improve the fit, the 'Delta Offset' is added as a fit parameter, as shown in the Model Options dialog box of Figure 15.52. Make sure that the 1/Wavelength Offsets box is checked. The 2\textsuperscript{nd} and 3\textsuperscript{rd} Delta Offset boxes are dispersion terms which are needed only if the window birefringence is very large, or if the spectral range of the instrument is very wide (e.g., the new JAW M-2000® SE systems).

Figure 15.52 Model Options dialog box.

By adding the Delta Offsets as fitting parameters, the model fit is greatly improved (Figure 15.53), and the in-plane window effect parameters are also determined.

**NOTE:** For optimum accuracy, the data used for analysis should be from the calibration which was used to determine the out-of-plane window parameters.
Model Fit, With Delta Offsets

2  si2_jaw  266.42 Å
1  intr_jaw  10 Å
0  si_jaw  1 mm

MSE=4.743
Thick.2  266.42±0.15
Angle0  74.985±0.00758
DelOff1  -6.3189±0.0528

Figure 15.53. Inclusion of Delta offset improves fit for both Psi and Delta and provides a measure of the in-plane window effects to be used on subsequent data.

The Delta Offset parameters determined above are then entered into the [Hardware] section of the HARDWARE.CNF file. This file is located in the C:\WVASE subdirectory, and can be edited with the Windows Notepad application. The syntax for the Delta Offset entry is:

[Hardware]
DelOffsets=2 -6.3189 0 0

where the '2' signifies 1/wavelength dispersion, and the next 3 numbers correspond to the values in the Delta Offset boxes of the Model Options dialog. The next time the ellipsometer hardware is initialized, the 'DelOffsets' entered in the HARDWARE.CNF file will become active, such that subsequently acquired data will be tagged with these values, and applied to the model calculation. If these values change, the HARDWARE.CNF file will need to be corrected.

NOTE: The Delta Offset parameters can be entered into the HARDWARE.CNF file automatically by opening the Model Options dialog, holding down the 'Ctrl', 'Alt', and 'Shift' keys and clicking the left mouse button on the 'Window Effects' button.

Acquiring/Analyzing Data with Window Effects

After the window effects have been determined using the procedures above, subsequently acquired ellipsometric data in WVASE® is 'tagged' with the previously determined window parameters. These parameters can be viewed by the File|Information menu option of the Experimental Data window, as shown in the dialog box on the next page. Furthermore, when the data is acquired, or when the data file is read into the Experimental window, the window effect parameters are automatically set in the Model Options. At model calculation time, window effect corrections are applied to the generated ellipsometric data, such that excellent model fits can be achieved, even with birefringent windows in the beam path.

NOTE: Be careful about loading saved models after an experimental data file has been loaded. Window effects in the model file will overwrite those set by the experimental data file.

With the rotating analyzer ellipsometer (RAE) configuration (which is implemented in J. A. Woollam Co. M-44® and M-88® systems), the window effects must be corrected at model calculation time, as the RAE system can not measure the 'handedness' of Delta, and therefore it is not possible to know (in general) at
In Situ Dynamic Data Analysis and Examples

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acquisition time whether to 'add' or 'subtract' the window effects from the measured data. In this case, the measured ellipsometric data does not represent the intrinsic Psi and Delta values of the sample; it also includes the effects of windows, which are then quantitatively accounted for in the model calculation. With the new J. A. Woollam Co. M-2000® system (which employs the rotating compensator ellipsometer configuration), window effects can be subtracted from the raw data at acquisition time, such that the 'true' ellipsometric parameters for the sample are stored in the data file, and no corrections are required at model calculation time.

Coating Problems

In most deposition systems the ellipsometer windows do become coated over time. Since ellipsometry measures a ratio, the accuracy of the measurement is not sensitive to decreases in the overall beam intensity caused by window coating. The S/N (precision) of the measurement does begin to degrade as the window becomes coated, though. Periodic checking of the window transmittance is highly recommended to insure the best measurement conditions.

Sample Alignment

When aligning the ellipsometer for an in situ measurement, it is usually not possible to tilt or raise and lower the sample as would be done in an ex situ environment. For in situ the alignment is done using the tilt stages on the ellipsometer input and output units and the X-Y translation adjustment on the output unit. A detailed alignment procedure can be found in the hardware manual that accompanies the ellipsometer.

Substrate Wobble

Figure 15.54 shows the geometry of the beam movement during substrate rotation, where $\Phi$ is the angle of incidence, $\theta$ is the angle between the substrate normal and axis of rotation (the substrate angular wobble), and ‘d’ is the substrate to detector distance. Simple trigonometry, shown in equations (15.1) and (15.2), predict the length ‘l’ and width ‘w’ of the ellipsoidal beam trajectory at the detector plane due to the substrate rotation.

$$l = 2 \cdot d \cdot \tan(\theta) \quad (15.1)$$

$$w = 2 \cdot d \cdot \tan(\theta) \cdot \cos(\Phi) \quad (15.2)$$

For example, if the angular wobble $\theta$ of the substrate is $\pm 0.1^\circ$, $d = 500$ mm and $\Phi = 75^\circ$, the reflected beam will move in a 1.7 x 0.5 mm ellipsoidal trajectory at the detector plane. While this would probably be acceptable for most ellipsometric measurements, in practice we typically observe beam trajectories which ranged from 2.5 times larger than this.
Since the aperture of the detector unit is only about 1 – 5 mm in diameter, it is important to collect as much of the beam reflected off the substrate as possible during rotation. If the beam trajectory due to substrate wobble is very large, then the size of the reflected ellipsometer beam at the detector aperture must be very big if the ellipsometer system is to collect light throughout the complete period of substrate rotation.

For optimal ellipsometer signal-to-noise, it is desirable to make the beam at the detector plane large enough such that a part of the beam is always collected while the substrate is rotating (see Figure 15.55). However, if the beam is too large, much of the light reflected from the sample is wasted, as it is never collected by the detector.

In this section a few examples of the analysis of in situ ellipsometric data are presented. These examples demonstrate different techniques for determining physical parameters such as growth rates, optical constants, and layer thicknesses.

The real-time data used in these examples are included in the WVASE® software package. The user can load the ellipsometric data files for the examples
given in this chapter into the WVASE® program for practice. These data files are saved under the “Examples” subdirectory. In situ measurements acquire data at many wavelengths simultaneously. Typical film deposition or etching processes will last for more than 30 minutes, which leads to very large experimental data files. For this reason, the ‘Maximum # of Data Points’ in the memory allocation of the ‘Defaults’ option of the ‘Global’ menu should be set to at least 55000 before loading these example data files.

Any J.A. Woollam Co. ellipsometer system can be used in situ to acquire real-time ellipsometric data. However, because of the relatively slow scanning rate of the monochromator in the VASE® system, it is restricted to slow deposition or etching processes. On the other hand the M-44®, M-88®, and M-2000® systems acquire ellipsometric data at many wavelengths simultaneously, such that the minimum time between acquisitions of complete spectra is less than 1 second, which is fast enough for most thin film growth or etch processes.

The following example data sets were acquired with various M-series ellipsometers from the J. A. Woollam company or simulated using WVASE®. The experimental conditions are briefly described for each example.

**Al₂O₃ on Si**

In this example, the optical constants and thickness of an Al₂O₃ film on glass are determined using a growth rate analysis. The data represent the growth of approximately 1800Å of Al₂O₃ on Si. Data were acquired every 1.5 seconds during deposition. The data for this example are in the file ‘Dyn-1800 Al₂O₃ on Si.bdt’ in the \WVASE\Examples directory. The Psi and Delta data for this example are shown in Figure 15.56. The Range Select menu item from the Experimental Data window was used to select three wavelengths for viewing, as displaying all of the wavelengths would result in very cluttered graphs. Notice that the deposition starts at about 1.0min. and ends at about 7.0min. The film is obviously transparent since interference effects are seen for all of the wavelengths.

![Figure 15.56. Ellipsometric (a) psi and (b) delta data for the deposition of 1800Å of Al₂O₃ on Si displayed at three wavelengths.](image)

It would be good practice at this point to try and work this example in the same way as the Ni on Si example was worked at the beginning of the Basic Analysis Strategies section of this chapter, using the Al₂O₃ optical constants found in the Dielectrics folder to fit the data. Start by selecting the time range of 0min. to 0.9 min. which represents the substrate before the film growth starts. Build a model for the substrate (Si with a native oxide) as shown in Figure 15.57 and select the oxide thickness and angle of incidence as fitting parameters. Since this is dynamic data, WVASE® assumes any layer on the substrate is grown starting at 0 time. In this case the SiO₂ layer is present before the data is acquired. This means we need to trick WVASE. We do this by setting the growth rate of the SiO₂ layer to a very large...
number – like 1000000Å/sec. Set the growth rate to this very large number and then perform a normal fit. The resulting thickness should be 18.1Å and the Angle of Incidence should be 75.07°. Now fix these fit parameter values for the rest of this example.

![Figure 15.57. The model representing the SiO₂/Si substrate for this example.](image)

Next, add the Al₂O₃ layer to the model (choosing the Al₂O₃ optical constants from the Dielectrics directory) and set the thickness as a fitting parameter and perform a point by point fit. The results should look like Figure 15.58. The poor fit indicates that the book value Al₂O₃ optical constants do not adequately represent this film.

![Figure 15.58. The (a) psi and (b) delta data fit for the Al₂O₃ thickness using the Al₂O₃ optical constants from the Dielectrics directory.](image)

Since the Al₂O₃ optical constants from the WVASE® library did not work for this film, we will have to fit for the optical constants ourselves. This will be done using the growth rate analysis technique. Start by setting the growth rate of the Al₂O₃ layer to 4.5Å/sec as this is the nominal rate given at the beginning of this example. You will also need to add a delay layer between the SiO₂ layer and Al₂O₃ layer and set the delay time to 1.0min. so WVASE knows the layer growth doesn’t start until the 1 minute mark. Generate data to see how well the nominal growth rate analysis model represents the data. The model and the generated data are shown in figures 14.59 and 14.60.

![Figure 15.59. The model used to perform the growth rate analysis method on the Al₂O₃ film. The Delay layer is used to specify that the layer doesn’t start growing until one minute after data acquisition begins.](image)
To get the optical constants and growth rate values close, we will start by selecting a small subset of the growth data and fitting only for the optical constants, and then we will add the growth rate. Select the time range from 0-2 min. This time range is selected because we only want a small part of an interference effect included in this initial fit. This makes fitting easier if our initial fit parameter values are quite wrong. Not select only the optical constants of the Al₂O₃ film as fit parameters and perform a normal fit. Once the fit is done, add the growth rate of the Al₂O₃ layer as a fit parameter and perform the fit again. By now the fit should look pretty good. Extend the time range to 4 min. and fit again. The MSE should be about 13.4.

Now that our optical constants and growth rate are well defined, select the entire time range and then generate data. The psi and delta graphs should look Figure 15.61.

From the graphs in Figure 15.61, it appears that the optical constants and growth rate of the Al₂O₃ layer are pretty much correct but our nominal film thickness is too thin. We will fix this now by unselecting the optical constants and growth rate of the Al₂O₃ layer and fitting only for the thickness of the layer. Perform the fit now. The new thickness should be ~1873Å. Now, add the optical constants and growth rate of the Al₂O₃ layer, and the Delay layer time as fit parameters and perform a final fit. This should result in an MSE of 13.4, a film thickness of 1848Å, and a growth rate of 5.11Å/sec. and data fits that look Figure 15.62.
GaAs and AlGaAs growth at 600°C

In this example we wish to determine the optical constants and growth rate for GaAs and AlGaAs films grown by MBE at 600°C. We will incorporate two analysis techniques: (1) The virtual substrate approximation and (2) growth rate analysis. The experimental data for this example can be found in the file 'gaas600c.bdt' in the 'WVASE\Examples' directory.

Al$_{0.1}$Ga$_{0.9}$As was grown on a GaAs substrate at 600°C in an MBE chamber with solid sources. A GaAs cap layer was then grown on top of the Al$_{0.1}$Ga$_{0.9}$As layer. Ellipsometric spectra were acquired throughout the entire growth with an M-44$^e$ instrument mounted on the MBE chamber. These experimental data are shown in Figure 15.63.

**Determination of the substrate optical constants at 600°C**

We will first determine the growth temperature optical constants of the GaAs substrate by analyzing the data acquired before the growth was performed. Select the data from the time = 0 to 1.4 minutes using the ‘Range Select’ option from the menu bar of the Dynamic Experimental Data window. These data were acquired after the oxide blow off. During this period of time, no crystal was grown, and as a result the data in Figure 15.63 show no time dependence for times less than 1.4 minutes after the start of the data acquisition.

Build a model using the room temperature GaAs material file gaas.mat as a substrate with no other layers, as shown in Figure 15.64.
Figure 15.64. Model for fitting the experimental data acquired before the start of the growth.

Define the optical constants \( n \) and \( k \) in the room temperature GaAs material file as fit parameters and perform a normal fit. After a few iterations, a nearly perfect fit is obtained. This is not surprising as we are fitting for all of the possible fit parameters.

The best-fit optical constants of the GaAs substrate at 600°C are shown in figure 15.65. This plot was obtained by clicking on the GaAs layer and then clicking on the ‘Optical Constants’ button. Save the optical constants as gaas600.mat.

Figure 15.65. The best-fit optical constants for the GaAs substrate at 600°C.

Growth of \( \text{Al}_{0.1}\text{Ga}_{0.9}\text{As} \) on GaAs at 600°C

To fit the data for the first AlGaAs film, we will break the analysis into two parts. In the first part we select just the beginning part of the growth such that less than one interference effect is observed in the data (Figure 15.63). We do this in order to get the optical constants and growth rate closer to their correct values before adding all of the data. In the second part we will select all of the data and perform the fit again.

Start by selecting the experimental data from 0 min. to 4 min. This represents the very initial start of the film growth as the \( \text{Al}_{0.1}\text{Ga}_{0.9}\text{As} \) layer growth began at about time=1.4min.

Build the model shown in Figure 15.66. GaAs is again selected to provide initial optical constant values for the \( \text{Al}_{0.1}\text{Ga}_{0.9}\text{As} \) layer since we do not know the optical constants of this material at 600°C. We will analyze this part of the data using a growth rate fit. In growth rate fit analysis the growth rates of the individual layers are fit parameters rather than the actual layer thicknesses. This technique will work when the growth rate does not change significantly during the growth of each film.

NOTE: When performing a growth rate analysis it is important to give the growing layer a thickness that is greater than that represented by the data, as the model assumes that the film stops growing after the indicated thickness is reached.

Figure 15.66. Model for fitting the AlGaAs film growth.
We will start by trying to get the optical constants close to their initial values. To do this, we will initially fit only for the optical constants of the growing film. Unselect the optical constants of the substrate as fitting parameters and then select the optical constants of the film for fitting. The resulting MSE should be close to 2.7. Now, add the growth rate as a fitting parameter (choose the 'Growth' menu from the Model window) and perform another normal fit. Now the MSE should be close to 1.15 and the fit should look like Figure 15.67.

![Figure 15.67](image)

*Figure 15.67. Initial fit to the ellipsometric psi data, after defining n and k of the virtual substrate and the growth rate as fit parameters.*

Although this fit looks pretty good, notice that it appears in Figure 15.67. that the beginning growth time may be not be exactly correct. We will fix this by adding the delay time as a fit parameter. Add the delay layer time as a fit parameter and perform another fit. Now the MSE is 0.64 and the fit looks perfect.

Now that we know the optical constants and growth rate values are well seeded, we will add the rest of the data for this layer growth and perform the final fit. Select the data from 0min. to 9min. and perform a normal fit. The fit quickly converges and results in an excellent fit to all of the data. The final MSE is ~0.7, the growth rate is 1.97Å/s and the delay layer time is 1.51min.

![Generated and Experimental](image)

*Figure 15.68. Final fit to the ellipsometric psi data, after defining n and k of the virtual substrate, the growth rate, and the delay layer time as fit parameters.*

Although the “best” fit has been achieved, it is not necessarily true that all of the fitting parameters are physically realistic. At this point the user should examine the best-fit values of the fit parameters. The best-fit optical constants of the Al$_{0.1}$Ga$_{0.9}$As layer are plotted in figure 15.69. These optical constants seem reasonable. Save these optical constants as algas600.mat. The other fit parameter
(growth rate) is found to be 1.97Å/sec. This value of the growth rate was in agreement with the growth rate obtained from MBE flux measurements.

Figure 15.69. Calculated optical constants of the Al$_{0.1}$Ga$_{0.9}$As film at 600°C. The solid line is the index of refraction (n) and the dashed line is the extinction coefficient (k).

**GaAs layer**

To analyze the next layer (GaAs) growth between 9 and 14 minutes, one can add a GaAs layer and solve for its growth rate. However, we will analyze the GaAs growth using a virtual substrate, defined at time $t = 10.14$ minutes. This virtual substrate allows us to replace the entire growth history (from time = 0 to 10.14 minutes) by a pseudo-substrate represented by the pseudo-optical constants obtained by inverting $\psi$ and $\Delta$ data at time $t = 10.14$. It is very important to know that this virtual substrate is an approximation which works very well for semiconductor layers on semiconductor substrates. The approximation does not work at all for dielectric materials.

Select the data in the range from time 10.14 to 14 minutes. The GaAs layer starts to grow about 9.6 minutes after the start of data acquisition. Build a model as shown in figure 15.70. Define the virtual substrate at time=10.14 min. Set up a delay layer at time=10.14 min assuming there is no growth before this time. Add the layer `gaas600.mat` (the optical constants for which were obtained during the substrate analysis). Define the `gaas600` layer growth rate as a fit parameter.

$$
\text{Figure 15.70. Model used to fit the dynamic data acquired during the GaAs film deposition, in the time range 10.14 - 14 minutes after the start of data acquisition.}
$$

Perform a normal fit. This will yield a very good fit, as shown in figure 15.71. The MSE should be ~0.95. Here it appears that the substrate optical constants (`gaas600`) represent the top GaAs layer very well. (However, in some situations it may be necessary to fit for both the optical constants and growth rate).
In this example, we will demonstrate how to obtain accurate layer thicknesses using the virtual substrate approximation by characterizing the MBE growth of AlGaAs/GaAs quantum well structures. The ellipsometric data (data file qw.bdt) which we will fit in this example were acquired during an MBE growth of AlGaAs/GaAs/AlGaAs multiple quantum wells. The ellipsometric data are shown in Figure 15.72, while the nominal structure of the multiple quantum wells is shown in figure 15.73. The nominal composition of the AlGaAs layers is 30% Al and 70% Ga.

![Generated and Experimental](image1)

**Figure 15.72.** Experimental ellipsometric (a) psi and (b) delta data acquired during the growth of AlGaAs/GaAs/AlGaAs.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>AlGaAs</td>
<td>500Å</td>
</tr>
<tr>
<td>GaAs</td>
<td>25Å</td>
</tr>
<tr>
<td>AlGaAs</td>
<td>200Å</td>
</tr>
<tr>
<td>GaAs</td>
<td>50Å</td>
</tr>
<tr>
<td>AlGaAs</td>
<td>200Å</td>
</tr>
<tr>
<td>GaAs</td>
<td>75Å</td>
</tr>
<tr>
<td>AlGaAs</td>
<td>200Å</td>
</tr>
<tr>
<td>GaAs</td>
<td>100Å</td>
</tr>
<tr>
<td>AlGaAs</td>
<td>500Å</td>
</tr>
<tr>
<td>GaAs</td>
<td>Substrate</td>
</tr>
</tbody>
</table>

**Figure 15.73.** The nominal structure of the multiple quantum wells.
Load the experimental data file qw.bdt into the Experimental Data window. The delta data are noisier when they are close to 0° or 180°, which is an inherent disadvantage of the simple rotating analyzer ellipsometer. This is not an issue with rotating compensator ellipsometers such as the M2000. However, the WVASE® program should be able to extract accurate physical parameter even in the presence of noise. This is not a ‘special’ capability of WVASE®, rather it is a consequence of the fact that even noisy data points still contain information about the sample, we simply use WVASE® to extract the useful information from amidst the noise.

After the angle of incidence is determined from the substrate, a layer-by-layer approach will be used to determine the thickness, growth rate, and optical constants of each layer, as demonstrated in the previous example. In this example we will perform the analysis of the first two layers. The rest of the analysis is similar to the analysis of the first two layers and is left as an exercise.

**Determining the Angle of Incidence**

To start this experiment, the angle of incidence will be determined by looking at the data from 0 minutes to 3.0 min., which represents the substrate before film growth starts. Select the data between 0min. and 3min. and build the model shown in Figure 15.74. Add the Angle of Incidence as a fitting parameter and perform an normal fit. The resulting angle should be ~74.99°. Fix the angle at this value for the rest of this example.

![Figure 15.74. The model for the GaAs substrate. This model is used to determine the angle of incidence.](image)

**500 Angstrom AlGaAs layer**

The first film grown on the substrate is a 500Å AlGaAs layer. Select data in the time range from 0 to 6.8min using the ‘Range Select’ option from the Dynamic Experimental Data window menu bar, and build a model as shown in Figure 15.75. The growth temperature is 600°C, so we will use the optical constants of the AlGaAs layer obtained in the second example (algas600) as the starting values for the optical constants of AlGaAs layer in this example. The delay layer is used to model the delay between the start of data acquisition and the start of growth, just as in the previous example. In the model the virtual substrate is defined at time=3.25 and eight points are averaged to get the virtual layer parameters for the substrate to minimized the effect of noise. The virtual layer dialog as setup for this example is shown in Figure 15.76. Finally, set the growth rate to 2Å/s as this is what we found to be the case for this material in the previous example.

![Figure 15.75. Model used to fit the experimental data for the first 500 Angstrom AlGaAs layer](image)
Figure 15.76. The Virtual Interface layer dialog with the virtual interface set at 3.25 minutes and 8 points averaged to get the virtual interface parameters. Averaging is a good way to reduce the effect of noise on the virtual interface parameters.

After setting up the model, select ‘Generate Data’ from the Generated Data window menu bar and compare the data predicted by the initial (nominal) model with the measured data. Note that the data predicted by the nominal model does not match the experimental data very well (Figure 15.77), indicating that the optical constants of the AlGaAs are different than the nominal values. Also note that there is some odd behavior in the generated data for the 731.6nm wavelength. This is due to noise in Delta causing the virtual interface layer to pick different mathematical roots to best fit the data (or the noise in the data). To prevent this from happening, select the ‘Don’t try both branches’ option in the virtual layer dialog.

Figure 15.77. Generated (a) psi and (b) delta data from the nominal model for the growth of the AlGaAs layer.

Since the nominal model is not very close to the correct model, we will stage the fit as follows: 1) Fit only for the optical constants of the AlGaAs layer, 2) add the growth rate as a fitting parameter, and 3) add the thickness and delay time as fitting parameters bring the total number of fit parameters to 3 plus the optical constants at each wavelength.

Define the optical constants of the AlGaAs layer as fit parameters and perform a normal fit. The resulting MSE should be ~6.4 and the model data should be much closer to the experimental data.

Now add the AlGaAs layer growth rate as a fit parameter and perform another fit. The MSE should now be 1.1 and the data fit should be very good.
Add the AlGaAs layer thickness and Delay layer thickness as fit parameters and perform the fit again. Finally add the optical constants of layer 0 (virtual substrate) as fit parameters and re-start a normal fit. Fitting the pseudo-optical constants will smooth out noise in the data. The final fits are shown in Figure 15.78. The MSE should be less than 1.0, the growth rate ~2.52, and the thickness of the AlGaAs layer should be 504.1 Å.

The thickness of the AlGaAs layer was found to be 504 Å, the growth rate was 2.49 Å/sec, and the final MSE was 1.06. The best-fit optical constants determined for the AlGaAs layer are shown in figure 15.79.

The thickness of the AlGaAs layer was found to be 504 Å, the growth rate was 2.49 Å/sec, and the final MSE was 1.06. The best-fit optical constants determined for the AlGaAs layer are shown in figure 15.79.

### 100 Angstrom GaAs Layer

Select the time range from 6.7 to 8.2min using the ‘Range Select’ option from the Dynamic Experimental Data window menu bar, and build a model as shown in Figure 15.80. Again, the material file gaas600.mat (obtained from the second example ) is used to model GaAs growth at 600°C. The virtual interface is now defined at 6.95 min with 8 points selected for averaging. The delay layer of 6.95min indicates that there is no growth until 6.95min. A GaAs growth rate of 2 Å/sec should be a good starting value.

```
2 gaas600
1 delay 6.95 minutes
0 virtual (fixed, time=6.95)
```
Figure 15.80. The model to be used to fit the ellipsometric data acquired during the growth of the 100 Angstrom GaAs layer.

Generate data. Note again that the data predicted by the nominal model match the experimental data rather closely, indicating the real sample structure is very close to the nominal sample structure.

Now define the GaAs layer thickness, GaAs growth rate, and Delay layer time as fit parameters, and initiate a normal fit. Good fits to the $\psi$ and $\Delta$ data are obtained. The layer thickness is found to be about 97.2Å and the growth rate is about 1.76Å/sec. We encourage the user to analyze the rest of the layers using the approach described above.

**InP Temperature Measurement and Oxide Removal**

A standard procedure for most epitaxial semiconductor growth is to heat the substrate to an elevated temperature to remove the oxide and/or any other contaminating overlayer from the surface before initiating the layer growth. This is an extremely critical part of the growth process, as any imperfections in the crystalline quality of the substrate surface will adversely affect subsequent epitaxial film growth. Since this process is so important, it would be very useful to monitor in real-time the substrate temperature and overlayer thickness. Ellipsometry is sensitive to both the oxide overlayer thickness and the substrate temperature. In this example, an InP substrate temperature is raised to 550°C to desorb the oxide and then brought down to 450°C before starting a layer growth. The data for the example can be found in the file 'InP Temp Example.bdt' in the `\WVASE\Examples` directory.

To analyze the data for this example, start by building the model shown in Figure 15.81. The material files can be found in the `\WVASE\Examples` directory. Notice that the 'inp-t.mat' file is a temperature dependant optical constant library. The 'inp-ox.mat' file represents InP's oxide. The parameters to select for fitting are the InP temperature, the oxide thickness, and the Angle of Incidence. It is reasonable to expect large changes in the temperature to induce changes in the angle of incidence due to thermal expansion of the substrate manipulator. It is also necessary in this case to allow the thickness of the oxide to go negative, as this thickness is relative to the oxide thickness on the wafer used to measure the InP oxide thickness. Do this by choosing the 'Edit Parms' menu item from the Fit Window. In the dialog (Figure 15.82) select the oxide thickness parameter (Thick.1) from the list of parameters and then enter –100 into the 'Minimum' box and press the ‘Change Parm Coupling’ button. Now the dialog should look like Figure 15.82.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>inp-ox</td>
<td>0 Å</td>
</tr>
<tr>
<td>inp-t Temp=22</td>
<td>1 mm</td>
</tr>
</tbody>
</table>

Figure 15.81. The model used to fit for the InP temperature and oxide thickness. The fit parameters are the substrate temperature, oxide thickness, and angle of incidence.
In Situ Dynamic Data Analysis and Examples

In Situ Dynamic Data Analysis and Examples

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Figure 15.82. The Edit Fit Parms dialog. The oxide thickness fit parameter needs to be modified to allow it to become negative, as it is a measure of the oxide thickness 'relative' to the thickness on the wafer which was used to measure the temperature dependant optical constant library.

Finally, perform a point-by-point fit. When the fit is done, the psi and delta fits should look like Figure 15.83. Next, look at the fit parameter values versus time by activation the graph window and then choosing 'Point by Point Fit Parms' from the 'Data' menu. The graphs of the Temperature and Oxide thickness should look like those in Figure 15.84. Notice that the oxide starts to desorb at ~34min. and is completely removed by 40min.

Figure 15.83. The (a) psi and (b) delta data fits for the InP temperature example.

Figure 15.84. The results of fitting for the InP temperature and oxide thickness. The oxide starts to desorb when the temperature gets to ~500°C.
InGaAs composition

In this example, the FastDyn layer will be used to measure the composition, thickness, growth rate, and surface roughness of an InGaAs film grown on InP. The growth temperature was 450°C. The data is in the file ‘InGaAs Comp.bdt’ in the \WVASE\Examples directory. This example is explained with the assumption that the default settings are set to display wavelength in eV and thickness in Å. Psi and Delta data at three wavelengths are displayed in Figure 15.85.

Figure 15.85. The (a) psi and (b) delta data for the InGaAs composition example.

For the analysis of this layer, the Surface+Layer analysis capability of the FastDyn layer will be used. Start by building the model shown in Figure 15.86. The ‘inggaas comp.mat’ file can be found in the \WVASE\Examples directory. Set the initial value for the ‘inggaas comp’ temperature to 450°C – the other values will be set in the FastDyn layer dialog.

Figure 15.86. The model used to fit for the InGaAs composition, growth rate, and surface roughness.

The next step is to setup the FastDyn layer parameters. In this example we are fitting for the thickness of the layer and the near surface composition. This
means we need to use the 'Surface+Layer' analysis of Fastdyn. Select the 'Surface + Layer' option now. The '# of Data Points for Fit' box contains the number of points to include when determining the near surface composition. Ten is a good default value. If the layer is growing very slowly then you may want to increase the number of points to use to decrease noise in the fit results. On the other hand, if the composition is changing quickly you may need to use fewer points to better track the changes, although you will have to live with more noise in the composition results.

As discussed in the FastDyn layer section earlier in this chapter, the Surface + Layer analysis actually fits the data twice, once for the layer thickness and again for the near surface composition. These two fits will typically use different wavelength ranges, as sensitivity to thickness occurs at spectral ranges where the material is less absorbing and sensitivity to near surface composition usually occurs where the film is more absorbing. In this example, all of the wavelengths are selected for composition fitting and only the 1.6-3.0eV spectral range will be selected for the thickness fit.

In this example, the film starts growing at approximately 2.3 minutes so the Selection Start Time and Layer Start Time need to be set to 2.3 minutes. Also, the growth rate, composition, surface interface thickness (roughness), and calculated thickness need to be set as fit parameters. Minimum thicknesses for growth rate and composition fitting should be set to 100Å or so since there is very little sensitivity to these parameters when the film is very thin. It is also a good idea to fit for the virtual interface parameters. When all of the parameters are setup the FastDyn dialog should look like Figure 15.87.

![Figure 15.87. The FastDyn layer dialog setup to fit for growth rate, composition, surface roughness, film thickness, and virtual interface parameters. The growth rate, composition, and virtual interface parameters will not be fit for until the film is at least 100Å thick.](image)

Finally, perform a point by point fit. There will be a dialog that appears asking the user to confirm the initial starting values (Figure 15.88). Notice that the layer thickness (Thick.0) starts off at a very large value. You should set the value close to the initial layer thickness or the fit will fail. In this case enter a number such as 100 for Thick.0 and press OK. Click OK again when the change starting parameters dialog appears. Figure 15.89 shows the results of the fit.
Figure 15.88. The Starting Parameter Values dialog allows the user to change the initial starting values for a fit.

Notice in Figure 15.89 that the parameter values start at the values we gave as initial starting values and then, after four or five minutes, change to the best fit values. This is caused to the 100Å minimum thickness values we entered into the FastDyn dialog. We essentially told FastDyn to trust our initial values until the film has grown to a thickness of 100Å. Now that we can see our initial values were a little off, open up the FastDyn layer dialog again and enter values close to the average of the fit parameter results (i.e. composition = 0.531, roughness = 3.25, growth rate = 1.36). Perform the fit again. This does not change the fit results after the 100Å minimum thickness has been reached but it does produce graphs that make more sense (Figure 15.90).
Figure 15.90. The final results for the thickness, composition, growth rate, and surface roughness of the InP film.

15.7 References


Appendix A Analysis File Formats

Experimental and generated data files

Column formatted ASCII data files are used to store the experimental data (ellipsometric, reflection, and/or transmission) used by the WVASE™ program. The columns may be separated by any number of spaces or tabs (but not commas). The first line of the any WVASE™ data file contains a description (or comment) for the data. The remaining lines of the file depend on the type of data file, and are described in the following sections.

The second line of the data file describes the units used to specify the wavelength of light, and is optional. The acceptable specifiers are: 'Angstroms', 'nm' (nanometers), 'eV' (photo energy), 'um' (microns), and '1/cm' (wavenumbers). If this line is omitted, the default units are Angstroms. If the word 'TRIG' follows the units specifier, the ellipsometric data are stored in Tan(Psi) / Cos(Delta) format, as opposed to the default Psi / Delta format.

The remaining lines of the file list the experimental data. The column definitions are as follows (each line may have a different data type, i.e., it is possible to mix different types of experimental data within the same file). Note that if the data format does not explicitly give the standard deviation for the measurement, the WVASE™ program will assign a value for the standard deviation on the measurement. The default standard deviation value can be modified in the wvase.cnf file.

Ellipsometric data
Ellipsometric data: Wavelength Angle Psi Delta
Dynamic data: Wavelength Angle Psi Delta Time
Ellipsometric data with error bars: Wvl Angle Psi Delta dPsi dDelta
(dPsi and dDelta are the standard deviations in Psi and Delta)
Dynamic data with error bars: Wvl Angle Psi Delta dPsi dDelta Time
Units: Psi and Delta are in degrees, unless the TRIG option is specified. The Angle of incidence is also in degrees. Time is specified in minutes.
Reflection and transmission data

xx  Wavelength  Angle  R/T  dR/T

where 'xx' is:

pT  for p-polarized transmission data
sT  for s-polarized transmission data
uT  for user-polarized transmission data

(the substrate backside reflection is accounted for with any transmission data)

pR  for p-polarized reflection data
sR  for s-polarized reflection data
uR  for user-polarized reflection data

(the substrate backside reflection is not accounted for with this type of reflection data)

pRb for p-polarized reflection data, with backside reflections
sRb for s-polarized reflection data, with backside reflections
uRb for user-polarized reflection data, with backside reflections

(the substrate backside reflection is accounted for with this type of reflection data)

The 'R/T' column is the transmission or reflection value (between zero and one). The 'dR/T' column is optional, and contains the standard deviation of the measurement.

Neutron reflection data

N  k  R  dR

where 'k' is the neutron momentum (in Å⁻¹), 'R' is the neutron reflectivity, and 'dR' is the standard deviation of the measurement.

Experimental data file examples

This file contains ellipsometric data, stored in Tan(Psi) / Cos(Delta) format, with the wavelength in nanometers:

Example file #1

nm  TRIG
300  70  .245  .123
400  70  .283  .034

The next file contains ellipsometric data, in Psi /Delta format with standard deviations, with the wavelength in eV:
Example file #2

<table>
<thead>
<tr>
<th>eV</th>
<th>1.5</th>
<th>70</th>
<th>20.32</th>
<th>140.32</th>
<th>.12</th>
<th>.15</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5</td>
<td>70</td>
<td>18.23</td>
<td>170.32</td>
<td>.08</td>
<td>.32</td>
<td></td>
</tr>
</tbody>
</table>

The following file contains both unpolarized transmission data and ellipsometric data, with the wavelength in the default units of Angstroms:

Example file #3

<table>
<thead>
<tr>
<th>uT</th>
<th>3000</th>
<th>8.5</th>
<th>0.6734</th>
</tr>
</thead>
<tbody>
<tr>
<td>uT</td>
<td>4000</td>
<td>8.5</td>
<td>0.2323</td>
</tr>
<tr>
<td>3000</td>
<td>70</td>
<td>23.23</td>
<td>98.03</td>
</tr>
<tr>
<td>4000</td>
<td>70</td>
<td>18.27</td>
<td>110.24</td>
</tr>
</tbody>
</table>

---

**Optical constant files (material files)**

The following material file formats are supported by the WVASE™ program: interpolation tables, semiconductor alloys, and temperature dependent materials (Cauchy, Lorentz oscillator, EMA, graded, and user-defined dispersion materials can be defined and saved from within the WVASE™ program, and therefore the file format for these materials will remain undocumented). Column formatted ASCII data files are used to store the optical constant data that describes the material.

**Interpolation table**

- The first line of the data file contains a description (or comment) for the material.
- The second line of the data file sets the units used to specify the wavelength of light. The acceptable specifiers are: 'Angstroms', 'nm', 'eV', 'um', and '1/cm'.
- The third line of the data file is either 'NK' or 'e1e2', denoting whether the optical constants are tabulated in terms of refractive index or dielectric function. Note that in the WVASE™ program, the extinction coefficient 'k' should be positive. This is opposite of the convention used in the earlier J.A. Woollam Co., Inc. analysis programs.
- The remaining lines of the file contain three columns: Wvl  n  k
  (Wvl is in the specified units; replace 'n' & 'k' with 'e1' & 'e2' if the third line of the file is 'e1e2')
- Look at the si.mat and ag.mat data files for examples of the interpolation table file format.

**Semiconductor alloy**

A critical point dependent spectrum shifting / weighted averaging algorithm (from P.G. Snyder et. al., J. Appl. Phys. 68, 5925 (1990) ) is used to describe the alloy dependent effects in compound semiconductors. The following file format contains all of the parameters required by the alloy algorithm.
The first line of the data file contains a description (or comment) for the material.

The second line of the data file must be 'ALLOY'.

The third line of the data file describes the units used to specify the wavelength of light. The acceptable specifiers are: 'Angstroms', 'nm', 'eV', and 'um'.

The fourth line of the data file is either 'NK' or 'e1e2', denoting whether the optical constants are tabulated in terms of refractive index or dielectric function.

The fifth line specifies the number of alloy fractions.

The sixth line lists the value of the alloy fractions.

The seventh line lists the number of critical points.

The next lines give the coefficients of the third degree polynomials that assign the critical point positions (in eV) as a function of alloy fraction.

The rest of the file contains the optical constant data at the different alloy fractions. A three column format, identical to the interpolation table format, is used. Blank lines are used to separate the optical data from different alloy fractions.

Look at the alx_gaas.mat material file for an example of the semiconductor alloy file format.

**Temperature dependent**

A simple interpolation algorithm is used to calculate the optical constants of a material at an arbitrary temperature, given the optical constants at number of reference temperatures.

The first line of the data file contains a description (or comment) for the material.

The second line of the data file must be 'TEMP'.

The third line of the data file describes the units used to specify the wavelength of light. The acceptable specifiers are: 'Angstroms', 'nm', 'eV', 'um', and '1/cm'.

The fourth line of the data file is either 'NK' or 'e1e2', denoting whether the optical constants are tabulated in terms of refractive index or dielectric function.

The fifth line specifies the number of temperatures.

The sixth line lists the value of the temperatures.

The rest of the file contains the optical constant data at the different temperatures. A three column format, identical to the interpolation table format, is used. Blank lines are used to separate the optical data from different temperatures.

Look at the gaas_tmp.mat material file for an example of the temperature dependent file format.
Appendix B Configuration File Formats

Overview

WVASE™ uses three files to keep track of the current program and system configuration: \textit{wvase.cnf} (stores user preferences for the WVASE™ program), \textit{hardware.cnf} (describes the current configuration of a J.A. Woollam Co., Inc. ellipsometer which is interfaced to the system), and \textit{ch Rae.cnf} (contains the current motor settings for the J.A. Woollam Co., Inc. beam-chopped rotating analyzer ellipsometer). All three of these files must be located in the c:\wvase subdirectory. The format of the \textit{ch Rae.cnf} file is undocumented, as this file should never be modified by the user.

WVASE.CNF

A sample \textit{wvase.cnf} file is printed below, followed by comments as to the functionality of the entries. If \textit{wvase.cnf} is deleted from the c:\wvase subdirectory, the WVASE™ program will create a new \textit{wvase.cnf} file using default values for all of the entries. Most of the entries in this file should not be directly modified by the user, but should be changed only with WVASE™.

Sample \textit{wvase.cnf} file:

\begin{verbatim}
[Windows]
MAIN= 0 0 640 416 0
MODEL= 0 0 330 158 1
GRAPH= 240 145 400 297 1
GEN= 0 158 261 99 1
EXP= 330 0 344 158 1
FIT= 0 257 261 185 1
HARDWARE= 50 50 500 300 0
Maximize= 1
Focus= 3
\end{verbatim}
[Graphics]
Font=Arial

[Fit]
dVASE=0.001
dRefl=0.01
dTrans=0.005
Derivative Incr=0.001
Type= 114

[VASE]
Units= 0 0 1
Handedness= 1
Wvl Start=4000
Wvl End=10000
Wvl By=25
Ang Start=70
Ang End=80
Ang By=5
Dir=c:\wvase\neutron
DefSubThickness=1

[Memory]
MaxLayers= 50
MaxFitParms= 25
MaxWvls= 200
MaxData= 3000

All of the entries under the [Windows] section describe the size and position of the various windows on the WVASE™ screen. Do not modify these entries directly; they are automatically saved by WVASE™ at the end of each session, such that the window configuration set up by the user is maintained when the program is restarted.

Under [Graphics], the font used for the 'Graph' window is specified (in this case the font is 'Arial'). It should be changed only with the 'Graph Edit Font' menu option.

The 'dVASE', 'dRefl', and 'dTrans' entries define the default standard deviations for data that is read into the Experimental Data window. The 'Derivative Incr' and 'Type' should be changed only with the 'Fit Defaults' menu option.
The entries in the [VASE] section store the default Units, Handedness fix, Wavelength and Angle ranges, and User Directory. Do not change these entries directly, instead use the appropriate menu options within WVASE™ to specify your preferences.

The ‘DefSubThickness’ option may be directly modified in this file. It is used to specify the default thickness (in mm) of any substrate added to the model.

The [Memory] options control how much memory WVASE™ allocates for model layers, fit parameters, wavelengths, and data. The higher these values are set, the more system memory WVASE™ will require.

---

**HARDWARE.CNF**

A typical hardware.cnf file is shown below. Note the file is internally documented by the comment lines which start with ‘;’. For your J.A. Woollam Co., Inc. ellipsometer hardware to work properly, it is extremely important that all of the entries in the hardware.cnf file match your ellipsometer. Included with this manual is a sheet that lists the correct settings in the hardware.cnf file for your system.

```plaintext
[Hardware]
;type should be 'RAE' or 'insitu'
Type=RAE
;for IR filt set: 4200 6000 10400, for 'old' filt set: 3900 5000 8000
FilterWvls=4200 6000 10400
;SolarBlind is the wvl range where the solar blind is 'in', should be '0 0' if no solar blind is present
SolarBlind=2000 3000
;DMA should be 1 or 3 (the Dash16 card must be set accordingly)
DMA_Channel=1
;IRDet should be 'yes' or 'no'
IRDet=yes
IRDetSwitchWvl=10500
Dash16BASE=768
PIO24BASE=784
PIO24#2BASE=800
;IBM should be 'yes' or 'no'
IBM=no
;Dash16Clk should be 1 or 10 (the Dash16 card must be set to 1 or 10 Mhz)
Dash16Clk=1
;Monocromator should be either PTI or DK
Monochromator=PTI
DKComPort=1
;GratingSwitch is the wvl which the DK mono should automatically switch gratings
```
GratingSwitch=6500
;Translation should be 'none' or 'r-theta'
Translation=none
;Base should be 'vert' or 'horz'
Base=vert

[Motors]
;the format for the Motors section is:
; motor name = steps/unit Delay
; for Delay, enter a floating point number to determine the motor speed
Polarizer=200 .002
Monochromator=.4 .004
Sample=400 .004
Detector=400 .004
Filter=100 .012
iPol1=200 .002
iPol2=200 .002
rTrans=393.7007874 .001
thetaTrans=50 .0001
Absolute minimum

An absolute minimum is defined as the lowest possible value of the MSE which may be obtained for a given set of model parameters. There may be more than one set of model parameters which yield absolute minimum MSE value, in which case the best-fit set of model parameters is not unique.

Absorption coefficient

The absorption coefficient is defined as $2\pi$ times the extinction coefficient (at a given wavelength) divided by the wavelength.

Absorption edge

An absorption edge is defined as the onset of absorption which occurs at the bandgap energy for semiconductor and dielectric materials. The material will be transparent for energies less than the bandgap energy (below the absorption edge) and absorbing for energies greater than the bandgap energy (above the absorption edge).

Accuracy

The accuracy of an optical experiment relates to how close the parameters determined by the optical experiment are to their actual values. For example, a very accurate experiment would yield layer thicknesses which are very close to the true layer thicknesses. The measurements may be very noisy, but as long as the averages of the parameter values (thicknesses, for example) over many measurements are very close to the true parameter values, the measurement is considered to be accurate.

Alignment detector

The alignment detector is a four-quadrant silicon photodiode detector with a small hole bored through the center, at the intersection of the four quadrants. When the alignment detector is mounted on the ellipsometer (on the input arm, just after the input polarizer), the light beam passes through the hole, is reflected from the sample (at normal incidence), and returns to strike the alignment detector. If the sample is perfectly aligned, the signal from each of the four quadrants will be equal.
Alignment jig

The alignment jig is used in M-44® systems to perform the fundamental optical alignment of the system.

Alloy layer

An alloy layer is a special parametric model for compound semiconductors. This model parameterizes the optical constants of a given alloy system in terms of a single parameter, the alloy fraction of one constituent of the alloy. Alloy layers are implemented in WVASE™ for AlGaAs, HgCdTe, InGaAs, and SiGe, for example.

Alloy-temp layer

An alloy-temp layer is a special parametric model for compound semiconductors. This model parameterizes the optical constants of a given alloy system in terms of two parameters, the alloy fraction of one constituent of the alloy and the temperature of the system. These layers are primarily used for analysis of data acquired in-situ during high temperature growth of compound semiconductor layers.

Ambient light

Ambient light is unwanted light which enters the detector of the ellipsometer from the surroundings.

Ambient medium

The ambient medium is the medium from which the light beam is incident upon the sample under test. The ambient medium is usually air (index of refraction of unity, no absorption), but other gases and liquids may be used as ambient media as well.

Analyzer

The word ‘analyzer’ is used to refer to the rotating polarizer (in a rotating analyzer ellipsometer) through which the light beam passes after it is reflected from the sample. It is called the analyzer because it is used to ‘analyze’ the polarization state of the light beam which passes through it.

Angle of incidence

The angle of incidence (usually denoted \( \phi_0 \)) in an optical experiment is defined as the angle between the incident light beam and the sample normal. The angle between the incident light beam and the sample surface will be \( 90^\circ \) minus the angle of incidence.

Angular spread

The range of angles of incidence at which the individual photons in the light beam struck the sample is termed the angular spread. This can be significant if the sample surface is curved or the light beam is poorly collimated.
**Anisotropic calibration scan**

An anisotropic calibration scan is a special type of spectroscopic scan which is accessed through the ‘Advanced Scan Options’ button in the spectroscopic scan dialog box (from the ‘Acquire data’ menu in the Hardware window). At each specified wavelength and angle of incidence, the Fourier coefficients of the detector signal are measured over a range of input polarizer positions, and these data are fit to determine the standard ellipsometric psi and delta values for the sample, as well as ratios of the off-diagonal to diagonal elements of the sample Jones matrix. This type of scan is useful for anisotropic or depolarizing samples.

**Anisotropic Cauchy layer**

An anisotropic Cauchy layer (acauchy.mat) is used to model uniaxially anisotropic materials in spectral regions where they are transparent. A three term Cauchy dispersion relation is used to model the dispersion of the index of refraction along the ordinary and extraordinary optical axes.

**Anisotropic layer**

An anisotropic layer is a layer (or substrate) in the optical model which may be optically anisotropic. *WVASE*™ contains two anisotropic layer types, standard anisotropic layers and anisotropic Cauchy layers (acauchy.mat).

**Anisotropy**

Anisotropy refers to a difference in some property of a material for different directions in the material. For example, an optically anisotropic material will exhibit different optical constants depending on what direction the light beam is propagating in the material.

**ASCII data file**

Most files stored by *WVASE*™ are stored as ASCII format text files. These are files which may be edited by any standard word processing program, and they may also be viewed and printed from the DOS prompt.

**Attenuation coefficient**

The attenuation coefficient is a calibration parameter of both the *VASE*® and *M-44®* systems. It is equal to the ratio of the gain of the amplifier circuits for the AC component of the detector circuits to the gain of the amplifier circuits for the DC component of the detector circuits. In other words, it specifies how much the AC component of the detector signal is attenuated with respect to the DC component.

**Back-surface reflection**

A back-surface reflected beam is defined as a component of the light beam which has penetrated the sample, reflected from the back surface of the substrate, and entered the detector of the ellipsometer. A back-surface reflected beam will not in general add coherently with the front-surface reflected (primary) beam(s), and requires special treatment when performing model calculations.
**Background scan**

A background scan refers to the measurement of the intensity of the light beam as a function of wavelength with the ellipsometer set in the straight-through configuration and no sample present. This scan must be performed prior to measurement of intensity type data, such as reflection or transmission.

**Bandgap**

Semiconductor and dielectric materials exhibit an energy bandgap. Photons with energy less than the bandgap energy cannot excite electrons in the material to higher energy levels. Optical absorption occurs at energies greater than the bandgap energy.

**Bandwidth**

The bandwidth refers to the range of wavelengths present in the light beam exiting the monochromator of the VASE® system (typically ~2 nm), or to the range of wavelengths which are incident upon a single element of the photodiode detector array in the M-44® system (typically ~12 nm).

**Best-fit model**

The best-fit model for a set of data is the model which yields the lowest MSE for that set of data.

**Binary data file**

Dynamic ellipsometric data may be stored by WVASE™ in a binary data format, designated by the file extension `.bdt`. This format requires much less disk space than the ASCII text format, but may not be viewed or printed by word processors or DOS.

**Birefringence**

Birefringence is a type of optical anisotropy in which a transparent material exhibits differing indices of refraction for right- and left-circularly polarized light. Birefringence may be due to crystalline anisotropy (quartz, for example), or due to stress in the sample (windows on a vacuum chamber, plastic substrates, for example).

**Brewster angle**

The Brewster angle is defined (for our purposes) as the angle of incidence (for a given wavelength) at which the sample exhibits an ellipsometric delta value of 90°. When the sample has coatings or layers on the surface, this angle of incidence is referred to as the pseudo-Brewster angle. This angle of incidence usually provides maximal sensitivity to the properties of the sample under test.
Bulk

A bulk sample is considered to be a thick substrate with no coatings or multilayers on its surface. Even though a true ideal bulk sample rarely occurs in practice, the bulk sample is a useful concept for analysis purposes.

Calibration

Calibration is a procedure which is performed on an experimental apparatus to determine the values of one or more internal (non-sample dependant) experimental parameters. For a rotating analyzer ellipsometer, a calibration procedure is required to determine the location of the axes of the input polarizer and the analyzer, and the relative attenuation of the AC component of the detector signal with respect to the DC component of the detector signal.

Calibration parameter

A calibration parameter is an instrument parameter whose value is determined by the system calibration.

Cauchy dispersion model

The Cauchy dispersion model is used to describe the dispersion of the index of refraction of materials in spectral ranges in which the given material is transparent. The Cauchy dispersion model is specified as follows:

\[ n(\lambda) = A + B/\lambda^2 + C/\lambda^4 \ldots \]

where the wavelength \( \lambda \) is given in microns, and A, B, and C are fit parameters. This model is very effective for describing the index of refraction of dielectric materials and semiconductors in spectral regions where they are transparent (i.e. where the extinction coefficient is zero).

Check box

A check box is used throughout WVASE™ to enable or disable fit parameters or program options. This is a small square box which is empty when disabled and will contain an ‘x’ when enabled.

Chop

This value is displayed in the ‘Display Signal’ screen and in the Hardware window during data acquisition. The ‘Chop’ parameter is proportional to the strength of the DC component of the detector signal.

Chop + 2A

This value is displayed in the ‘Display Signal’ screen and in the Hardware window during data acquisition. The ‘Chop + 2A’ parameter is proportional to the strength of the AC component of the detector signal.
Circularly polarized light

A light beam is circularly polarized if, when looking directly into the propagating beam, the tip of the electric field vector of the beam describes a circular path in the plane perpendicular to the propagating beam. A beam may be right- or left-circularly polarized if the tip of the electric field vector is precessing in a clockwise or counter-clockwise direction, respectively.

Coarse calibration

A coarse calibration may be performed to determine the approximate values of the calibration parameters. This type of calibration is typically performed when a fine calibration has been performed and failed to yield reasonable results. A coarse calibration consists of measurement of the signal Fourier coefficients over a very broad range of polarizer angles, followed by a fit to these measured data to determine the values of the calibration parameters and the sample psi and delta values.

Coherence

Coherence refers to the way in which two light beams will mix with each other. When two beams add coherently, the electric fields of the beams are summed, such that interference effects may occur and the resulting beam has a single well-defined polarization state. When two beams do not add coherently, the intensity of the beams is summed, such that interference effects do not occur and the resulting beam does not have a single well-defined polarization state. Beams reflected from the top and bottom surfaces of a thin film will add coherently, while beams reflected from the top and bottom surfaces of a thick (>0.1 mm, or so) substrate will not add coherently.

Compensator

A compensator is an optical component which is used to induce a phase change in the p- or s-component of a light beam relative to the other component. The combination of a variable compensator after a variable polarizer may be used to generate beams of any polarization state.

Complex dielectric function

The complex dielectric function \( \tilde{\varepsilon} \equiv \varepsilon_1 - i\varepsilon_2 \)\(^{\dagger} \) is one representation of the optical constants of a material. It is defined as the ratio of the displacement field to the applied electric field at a given point in a material, and is a measure of how polarizable a material is at the given wavelength (or photon energy). The imaginary part of the dielectric function is a measure of how much energy per unit volume and unit time a material will absorb from a light beam of the given wavelength.

Complex index of refraction

The complex index of refraction \( \tilde{n} \equiv n - ik \)\(^{\dagger} \) is one representation of the optical constants of a material. It governs the phase change and amplitude decay of a plane

electromagnetic wave (of the given wavelength) propagating in the material. The real part of the complex index of refraction determines how fast the phase of the propagating wave changes, while the imaginary part (the extinction coefficient k) determines how fast the amplitude of the wave decreases as the wave propagates.

**Composite layer**

A composite layer is a layer consisting of a mixture of two or more materials. The optical constants of the composite material are evaluated from the optical constants and volume fractions (or alloy fraction) of the constituent materials. An effective medium approximation (EMA) is usually used for this calculation.

**Confidence limit**

The confidence limit on a variable model parameter refers to the uncertainty (or error bar) on the final value of the parameter after a fit. WVASE™ calculates 90% confidence limits, which define the range of the parameter value in which there is a 90% probability that the true parameter value lies. The 90% confidence limits are calculated assuming that all errors in the experimental data are random, such that there are no systematic errors in the data.

**Configuration file**

WVASE™ uses several external configuration files to store parameters relating to the system hardware and the software configuration. The file extension '.cnf' is used to designate configuration files. The files hardware.cnf and wvase.cnf may be modified by the user, but the user should never modify other configuration files. Any configuration file should be modified with care, as incorrect values in these files may lead to incorrect functioning of the system and/or damage to the instrument.

**Convergence**

When the fit algorithm reaches a minimum and cannot reduce the MSE further, we say that the fit has converged, or that the algorithm has reached convergence. A fit may also terminate if the maximum number of iterations has been reached, or if the user terminates the fit.

**Convolution profile**

The convolution profile (specified in the ‘Options’ dialog box from the Model window) is used to specify the profile used for the convolution integration required when evaluating the thickness non-uniformity, monochromator bandwidth, or angular spread non-idealities. The width of the profile may be declared as a fit parameter.

**Correlation**

Correlation is a measure of the independence of parameters in the optical model. If two parameters are strongly correlated, there is no unique pair of values for these parameters which yields a best-fit minimum value of the MSE.
Correlation coefficient
Correlation coefficients are elements of the correlation matrix. Element $S_{ij}$ of the correlation matrix represents the correlation between the $i^{th}$ and $j^{th}$ fit parameters. The correlation coefficients may have values between -1 and 1, with values near -1 or 1 representing very strong correlation and values near zero representing nearly independent fit parameters.

Coupling
Coupling refers to the concept of linking two layers or variables together. Layers which are coupled together are forced to have the same optical constants. A fit parameter may be coupled to another fit parameter such that the first parameter always equals the second (or a constant multiple of the second, with the constant termed the coupling constant).

Current layer
The current layer is the layer in the Model window which is designated by the current layer indicator (‘>’, which appears to the left of the model). Pressing <Enter> will open the current layer when the Model window is active, and layers are always added just above the current layer. Also, the current layer optical constants may be displayed in the Graph window.

Current materials list
The current materials list is a list of the materials which are currently loaded in WVASE™. Any time a new layer is added to the model, this list is checked first to see if the material is already loaded.

Current selected range
The current selected range is specified in the ‘Range select’ dialog box from the Experimental Data window. In this dialog box, the user may select the data types, wavelength range, and angle of incidence range which will be fit and/or displayed by WVASE™.

DDE protocol
Dynamic Data exchange - a protocol used by Windows applications for exchanging data between each other.

Default materials directory
The default materials directory is always searched for the specified file when a layer is added to the model. This directory may be specified by the user (c:\wvase\my_mats, for example).

Delay layer
A delay layer is used in the analysis of dynamic data to represent a pause in the process during which nothing occurs.
Delta

The ellipsometric parameter delta (\( \Delta \)) is defined as the difference in phase between the p- and s-direction pseudo-Fresnel reflection coefficients of the sample at the given wavelength and angle of incidence. \( \Delta \) ranges from 0° - 180° for standard VASE® and M-44® systems, but will range from 0° - 360° when measured by systems with the auto-retarder option installed.

Depolarization

Depolarization occurs when interaction with the sample causes the reflected beam to be partially polarized. This will occur when the sample is extremely rough or exhibits back-surface effects, when a film on the sample is non-uniform or patterned, and when monochromator bandwidth or angular spread effects are significant.

Depth profile

A plot of the variation in optical constants versus depth into the sample, obtained in WVASE™ by selecting 'Data' from the Graph menu, then selecting 'Depth profile of optical constants'. This is usually used with respect to graded models.

Detector

A detector is an optical element which generates an electrical voltage (or current) proportional to the intensity of the light beam incident upon it. Common detector types are photomultiplier tubes (used in the past, but nonlinear, and require a large d.c. bias voltage), semiconductor photodiodes (silicon and InGaAs are used in the J. A. Woollam Co., Inc. VASE® ellipsometers), and semiconductor photodiode arrays (used in the J. A. Woollam Co., Inc. M-44® instrument).

Dielectric

A dielectric material is traditionally defined as a material which is a poor conductor of electricity. For optical experiments, we loosely define dielectric materials as materials which are transparent over most or all of the measured spectral range.

Dispersion

Dispersion is defined as the dependence of any quantity on the light beam wavelength (or photon energy). For example, dispersion of the index of refraction refers to the change of the index of refraction as a function of wavelength (or photon energy).

Dispersion model

A dispersion model is a functional model which specifies the dispersion of some quantity (usually the optical constants of a given material) in terms of a relatively small number of parameters. WVASE™ contains implementations of a large number of dispersion models, including Cauchy, Lorentz oscillator, user-defined, effective medium approximation, and parametric semiconductor models.
**Drude model**

The Drude model predicts the optical constant dispersion for absorption due to free carriers. This model is very useful for transparent conducting oxides, and may be obtained as a limiting case of a single Lorentz oscillator when the center energy of the oscillator is zero.

**Dynamic data**

Data acquired as a function of time from a sample which is changing as a function of time.

**Dynamic-spectroscopic mode**

Dynamic data may be viewed in the dynamic-spectroscopic mode. In this mode, full spectra which were acquired at selected instants in time are displayed.

**Effective medium approximation**

An effective medium approximation (EMA) is a mathematical model used to calculate the effective optical constants of a composite material given the optical constants and volume fractions of the constituent materials in the composite.

**Ellipsometric parameters**

The ellipsometric parameters psi and delta are measured in ellipsometric experiments.

**Ellipsometry**

An optical technique which measures the change in polarization state of a light beam reflected from or transmitted through the sample under study. Ellipsometry usually measures two real quantities (the ellipsometric parameters psi and delta) as functions of the wavelength and angle of incidence of the probing light beam.

**Elliptically polarized light**

A beam of light is elliptically polarized if, looking into the propagating beam, the tip of the electric field vector of the propagating wave precesses around an ellipse.

**Error bar**

The term error bar is generically used to represent uncertainty in measured data points (standard deviations) and fit parameters (90% confidence limits).

**ex-situ**

Refers to measurements from a sample acquired after the sample has been removed from the processing chamber.
**Exponential absorption model**

The exponential absorption model contained in the Cauchy dispersion model layer defines the extinction coefficient as an exponential function of the wavelength. This model sometimes works for the onset of absorption in semiconductors and dielectric materials.

**Extinction coefficient**

The extinction coefficient \(k\) is the imaginary part of the complex index of refraction, and governs the rate at which a propagating wave will decay as it propagates. If \(k\) is zero, the amplitude of the wave will remain constant as the wave propagates, and the material is said to be transparent.

**File extension**

Any file stored on an MS-DOS based personal computer will be stored with a file name consisting of a file prefix (up to eight characters) and a file extension (a period followed by up to three characters). For example, the file name ‘cauchy.mat’ has the file prefix ‘cauchy’ and the file extension ‘.mat’.

**Filter**

A filter is an optical element used to eliminate ranges of wavelengths from a light beam which passes through the filter. Order sorting filters are often used to eliminate higher order diffracted components in the beam leaving the monochromator.

**Fit**

A fit is the procedure performed to find the values of the variable parameters in the model which yield calculated data which best match the experimental data.

**Fit parameter**

A fit parameter is a model parameter which is allowed to vary during a fit.

**Fit statistics**

The fit statistics are the quantities calculated after a fit to evaluate the goodness of the fit, including the final MSE, the 90% confidence limits on the variable parameters, and the correlation matrix elements between the variable parameters.

**Fit weighting**

Fit weighting refers to the experimental data points are weighted with respect to each other in the evaluation of the MSE.

**Fourier coefficients**

The Fourier coefficients of the detector signal are obtained by Fourier analysis of the signal output from the detector, and are the basis for the measured psi and delta values.
Free carrier absorption

Free carrier absorption refers to the absorption of light by free (or nearly free) carriers in metals and semiconductors. The Drude model (obtained as a limiting case of the Lorentz oscillator model) is used to describe free carrier absorption.

Fresnel coefficient

A Fresnel coefficient is defined as a complex coefficient which describes the change in amplitude and phase of the electric field of a light beam which is reflected from or transmitted through an interface. Separate Fresnel coefficients describe the reflection or transmission of p- or s- polarized light, and light of arbitrary polarization state is treated by decomposing it into its p- and s-components. The Fresnel reflection and transmission coefficients of an interface are functions of the optical constants of the materials on each side of the interface (at the wavelength of the light beam), and the angle of incidence of the beam on the interface.

Function-based optical constant model

A function-based optical constant model is a mathematical parameterization of the optical constants as a function of wavelength (or photon energy) in terms of one or more parameters.

Fused silica

Fused silica, or fused quartz, is a very useful substrate material, exhibiting a very well-known and reproducible index spectrum and no absorption over the entire UV-VIS-NIR spectral range.

Generalized anisotropic ellipsometry

In a generalized anisotropic ellipsometric experiment the sample Jones matrix is not assumed to be diagonal, and in addition to the standard ellipsometric psi and delta values, ratios of the off-diagonal to diagonal elements of the sample Jones matrix are measured as well. This type of ellipsometry can be very useful for very rough or anisotropic samples.

Goniometer

A goniometer is a rotational stage used to precisely set the angle of incidence.

Graded layer

A graded layer is a layer whose optical constants change from top to bottom through the film.

Grading profile

The grading profile is the profile of the optical constants as a function of depth in a graded film.
Growth rate analysis

Growth rate analysis is a dynamic data analysis technique based on the assumption that the growth rates of individual layers are constant during the growth of the layer.

Handedness change

A handedness change is a wavelength where, as the wavelength increases, delta peaks at 180° or drops to a minimum at 0°. Technically, if we look into the propagating beam, the tip of the electric field vector changes the direction in which it is precessing at these points, thus the name ‘handedness-change’.

Hardware initialization

Hardware initialization is the procedure performed by WVASE™ to check that an ellipsometer is attached to the computer and is functional.

In-situ

Refers to measurements from a sample while it is being processed, usually in a vacuum chamber.

Index of refraction

The index of refraction ‘n’ is the real part of the complex index of refraction \( \tilde{n} = n - ik \). The index of refraction governs how the phase of a wave changes as it propagates in a material of the given index.

Interference

Optical interference occurs when two propagating waves add together coherently. An example is the addition of beams reflected from the top and bottom surfaces of a thin film.

Isotropic

A material is isotropic if its physical properties (optical constants, electrical conductivity, thermal conductivity, etc.) do not depend on the orientation of the material. In other words, in an isotropic material all directions are equivalent.

Jones matrix

A Jones matrix is used to describe the effect of an optical system on a totally polarized light beam (represented by a Jones vector). Since Jones vectors have two components, Jones matrices are 2×2 matrices. The diagonal elements of the Jones matrix determine change of amplitude and phase of the p- and s- components of the light beam, while the off-diagonal components (usually zero) specify the magnitude and phase of the p- (s-) component of the beam which is scattered by the optical system into the s- (p-) direction.
Jones vector

A Jones vector is a two component vector which completely specifies the polarization state and intensity of a totally polarized beam of light. The complex amplitudes of the p- and s-direction components of the electric field of the light beam are specified as the two components of the Jones vector.

Kramers-Kronig relation

The Kramers-Kronig relation is a special case of the Hilbert transformation integral which relates the real and imaginary parts of the complex index of refraction or complex dielectric function. This relation is derived from the principle of causality, and places constraints on the dispersion of the optical constants.

Linearly polarized light

If we look into a linearly polarized light beam propagating toward us, the tip of the electric field vector of the beam will move along a straight line intersecting the center of the beam.

Lorentz oscillator dispersion model

The Lorentz oscillator dispersion model is used to describe the dispersion of both the index of refraction and the extinction coefficient (or equivalently the real and imaginary parts of the complex dielectric function) of a material. The Lorentz oscillator model is Kramers-Kronig consistent, and describes the optical constants of a material as a sum of contributions from individual oscillators, each parameterized by a center energy, amplitude, and broadening. WVASE™ supports Lorentz oscillator layers with up to seven oscillators. This model works well for transparent conducting oxide materials, metals, and resonant absorption features (such as a dye line).

Material files

Files which specify the optical constants of a given material. The optical constants may be specified in tabular form or by a functional representation.

Menubar

The bar at the top of the screen containing a list of menu titles. Clicking on any menu title will open that menu. The WVASE™ menubar contains different menu titles depending on which window is active.

Model

An optical model consists (most simply) of the optical constants and layer thicknesses of all materials and layers in the sample, plus the equations required to predict the experimental data as a function of these parameters.

Monochromator

A monochromator is used to separate light of a given wavelength from a white light beam.
MSE

The mean-squared error (MSE) is the sum of the squares of the differences between each measured and experimental data point, divided by the standard deviation of the experimental data point. When the MSE is unity, the calculated data (on the average) lie within one standard deviation of the experimental data.

Multiple sample analysis

A multiple sample analysis is performed by simultaneously fitting the data from two or more samples. Fit parameters are coupled between the models to take advantage of the additional information provided by the use of multiple samples.

NAN

‘NAN’ is an abbreviation for ‘not a number’ which will sometimes appear in place of a number for the correlation matrix elements or 90% confidence limits if the fit is extremely correlated.

Native oxide

The native oxide on a sample is the surface oxide layer which grows naturally in atmosphere.

Normal fit

A normal fit consists of varying all defined fit parameters simultaneously to fit the active experimental data.

Normal incidence

At normal incidence the incident and reflected beams are collinear, and the angle of incidence is 0 degrees.

Optical constants

Material parameters which specify how the given material will respond to an applied electric field which is oscillating at optical frequencies. \( \text{WVASE} \) represents the optical constants as the complex index of refraction or the complex dielectric function.

Optical model

A mathematical model used to calculate the optical response of a layered structure (sample). An optical model must specify the thicknesses of all layers (except the substrate) in the sample, as well as the optical constants of all layers and the substrate (either directly or via a parametric function). In \( \text{WVASE} \), the optical model is represented graphically in the Model window.

Optical thickness

The optical thickness (or phase thickness) of a (transparent) film is given by the product of the index of refraction of the film and the physical thickness of the film.
**Optically thick**

A film or sample is said to be optically thick if it is opaque, or, more generally, if the front and back-surface reflections from the sample (or film) do not mix coherently.

**p-direction**

The p-direction (or p-plane) is one of the two orthogonal basis directions used to specify the electric field (or polarization state) of an arbitrarily polarized beam of light. The p-direction lies in the plane of incidence (the plane which contains the incident and reflected light beams and the sample normal), and always points away from the surface of the sample (in other words, the component of the p-direction along the z-axis is always positive). The p-direction, s-direction, and the direction of propagation of the light beam at any point along the beam always form a right-handed Cartesian coordinate system.

**Parameter limiting**

Parameter limiting is used to constrain parameters such that they do not attain unphysical values during a fit. For example, a layer thickness may be constrained such that it cannot become negative.

**Parametric dispersion model**

See definition of function-based optical constant model.

**Parametric semiconductor dispersion model**

The parametric semiconductor dispersion model is a very sophisticated parametric model for the dispersion of the optical constants of dielectric and semiconducting materials. It is similar to the Lorentz oscillator model in principle (Kramers-Kronig consistent, based on a sum of contributions from one or more oscillators), but is much more flexible. This is the model of choice when working with semiconductor films such as poly-Si.

**Partially polarized light**

A partially polarized beam of light may be broken down into two or more components which are totally polarized. The total beam, however, does not exhibit a single well-defined polarization state.

**Penetration depth**

The penetration depth for a material at a given wavelength is a measure of how far a beam of light of that wavelength will penetrate into the material. A propagating beam will be attenuated to $1/e$ of its original amplitude after propagating a distance equal to the penetration depth. The penetration depth equals the wavelength divided by two times pi times the extinction coefficient.

**Phase thickness**

See the definition of optical thickness.
**Plane of incidence**

The plane of incidence is defined as the plane which contains the incident and reflected light beams and the sample normal. The p-direction lies in the plane of incidence.

**Point-by-point fit**

In a point-by-point fit, the data at each single wavelength (or at each single instant of time if dynamic data are being fit) are fit separately. This type of fit works best when fitting for one set of optical constants only, in which case it is much faster than a normal fit.

**Polarizer**

A polarizer is an optical element which will transform a light beam of any polarization state into a linearly polarized light beam, with the linear polarization lying along the axis of the polarizer (which defines the polarizer axis).

**Polarizer tracking**

Polarizer tracking refers to the practice of moving the polarizer at each measurement such that the polarizer azimuthal angle P roughly equals the measured psi value. This condition minimizes systematic errors in the data due to errors in the calibration parameters.

**Precision**

The precision of an optical experiment relates to how repeatable the measurement is, independent of how accurate the measurement is. If multiple determinations of a layer thickness via ellipsometry yield nearly the same value every time, the experiment is very precise, regardless of whether the measured layer thickness is close to the true thickness of the layer.

**Pseudo-**

The prefix pseudo- is used to designate quantities which were calculated from the experimental data using a bulk model, regardless of whether the sample is actually a bulk sample or not. Pseudo-optical constants and pseudo-Fresnel coefficients are commonly encountered in the literature.

**Psi**

The ellipsometric parameter psi (ψ) is defined as the magnitude of the ratio of the p-to s-direction pseudo-Fresnel reflection coefficients of the sample at the given wavelength and angle of incidence. ψ equals the square root of the ratio of the p- to s-direction reflectances at the given wavelength and angle of incidence. ψ ranges from 0° (at which the p-reflectance is zero) to 90° (at which the s-reflectance is zero).
Randomly polarized light

In a randomly polarized beam of light, the individual photons in the beam are each polarized, but the photon polarizations are random. As a result, the total beam does not exhibit a well defined polarization state.

Reflectance

The percentage of a light beam which is reflected from a given sample. This is an absolute intensity measurement which is usually performed at normal incidence, but may be performed at oblique angles of incidence as well.

Regression

Regression is a numerical procedure used to find the values of variable parameters in a function which yield calculated data from the function which match a given set of (experimental) data as closely as possible. For optical data analysis, multivariate non-linear regression algorithms are usually required.

Relative minimum

Also known as a local minimum, a relative minimum of the MSE can cause the fitting algorithm to converge to the wrong solution. A relative minimum is a minimum value of the MSE which is not the lowest attainable value.

Retarder

An optical retarder will induce a phase delay in one of the orthogonal electric field components of a beam propagating through the retarder (with respect to the other field component). A quarter-wave retarder can convert a linearly polarized beam into a circularly polarized beam.

Reverse direction ellipsometry

Reverse direction ellipsometric data are acquired from the back surface of a film or film stack, with the beam incident through the substrate (which must be transparent).

Rho

The complex ellipsometric parameter rho (\(\rho\)) and the real ellipsometric parameters psi (\(\psi\)) and delta (\(\Delta\)) are defined in terms of the pseudo-Fresnel reflection coefficients of the sample as follows.

\[
\tilde{\rho} \equiv \tan(\psi) \exp(i\Delta) \equiv \frac{\tilde{R}_p}{\tilde{R}_s},
\]

where the p- and s-direction pseudo-Fresnel reflection coefficients are denoted by \(\tilde{R}_p\) and \(\tilde{R}_s\), respectively. Specifying the complex ellipsometric parameter \(\rho\) is equivalent to specifying both of the real ellipsometric parameters \(\psi\) and \(\Delta\).
Rotating analyzer ellipsometer

This is an ellipsometer configuration in which the light beam leaves the light source, passes through a fixed (input) polarizer, is reflected from the sample, passes through a rotating polarizer (the analyzer) and then strikes the detector. A monochromator may be placed between the light source and the input polarizer (as is the case for the J. A. Woollam Co., Inc. VASE® instrument), or a dispersive element may be placed after the rotating analyzer, such that the light beam is then spectrally dispersed onto a detector array (as is the case for the J. A. Woollam Co., Inc. M-44® instrument).

s-direction

The s-direction is one of the two orthogonal basis directions used to specify the electric field (or polarization state) of an arbitrarily polarized beam of light. The s-direction points perpendicular to the plane of incidence and parallel to the surface of the sample. The p-direction, s-direction, and the direction of propagation of the light beam at any point along the beam always form a right-handed Cartesian coordinate system.

Sample normal

The sample normal is a unit vector which is perpendicular to the surface of the sample and points away from the sample.

Semiconductor

A semiconducting material is traditionally defined as a material which exhibits medium resistivity (between a dielectric and metal), and for which the resistivity is a strong function of impurity concentration and temperature. For optical experiments, semiconductors are defined as materials which are absorbing below some cutoff wavelength and transparent above the cutoff wavelength. The cutoff wavelength usually lies within the measured spectral range.

Sensitivity

The sensitivity of the experimental data to a given parameter in the optical model is an important concept in optical experiments. If a small change in some model parameter (a layer thickness or optical constant, for example) causes a significant change in the data calculated from the optical model, the experimental data are sensitive to the model parameter. If changing the model parameter does not yield changes in the calculated data, the experimental data will not be sensitive to the given parameter, and that parameter should not be varied during a fit. Attempting to vary a parameter to which the experimental data are not sensitive will usually lead to the “Singular matrix” error.

Singular matrix

A singular matrix is a (square) matrix which cannot be inverted.

Specular reflection

Specular reflection occurs when the beam is reflected from the sample at the same angle at which it was incident (as in reflection from a mirror). Roughness can cause significant non-specular reflection.
Standard calibration sample

This sample is provided with every VASE and M-44 system, and consists of ~ 25 nm of thermal silicon dioxide on silicon. Calibrating on this sample at 500 nm and 75° angle of incidence will always yield good results.

Standard deviation

In lieu of a full statistical definition of the standard deviation, it can be considered to be a measure of how noisy (or uncertain) a given data point is.

Standard sample

In this manual the phrase ‘standard sample’ refers to the 3” silicon wafer provided with the VASE® or M-44® instrument. This wafer consists nominally of ~20 - 30 nm of thermal silicon dioxide on crystalline silicon, and is an ideal sample on which to calibrate either ellipsometer (use 75° angle of incidence, 500 nm wavelength for UV detector, 1300 nm for NIR detector).

Straight-through configuration

In the straight-through configuration, the light beam leaves the input polarizer and propagates directly into the rotating analyzer and detector. With no sample in place, this should yield a measured psi value of 45 degrees and a measured delta value of zero.

Superlattice

A superlattice is technically a periodic crystalline structure, although we tend to use to term to refer to any periodic layered structure (i.e. structures in which two or more layers are repeated).

Trajectory plot

A trajectory plot is a plot of psi versus delta, usually for a time-varying process.

Transmission ellipsometry

Transmission ellipsometry refers to ellipsometric experiments conducted in transmission through the sample.

Transmittance

The percentage of a light beam which is transmitted by a given sample. Usually performed at normal incidence as a function of wavelength.

Transparent conducting oxide

Transparent conducting oxides are a class of materials which are transparent (or nearly transparent) over much of the visible spectral range, but due to a very high concentration of free carriers are electrically conducting and optically absorbing in the infrared.
**Uniaxial anisotropy**

Uniaxial anisotropy refers to a type of anisotropy in which the material exhibits the same optical constants along two of the Cartesian axes, but exhibits different optical constants along the third axis. In this case the dielectric tensor for the material is diagonal.

**Uniqueness**

A best-fit model (or set of model parameters) is unique if it is the only set of parameter values which yield the minimum (best-fit) MSE value.

**VB-200**

The VB-200 is the electronic control box which interfaces the computer running WVASE™ to the ellipsometer hardware.

**Virtual interface**

The virtual interface is a mathematical construct used for the analysis of dynamic data. The virtual interface is placed just below the surface of the growing film, and everything below the virtual interface is treated as the (virtual) substrate. This approximation (the virtual substrate approximation) works well for semiconductor and metal films, but usually does not work as well for dielectric films.

**Win32s**

32-bit extensions to the Windows operating system. Win32s must be installed to run WVASE.

**Window effects**

Polarization changes may be induced in the light beam when propagating through windows on a vacuum chamber due to stress birefringence in the window.

**WSCRIPT**

The WVASE script file reader, which may be used to automate the acquisitions and/or analysis of data.

**Zone averaging**

Zone averaging refers to averaging measurements acquired with the polarizer axis positioned in different quadrants. This type of measurement is performed to minimize systematic errors due to errors in the polarizer axis calibration.
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