7.1 INTRODUCTION.

Ellipsometers, or reflection polarimeters, are optical instruments which measure changes in the state of polarization of collimated beams of monochromatic polarized light caused by reflection from the surfaces of substances. An ellipsometric measurement involves irradiating the surface of a sample with a collimated beam of monochromatic light having a known, controllable state of polarization, at a known angle of incidence, and determining the differences between the states of polarization of the incident and reflected beams. The measured optical parameters, which characterize the differences between the states of polarization of the incident and reflected beams, in combination with a physical model of the film-covered surface, permit various properties of that sample to be computed (the specific combinations of sample properties that can be computed are discussed at length in Paragraph 4.9).

Ellipsometry has several advantages over other methods of measuring film thickness:

- It can measure film thicknesses at least an order of magnitude smaller than can be measured by other methods such as interferometry.

- It can permit determination of the index of refraction of thin films of unknown thickness. Neither interferometry nor reflectometry permit this determination.

- It can make measurements in optically transparent environments such as air or liquids.

- It does not require special conditions, such as vacuum, heat, or electron bombardment, that may change the optical properties of surfaces being studied, but does permit measurements under such conditions, if desired.

- Nulling ellipsometers (such as the AutoEL) have the advantage that the measured quantities are usually azimuth angles (of rotation of the polarizing components), which can be measured with high resolution and accuracy. This almost completely eliminates effects caused by variations of intensity of the incident light beam, variations in total reflectance of the samples being measured, and variations in sensitivity of the detector-amplifier system used to measure the intensity of the reflected beam.
7.2 BASIC THEORY OF ELLIPSOMETRY.

7.2.1 ELECTROMAGNETIC REPRESENTATION.

The instantaneous amplitude of a single-frequency harmonic oscillation can be represented by

\[ \tilde{E}(t) = E e^{i(\omega t + \tau)} = E e^{i\omega t} \cdot e^{i\tau} \]  \hspace{1cm} (1)

where \( e^{i\tau} \) is time-dependent, and both \( E \) and \( e^{i\tau} \) are time-independent.

The above equation can be used to represent the collimated beams of monochromatic polarized light used in ellipsometry, where \( \tilde{E}(t) \) is the complex instantaneous amplitude of the electric field, \( E \) is the real amplitude of the electric field, and \( \omega \) is the time-independent phase of the light wave.

The reflection process is shown in Figure 7.2. If a collimated beam of monochromatic polarized light is incident on a reflecting surface at an angle of incidence \( \Phi_0 \) (PHI-zero, commonly called PHI) with respect to a normal to the surface at the point of incidence, the angle of reflection of the reflected beam with respect to the normal will be equal to the angle of incidence. Since the two angles are always equal, it is customary to refer to both as angles of incidence. The incident beam, the reflected beam, and the normal to the surface at the point of incidence, all lie in a plane called the plane of incidence.

The electric fields of the incident beam and the reflected beam can each be resolved into two orthogonal linearly-polarized components: The \( p \) component, with its electric field vector parallel to the plane of incidence, and the \( s \) component, with its electric field vector normal to the plane of incidence. The \( p \) and \( s \) components of each beam may have different phases and different amplitudes. The state of polarization of a beam is determined by the relative amplitude (amplitude ratio) of the \( p \) and \( s \) components and by the relative phase (phase difference) between the \( p \) and \( s \) components. If the phase difference between the \( p \) and \( s \) components is either 0° or 180°, the beam is linearly polarized; all other phase differences result in elliptical polarization (of which circular polarization is a special case). At phase differences of 90° or 270°, the major and minor axes of the ellipse will be oriented parallel to the planes of polarization of the \( p \) and \( s \) components.

When a collimated beam of monochromatic polarized light is reflected from a surface, there will generally occur changes in the relative phases and the relative amplitudes of the \( p \) and \( s \) components. These changes determine two angles, \( \Delta \) (DELTA) and \( \Psi \) (PSI), which are derived in the following paragraphs.
7.2.2 DEFINITIONS.

First, let the following quantities be defined:

\( \tilde{E}_p(t) \) and \( \tilde{E}_s(t) \), the instantaneous complex amplitudes of the incident \( p \) and \( s \) components.

\( E_p \) and \( E_s \), the time-independent real amplitudes of the incident \( p \) and \( s \) components.

\( \alpha_p \) and \( \alpha_s \), the time-independent phases of the incident \( p \) and \( s \) components.

\( \tilde{R}_p(t) \) and \( \tilde{R}_s(t) \), the instantaneous complex amplitudes of the reflected \( p \) and \( s \) components.

\( R_p \) and \( R_s \), the time-independent real amplitudes of the reflected \( p \) and \( s \) components.

\( \beta_p \) and \( \beta_s \), the time-independent phases of the reflected \( p \) and \( s \) components.

7.2.3 REFLECTION COEFFICIENTS.

The reflection of the \( p \) and \( s \) components of an incident beam from any surface can be described by defining a complex reflection coefficient \( \tilde{r}_p \) for the incident and reflected \( p \) components, and a complex reflection coefficient \( \tilde{r}_s \) for the incident and reflected \( s \) components, as follows:
\[ \tilde{r}_v \equiv \frac{\tilde{R}_v(t)}{E_v(t)} \quad v = p \text{ or } s \]  

(2)

Since, from equation (1), \( \tilde{E}(t) = E e^{i\omega t} e^{i\epsilon} \), then

\[ \tilde{r}_v = \frac{R_v e^{i\omega t} e^{i\beta_v}}{E_v e^{i\omega t} e^{i\alpha_v}} \quad v = p \text{ or } s \]  

(3)

which can be simplified to give

\[ \tilde{r}_v = \frac{R_v}{E_v} e^{i(\beta_v - \alpha_v)} \quad v = p \text{ or } s \]  

(4)

where the amplitude attenuations caused by reflection are \( R_p/E_p \) and \( R_s/E_s \), and the changes in phase caused by reflection are \( \beta_p - \alpha_p \) and \( \beta_s - \alpha_s \).

### 7.2.4 EQUATIONS OF ELLIPSOMETRY.

The complex reflection coefficients \( \tilde{r}_p \) and \( \tilde{r}_s \) are not separately measurable, but their ratio \( \tilde{\rho} \) can be measured by ellipsometric methods. The ratio \( \tilde{\rho} \) is defined as

\[ \tilde{\rho} = \frac{\tilde{r}_p}{\tilde{r}_s} \]  

(5)

Substituting from equation (4) gives

\[ \tilde{\rho} = \frac{(R_p/E_p) e^{i(\beta_p - \alpha_p)}}{(R_s/E_s) e^{i(\beta_s - \alpha_s)}} \]  

(6)

which can be rearranged to give

\[ \tilde{\rho} = \frac{R_p/R_s}{E_p/E_s} e^{i(\Delta_r - \Delta_i)} \]  

(7)

where \( \Delta_i = \alpha_p - \alpha_s \) and \( \Delta_r = \beta_p - \beta_s \). Note that \( \Delta_i (\Delta_r) \) represents the phase difference between the \( p \) and \( s \) components of the incident (reflected) electric field.

Equation (7) can be further simplified to

\[ \tilde{\rho} = \tan \Psi e^{i\Delta} \]  

(8)

where \( \tan \Psi = (R_p/R_s)/(E_p/E_s) \) represents the change in the amplitude ratio upon reflection, and \( \Delta = \Delta_r - \Delta_i \) represents the change in the phase difference between the \( p \) and \( s \) components caused by reflection. Equation (8) is called the basic equation of ellipsometry.
Note that both \( \Delta \) (DELTA) and \( \Psi \) (PSI) are angles. The angle \( \Psi \) (PSI) may have any value between \( 0^\circ \) and \( 90^\circ \), and the angle \( \Delta \) (DELTA) may have any value between \( 0^\circ \) and \( 360^\circ \).

The reflection process, then, may be characterized by the optical angles \( \Delta \) and \( \Psi \), which may be determined by ellipsometry. The magnitudes of these angles depend on the characteristics of the reflecting sample, and the wavelength and angle of incidence of the incident light beam.

### 7.3 ELLIPSOOMETRIC MEASUREMENT OF DELTA (\( \Delta \)) AND PSI (\( \Psi \)).

#### 7.3.1 TYPES OF ELLIPSMETERS.

There are two basic types of ellipsometers. The first type, of which the AutoEL is an example, is the nulling type of ellipsometer; its configuration is illustrated in Figure 7.3.2. The second type is the rotating element (photometric) type, which commonly is implemented with a rotating analyzer (as in the Rudolph Research Model RR2436). The rotating analyzer configuration is illustrated in Figure 7.3.1.

![Rotating Analyzer (Photometric) Configuration](image)

**Figure 7.3.1. Rotating Analyzer (Photometric) Configuration**

Both types of ellipsometer have two optical axes, an incident-beam axis and a reflected-beam axis, which are adjustable to desired angles of incidence with respect to a sample located at the intersection of the axes. A source of collimated, monochromatic, unpolarized or circularly-polarized light is located at the far end of the incident-beam axis, away...
from the intersection of the two axes. The collimated beam of light from the source passes through any optical components that are mounted along the incident-beam axis, strikes and is reflected from the surface of the sample, and passes through any optical components that are mounted along the reflected-beam axis, until it enters a photodetector at the far end of the reflected-beam axis.

### 7.3.2 PCSA NULLING TYPE (AutoEL)

Nulling ellipsometers generally employ a polarizer, an analyzer, and a compensator, each aligned along the axis in which it is located. The polarizer is generally located in the incident-beam axis, the analyzer is generally located in the reflected-beam axis, and the compensator may be located in either axis. The most common configuration, employed in the AutoEL, is that with the compensator in the incident-beam axis. This is called the PCSA configuration, for Polarizer, Compensator, Sample, Analyzer, which describes the sequence in which the light from the source passes through the instrument. One of the three components (usually the compensator) is fixed at some azimuth angle about the optical axis, with respect to the plane of incidence established by the incident and reflected beams; and the other two (usually the polarizer and analyzer) are rotatable either manually (as in the Rudolph Research Type 436 and Type 437) or automatically (as in the AutoEL). A measurement consists of:

1. setting the incident-beam and reflected-beam axes at some desired angle of incidence with respect to a sample mounted with its surface at the intersection of the two axes,
(2) alternately rotating the polarizer and analyzer until the intensity of the reflected beam (as sensed by a photodetector after passage through the analyzer) is reduced to a minimum, and

(3) determining, at that null or ‘extinction’ condition, the angular azimuths \( P \) of the polarizer and \( A \) of the analyzer with respect to the plane of incidence. The azimuths \( P \) and \( A \) at null are directly convertible by means of simple linear equations into the polarization parameters \( \Delta \) and \( \Psi \).

The AutoEL is a PCSA nulling type ellipsometer. The AutoEL light source assembly produces a collimated, circularly or randomly polarized beam of light at a specified wavelength, \( \lambda \). This beam of light is converted to linearly-polarized light by a rotatable polarizer, and then to elliptically-polarized light by a quarter-wave compensator. The elliptically-polarized beam strikes the surface of a sample at an angle of incidence \( \Phi_0 \), is reflected at the same angle, passes through a rotatable analyzer and a wavelength filter, and then falls on a photodetector.

### 7.3.2.1 POLARIZER.

The linearly-polarized light from the rotatable polarizer has its polarization azimuth parallel to the polarization axis of the polarizer. The polarization azimuth of the beam thus rotates with the polarizer, and enters the compensator with the same azimuth as the polarization axis of the polarizer.

### 7.3.2.2 QUARTER-WAVE COMPENSATOR.

The quarter-wave compensator converts the linearly-polarized light from the polarizer into elliptically-polarized light which strikes the sample at the chosen angle of incidence, \( \Phi_0 \). The compensator has two orthogonal axes (the fast axis and the slow axis) in the plane perpendicular to the direction of transmission. The electric field of an entering beam which is linearly polarized along any other azimuth will be resolved into two components, one parallel to the fast axis and the other parallel to the slow axis. The fast-axis component will be transmitted at a greater velocity than the slow-axis component. The thickness of the quarter-wave compensator is such that the slow component is retarded by 90° or one-quarter-wave with respect to the fast component. When the fast and slow components emerge they recombine, but the phase shift between them causes the polarization form of the output to differ from that of the input. If the azimuth of the linearly-polarized input is 45° from the azimuth of the fast axis of the compensator, the output will be circularly polarized. If the axis of the linearly-polarized input is at any other angle with respect to the fast axis of the compensator, the output will be elliptically polarized, with an azimuth (orientation of the major axis of the ellipse with respect to the plane of incidence) and ellipticity (ratio of minor to major axes of the ellipse) determined by the orientations of the polarizer and the compensator. Compensators can be oriented with their fast axes at any azimuth, but are usually oriented with their fast axes at +45° or −45° to the plane of incidence (i.e., at azimuths of +45° or +315°, since all azimuth angles are considered positive when measured counterclockwise from the plane of incidence when looking in the detector-to-light-source direction).
Alternatively, it can be shown\(^1\) that the elliptically polarized light exiting the compensator may be completely described by the magnitude of the two components \(E_p\) and \(E_s\) (which lie in and normal to the plane of incidence, respectively) and their relative phase. If the compensator azimuth is fixed at \(\pm 45^\circ\), the relative phase, \(\Delta_i\) depends only on the polarizer azimuth \(P\). All values of \(\Delta_i\) between 0\(^\circ\) and 360\(^\circ\) may be generated by rotating \(P\) through 180\(^\circ\). For every sample there is a polarizer azimuth between 0\(^\circ\) and 180\(^\circ\) at which \(\Delta_i = -\Delta\). That is, the phase difference, \(\Delta_i\), between the incident \(p\) and \(s\) components is exactly equal and opposite to the phase change, \(\Delta\), caused by reflection, and the reflected light is linearly polarized with \(\Delta_r = \Delta + \Delta_i = 0^\circ\). Similarly, there is a polarizer azimuth between 0\(^\circ\) and 180\(^\circ\) at which \(\Delta_i = -\Delta + 180^\circ\) and the reflected light is linearly polarized, with \(\Delta_r = 180^\circ\).

7.3.2.3 ANALYZER.

The optical properties of the sample surface cause the data of polarization of the reflected beam to differ from that of the incident beam. The reflected beam passes through the analyzer prism and the narrow-band wavelength filter to the photodetector, which generates an output current proportional to the intensity of the beam entering the photodetector. If the state of polarization of the reflected beam is anything but circular, rotation of the analyzer will cause the intensity of the beam entering the photodetector, and thus the output current of the photodetector, to vary. As the analyzer is rotated, the photodetector output current will have minima at two azimuths that are 180\(^\circ\) apart. In general these minima will not correspond to true extinction, which can be achieved only if the reflected beam is linearly polarized.

For each sample, and for any compensator setting (e.g., +45\(^\circ\)), there is some polarizer azimuth at which the reflected beam is linearly polarized, so that true extinction can be obtained by orienting the analyzer with its transmission axis at 90\(^\circ\) to the polarization azimuth of the linearly-polarized reflected beam. This is achieved by alternately adjusting the polarizer and analyzer until a null corresponding to true extinction is obtained. The polarizer azimuth \(P\) at null is a measure of \(\Delta\), and the analyzer azimuth \(A\) at null is a measure of \(\Psi\). For the PCSA nulling configuration used in the AutoEL, the equations relating \(P\) and \(A\) at null to \(\Delta\) and \(\Psi\) are simple linear equations.

7.3.3 DETERMINATION OF DELTA (\(\Delta\)) AND PSI (\(\Psi\)).

There are 32 different combinations of polarizer, analyzer, and compensator settings which can result in a given pair of values of \(\Delta\) and \(\Psi\). Because any two azimuths of a polarizer, compensator, or analyzer that are 180\(^\circ\) apart are optically identical, the number of combinations of polarizer, analyzer and compensator settings giving any pair of values of \(\Delta\) and \(\Psi\), can be reduced to 16 if all azimuths are restricted to ranges less than 180\(^\circ\). The 16 pairs of linear equations relating \(\Delta\) and \(\Psi\) to \(P\) and \(A\) at null are summarized as follows:

---

\(^1\) See references 2 and 5 in the Bibliography, Appendix A.
\[ \Psi : A, \, 180^\circ - A \]
\[ \Delta : 2P - 90^\circ, \, 2P - 270^\circ, \, (2m - 1)90^\circ \pm 2P \]
where \( m = 1, \, 2, \, 3 \) or 4

\[ (9) \]

7.3.3.1 ZONES 2 AND 4.

The 16 pairs of equations represented by equation (9) can be reduced to two pairs of equations by restricting the compensator azimuths to one value, e.g., 45°, and the ranges of \( P \) and \( A \) to two zones. These restrictions are employed in the AutoEL for which the two zones, designated zone 2 and zone 4, are defined as follows:

\[ \text{Zone 2} : \quad -45^\circ \leq P_2 \leq 135^\circ, \quad 0^\circ \leq A_2 \leq 90^\circ, \quad C = 45^\circ \]
\[ \text{Zone 4} : \quad -135^\circ \leq P_4 \leq 45^\circ, \quad -90^\circ \leq A_4 \leq 0^\circ, \quad C = 45^\circ \]

\[ (10) \]

The equations relating \( \Delta \) and \( \Psi \) to \( P \) and \( A \) in each of the two zones are:

\[ \Delta_2 = 270^\circ - 2P_2, \quad \Psi_2 = A_2 \]
\[ \Delta_4 = 90^\circ - 2P_4, \quad \Psi_4 = -A_4 \]

\[ (11) \]

7.3.3.2 TWO-ZONE AVERAGING.

Although equally valid measurements can be made in either zone 2 or zone 4, the effects of imperfections in the compensator (retardation not exactly 90° and/or unequal attenuations for components parallel to compensator fast and slow axes) can be eliminated by making measurements in both zones, and averaging the results of those measurements to obtain the mean quantities \( \overline{\Delta} \) and \( \overline{\Psi} \).

\[ \overline{\Delta} = \frac{\Delta_2 + \Delta_4}{2} = 180^\circ - (P_2 + P_4) \]
\[ \overline{\Psi} = \frac{\Psi_2 + \Psi_4}{2} = \frac{A_2 + (-A_4)}{2} = \frac{A_2 - A_4}{2} \]

\[ (12) \]
7.4 THE MODELS.

Ellipsometers would only be of academic interest if the measured parameters $\Delta$ and $\Psi$ were not related to fundamental physical properties of the reflecting sample.

7.4.1 BARE SURFACES.

In the last century Fresnel derived equations for the reflection of light from a film-free surface, based on the assumption that the light reflection occurs at an infinite planar boundary between two media of different but uniform refractive indices. For such a film-free surface, $\Delta$ and $\Psi$ are each functions of the angle of incidence $\Phi_0$, the wavelength $\lambda$ of the light, the refractive index $n_0$ of the ambient medium, as well as the real part $n_3$ and the imaginary part $k_3$ of the substrate refractive index, $n_3 - ik_3$:

$$\Delta = f_3(\Phi_0, \lambda, n_0, n_3, k_3) \quad \text{and}$$
$$\Psi = g_3(\Phi_0, \lambda, n_0, n_3, k_3)$$

(13)
Since $\Phi_0$, $\lambda$, and $n_0$ are known, equations (13) may be solved uniquely and in closed form for $n_3$ and $k_3$, the optical constants of the substrate.\(^2\)

### 7.4.2 Single Films

Drude extended the Fresnel reflection equations to the single-film model. In this model, $\Delta$ and $\Psi$ depend on the real part $n_2$ and the imaginary part $k_2$ of the film refractive index, the film thickness $d_2$, as well as on all other parameters in equations (13):

\[
\begin{align*}
\Delta &= f_2(\Phi_0, \lambda, n_0, n_3, k_3, n_2, k_2, d_2) \\
\Psi &= g_2(\Phi_0, \lambda, n_0, n_3, k_3, n_2, k_2, d_2)
\end{align*}
\] (14)

Note that $k_2$ and $k_3$ are related to the absorption coefficients of the film and substrate, respectively. If $n_3$ and $k_3$ are known from previous measurements or other sources, and if the film is transparent (i.e., $k_2 = 0$), the film thickness $d_2$ and refractive index $n_2$ are the only unknowns in equations (14), and may be calculated from the results of a single $\Delta$ and $\Psi$ measurement. Unfortunately, equations (14) cannot be inverted to obtain $n_2$ (or $d_2$) as a function of $\Delta$ and $\Psi$. Instead, numerical techniques must be employed to determine $n_2$ and $d_2$. If the film is absorbing ($k_2 \neq 0$) it is not possible to determine uniquely $n_2$, $k_2$, and $d_2$ from a single $\Delta$, $\Psi$ measurement. A value for $n_2$ or $k_2$ must be assumed to permit computation of the remaining optical constant and thickness.

### 7.4.3 Double Films

For the two-layer film model, $\Delta$ and $\Psi$ depend also on $n_1$, $k_1$, and $d_1$, the optical constants and thickness of the top layer.\(^3\)

\[
\begin{align*}
\Delta &= f_1(\Phi_0, \lambda, n_0, n_3, k_3, n_2, k_2, d_2, n_1, k_1, d_1) \\
\Psi &= g_1(\Phi_0, \lambda, n_0, n_3, k_3, n_2, k_2, d_2, n_1, k_1, d_1)
\end{align*}
\] (15)

As above, equations (15) may be solved by numerical techniques for any two of the physical constants, provided the remaining constants are known. Further, if $d_1$, the thickness of the top film, is one of the physical constants being determined, the numerical technique is simplified and usually yields unique results.

\[
\begin{align*}
d_1 &= f(L, \Delta, \Psi, \Phi_0, n_0, n_1, k_1, d_1, n_2, k_2, d_2, n_3, k_3) \\
0 &= g(L, \Delta, \Psi, \Phi_0, n_0, n_1, k_1, d_1, n_2, k_2, d_2, n_3, k_3)
\end{align*}
\] (16, 17)

Every reflecting surface alters the polarization state of light upon refraction and hence possesses a $\Delta$ and $\Psi$ which can be measured by ellipsometry. The investigator then postulates a model, be it a bulk material, single layer, double layer, or multiple film system, to explain the observed values of $\Delta$ and $\Psi$.

---

\(^2\) See reference 5 in Bibliography.

\(^3\) See references 2, 5 and 11 in Bibliography.
The ellipsometer measures a value of Δ and Ψ at controlled values of wavelength λ, angle of incidence Φ₀, and ambient refractive index n₀. There are nine unknowns in equation 17 (double film case), or six unknowns if the equation is simplified to a single film case. The unknowns are the optical constants of the films and substrate together with the periodicity index L. Under the best of conditions, only two of the unknowns in equation (17) can be computed from a single Δ, Ψ measurement.

The simplest evaluation of equation (17) occurs when all the optical constants except the upper layer film thickness are known. The film thickness is computed for several integer values of L, and the investigator selects the thickness closest to the expected value. The film thickness solution is not unique due to the film thickness order effect (Paragraph 4.9.4) which shows up in equation (17) as the periodicity index L.

The known optical constants and the measured data are used to evaluate the right-hand portion of equation (17). If that computation does not produce a number close to zero, the accuracy of the measured Δ and Ψ, or the accuracy of the "known" optical constants must be questioned.

If, in addition to the unknown film thickness d₁, one of the other optical constants is also unknown (e.g., n₂ or d₂), the value of the second unknown optical constant may be obtained from equation (17) by numerical techniques (usually on a computer). Two numerical techniques are in widespread use. One involves the binary division of intervals, and the other utilizes the Newton-Raphson approximation to the roots of an equation. In both cases, the value of the second (unknown) optical constant is varied from an initial estimate until the right-hand side of equation (17) is arbitrarily close to zero, after which d₁ is evaluated using equation (16).

When the film thickness TU is known and the values of two of the other optical constants are desired, a two-dimensional numerical search in both unknown optical constants must be conducted to solve equations (16) and (17).

When more than two of the optical constants are unknown (e.g., n₁, k₁, and d₁) the problem is insoluble with only one Δ, Ψ pair. The investigator must endeavor to obtain independent measurements of Δ and Ψ by varying the measurement conditions, i.e., different angles of incidence, different ambient media, different substrates, or different underlying film thicknesses. Using the multiplicity of data thus obtained, a combination of numerical and graphical searches in three dimensions are carried out to determine the three unknown optical constants.⁴

⁴ See references 11 and 12 in the Bibliography.