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Ellipsometry Solutions

1A: Introduction to WVASE Data Analysis

Nina Hong

U Penn, February 2014

Session Outline

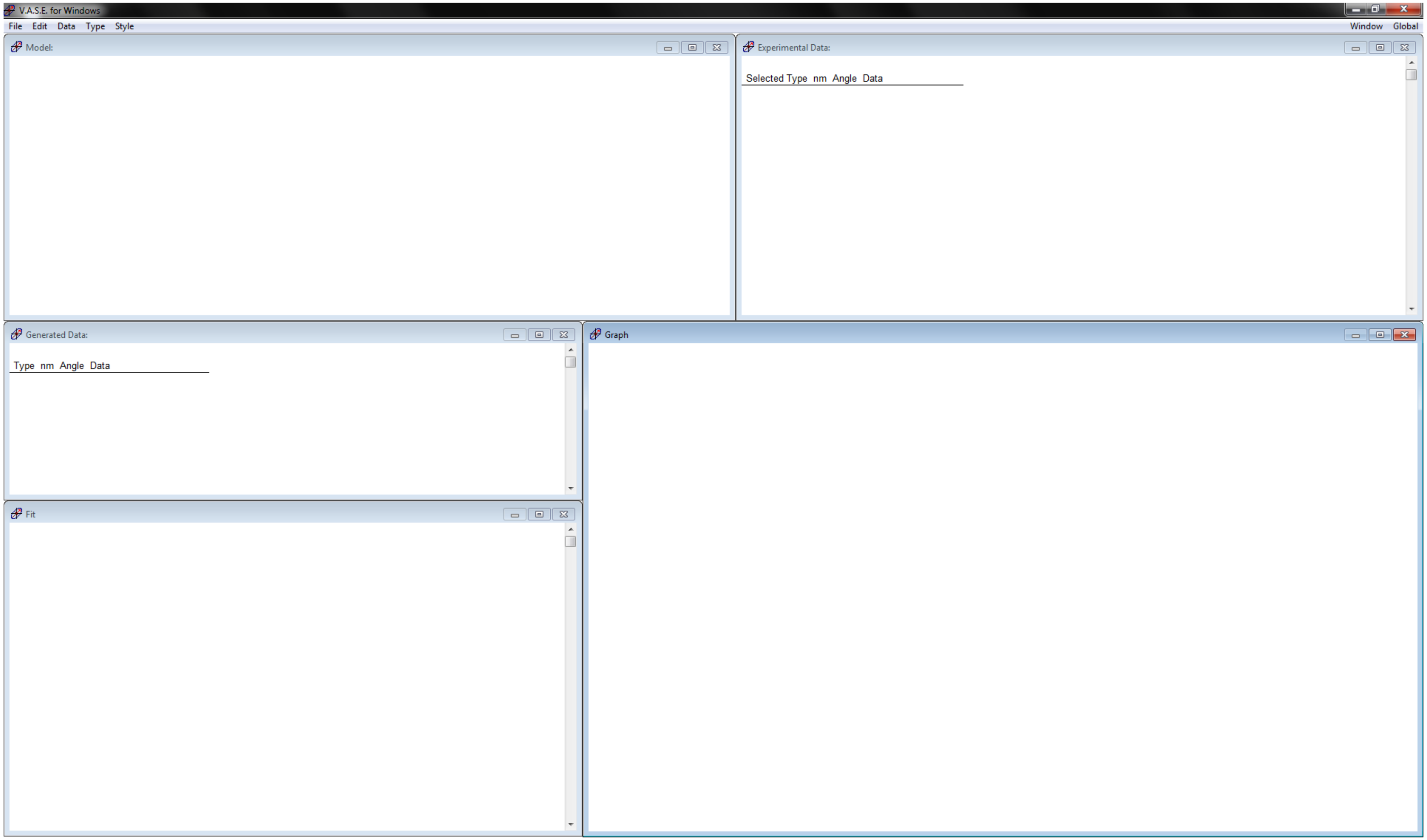
1. **Introduction to Ellipsometry.**
2. **Classification of Samples.**
   - Transparent
   - Semi-absorbing
   - Absorbing
   - Bare substrates, and coated samples.
3. **Oscillator Models and Genosc Layer.**
   - Types of oscillators.

Learning Outcomes:

- Basic operation of WVASE software.
- Fundamentals of spectral interpretation.

WVASE Software

Opening Screen.



Five Empty Windows. Click inside each.
How to use these windows?

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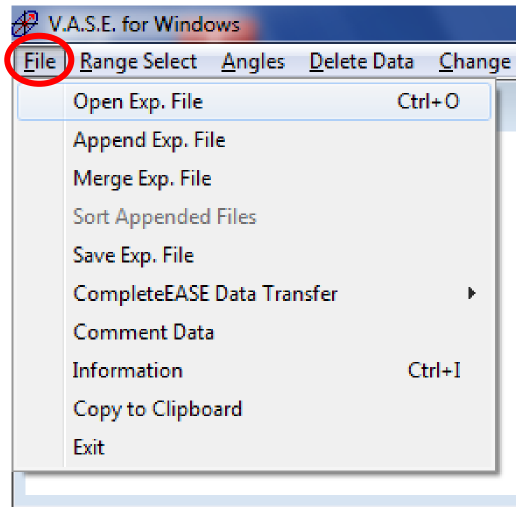
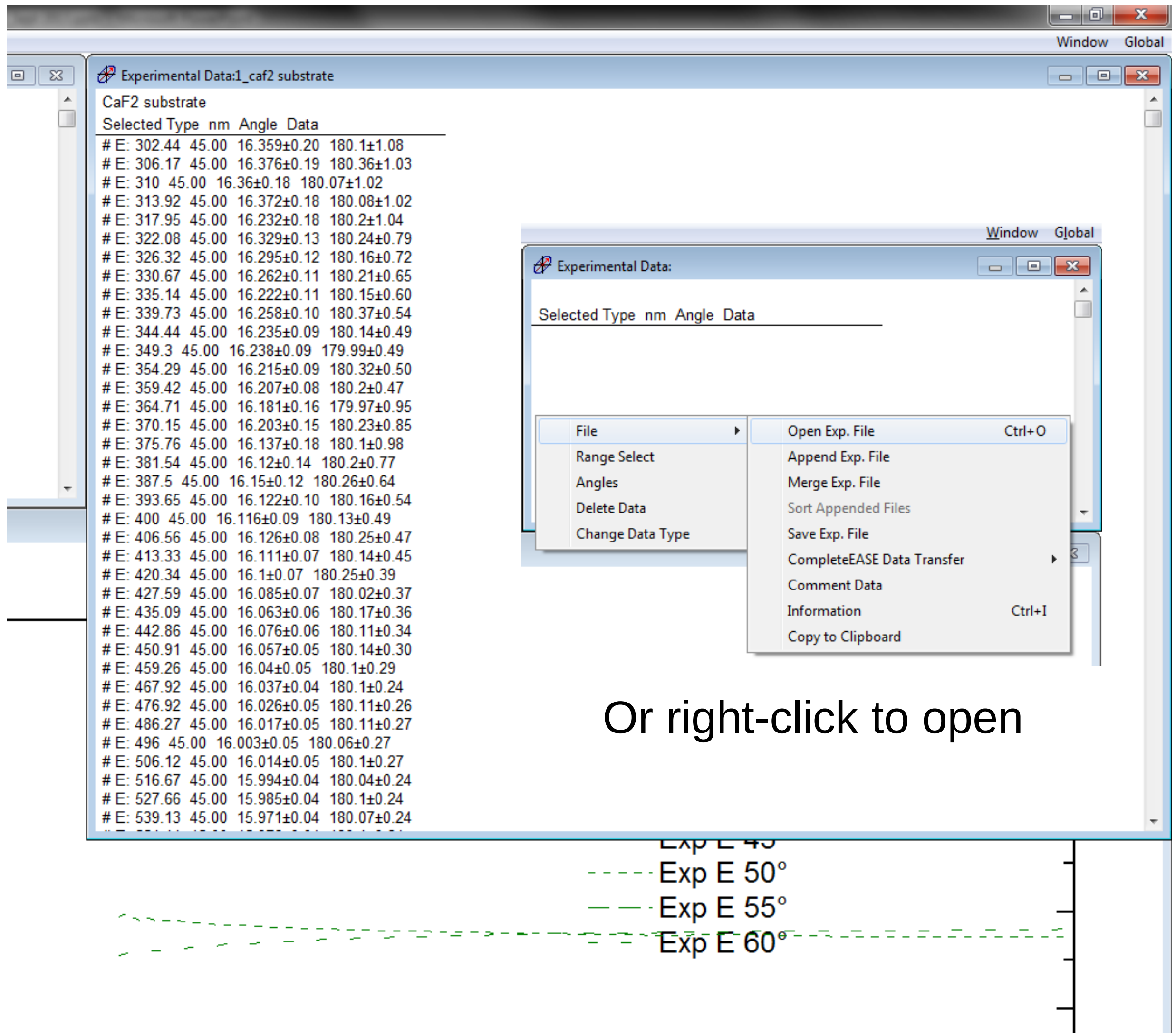
Experimental Data Window

Use to open data files.



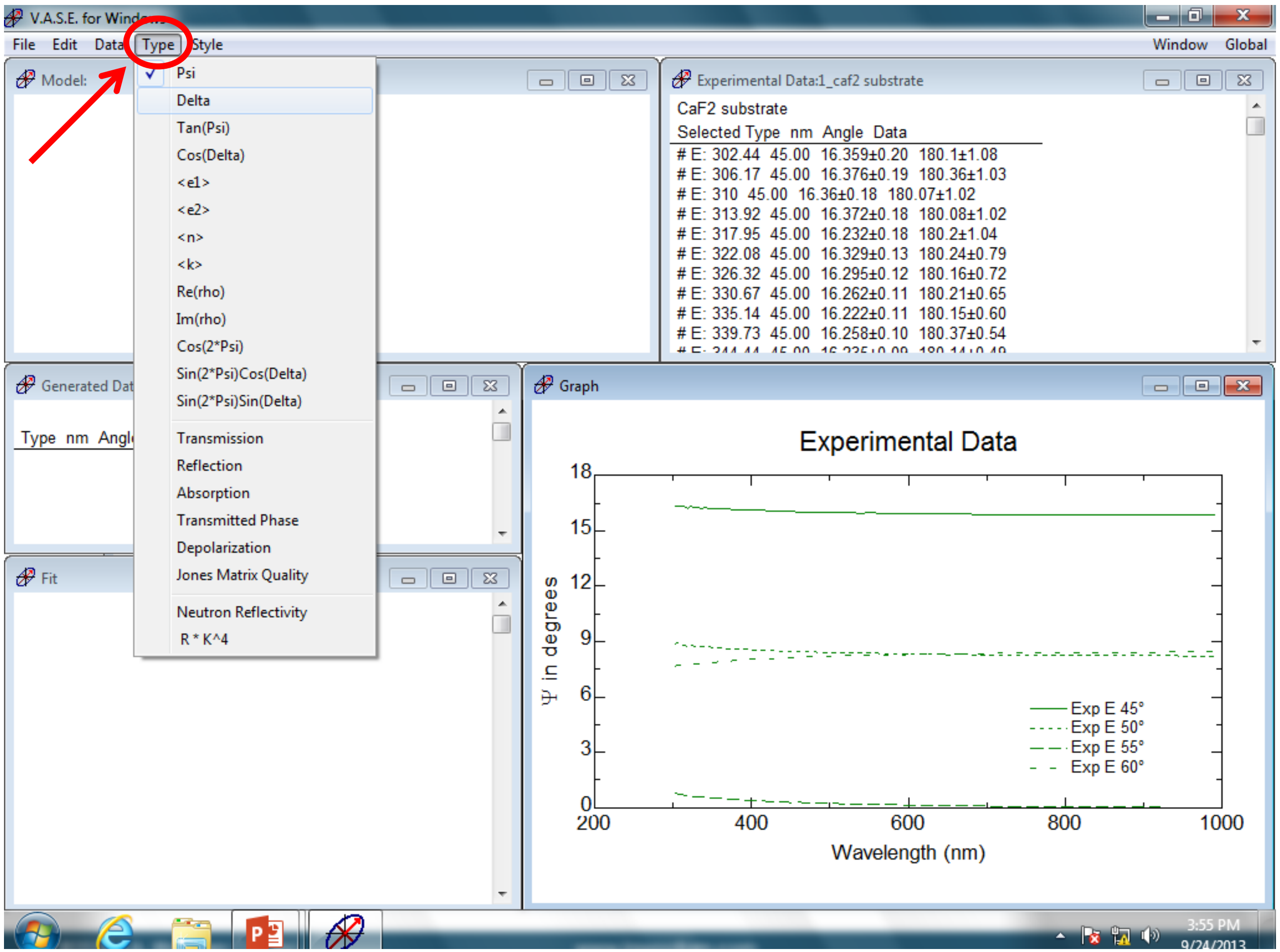
From upper-left.



Or right-click to open

Graph Window

Displays graphs of Experimental Data



Select “Type” to change graphs.

1 1_CaF2 Substrate.dat

Step 1:

- Select Experimental Data Window.
- Open data file: 1_CaF2 Substrate.dat

Step 2:

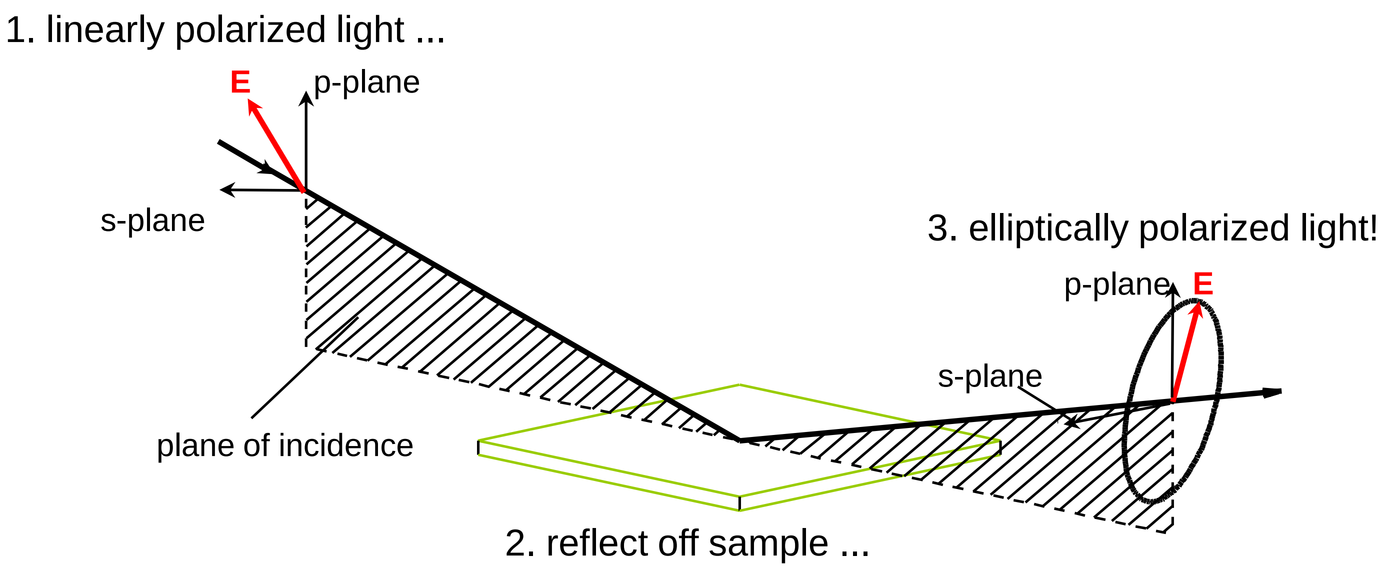
Select Graph Window

- **Plot Ψ and Δ data.**
- Ψ and Δ? **What are these?**
- **What do they mean?**

Learning Outcomes:

- Use Experimental Data and Graph Windows.
- Open data files. Display graphs of **Ψ and Δ**.

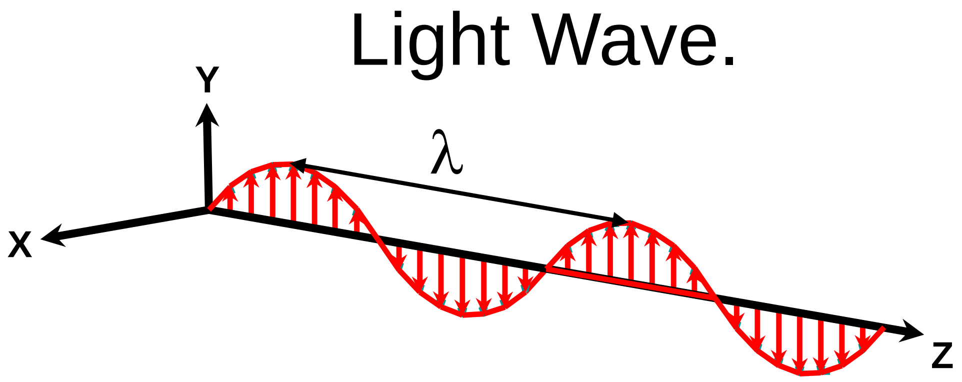
Ellipsometry Measurement



- Ellipsometry **measures the change in polarization state** of light reflected from a surface.
- Sample properties cause the change.
- Polarization is rotated, and becomes elliptical.

Next: What is polarized light? What is Ellipsometry?

Units: Wavelength, Photon Energy, & Wavenumber

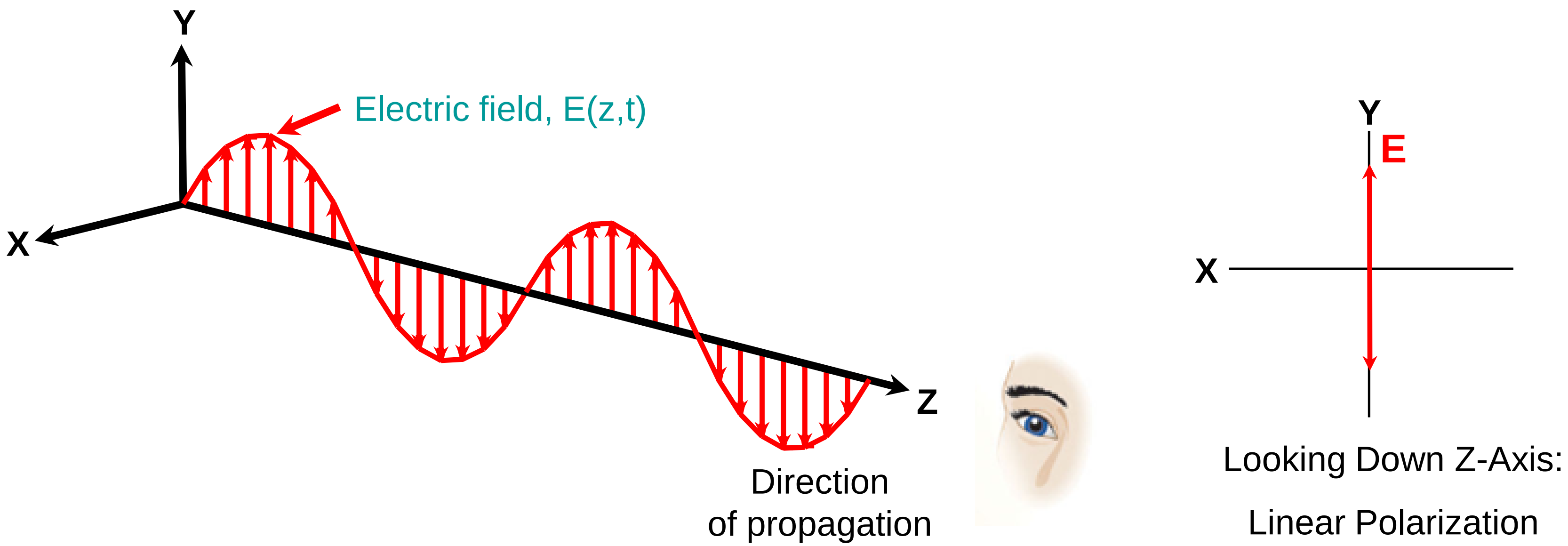


- **Wavelength**, λ (units in Å, nm, or microns)
- **Photon Energy** (eV). "Electron Volts"
- **Wavenumber** (cm^{-1}). Used Mid to Far IR.
- Unit conversions:

$$E_{eV} = \frac{12400}{\lambda_{Å}}, \quad E_{eV} = \frac{1240}{\lambda_{nm}}, \quad E_{eV} = \frac{1.240}{\lambda_{\mu m}}, \quad cm^{-1} = \frac{10000}{\lambda_{\mu m}}$$

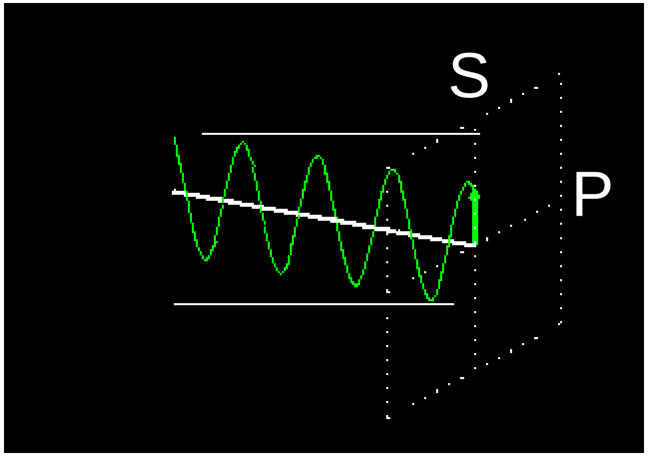
What is Polarization?

- "Shape" of the beam as it propagates towards us. (Looking down z-axis).

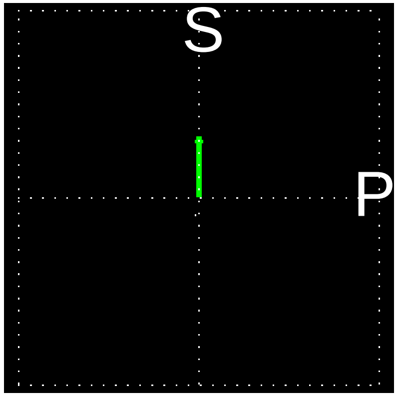


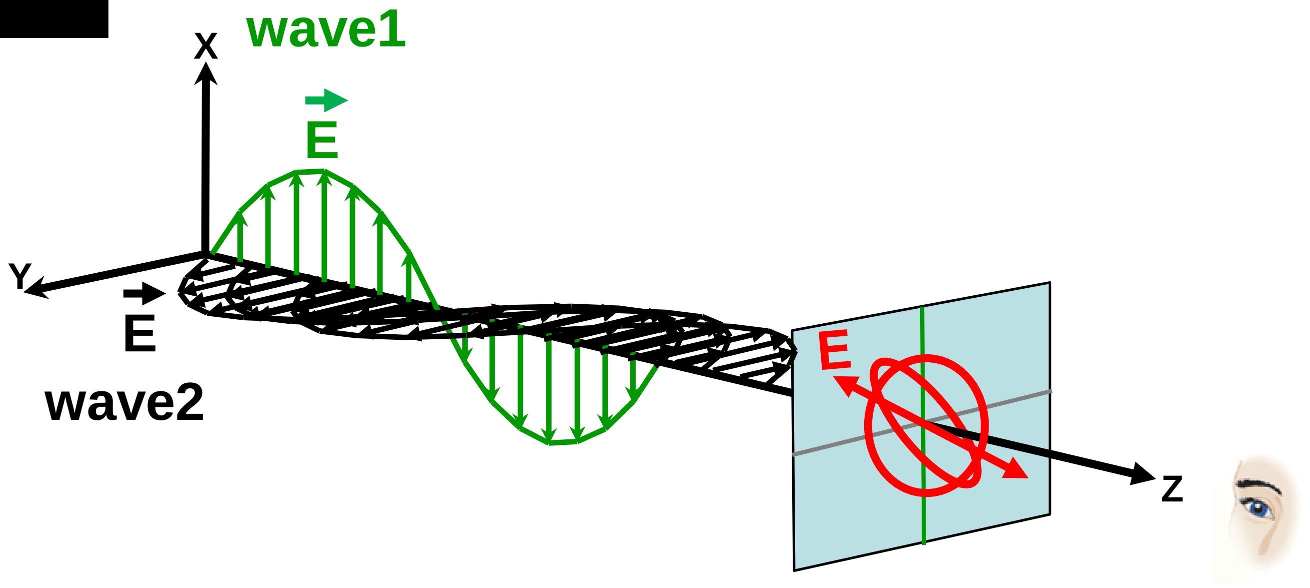
- Polarization state defined by orientation & phase of the E-field vector.

Polarized Light



- Polarization can be linear, circular or elliptical.
- *Superposition* of two orthogonal light beams (components).





ANIMATIONS FROM WWW.ENZIM.HU
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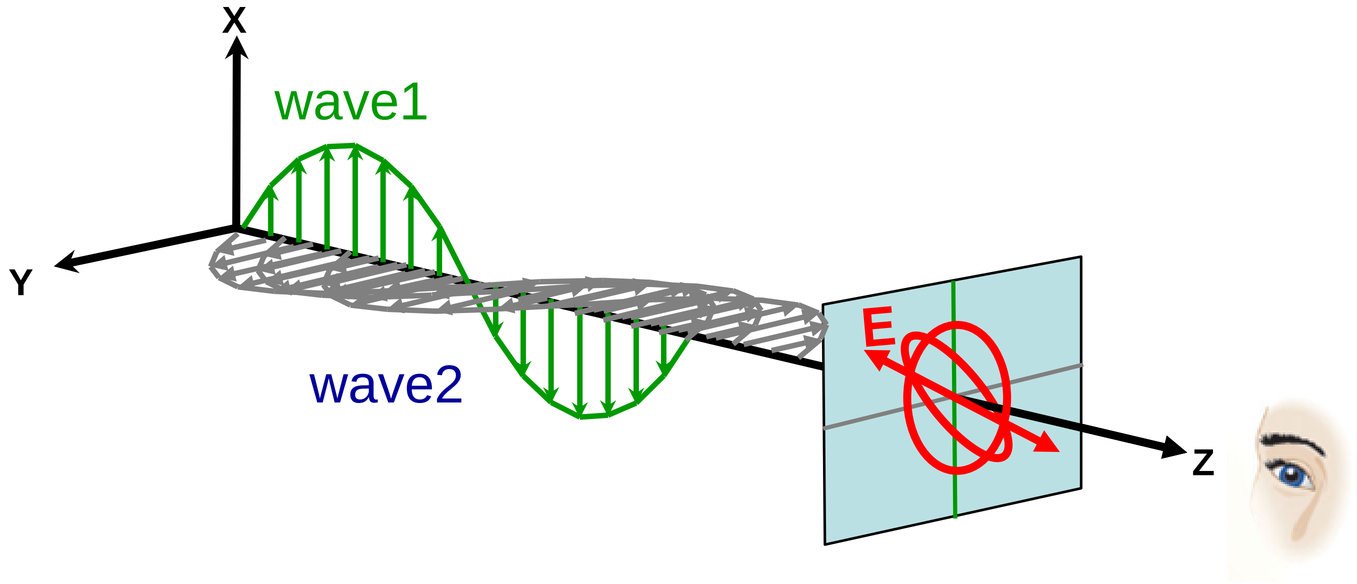
What is Polarization?

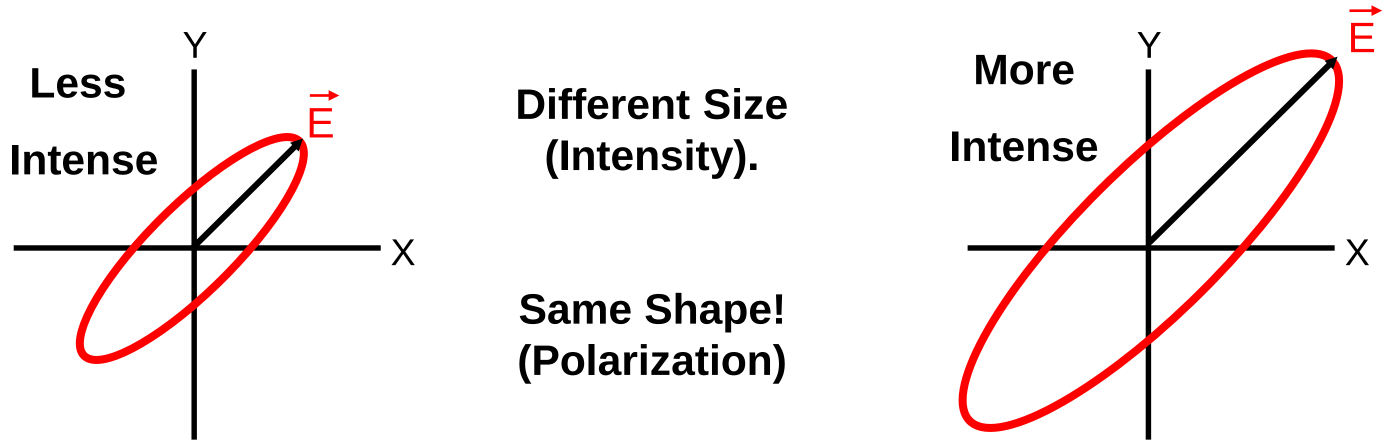
Polarization: Describes "shape" of electric field along the direction of travel.



- Linear: arbitrary amplitudes, in-phase.
- Circular: equal amplitudes, 90° phase difference.
- Elliptical: arbitrary amplitudes, arbitrary phases.

Intensity and Polarization

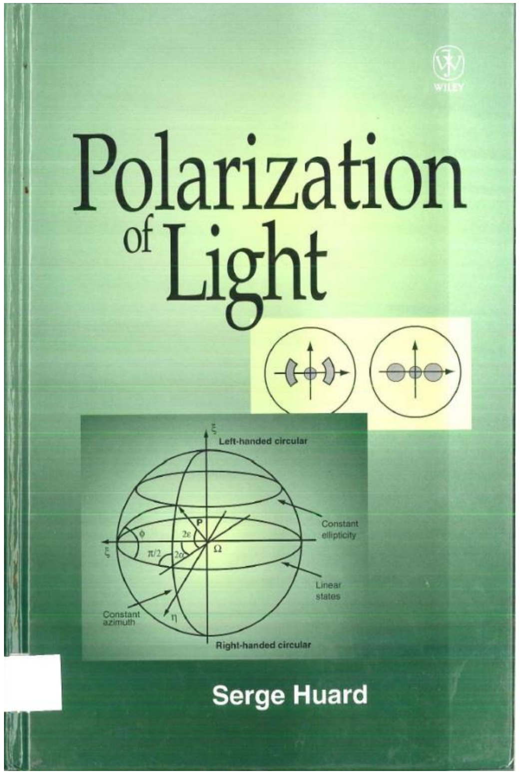
- Light Intensity = **"Size" of the Ellipse.**
  - One Number Describes Wave Amplitude (E).
  - Intensity is proportional to E^2…"Brightness". $I \propto E^2 = (E_x{}^2 + E_y{}^2)$



- Polarization = **"Shape" of Ellipse.**
  - **2 numbers required**: ellipse **Azimuth and Ellipticity**.
  - Independent of ellipse size. Independent of intensity
  - **Ellipsometry always measures 2 numbers: Ψ & Δ.**

Light and Polarization

- For more details…



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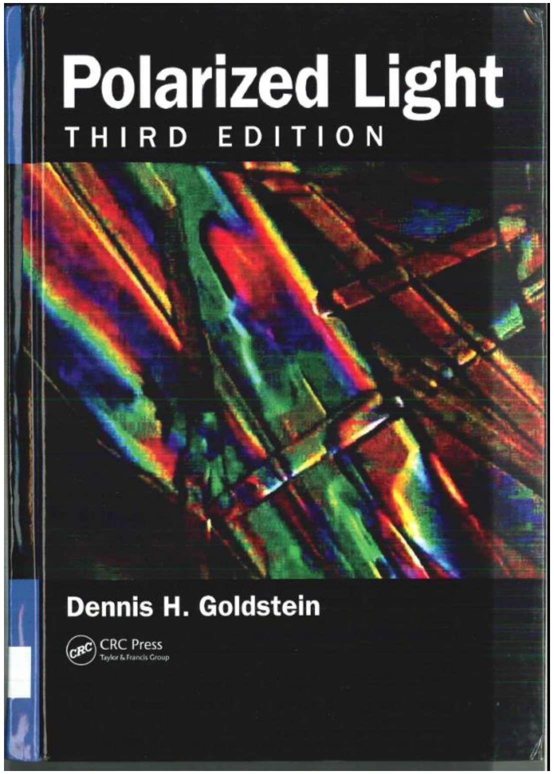

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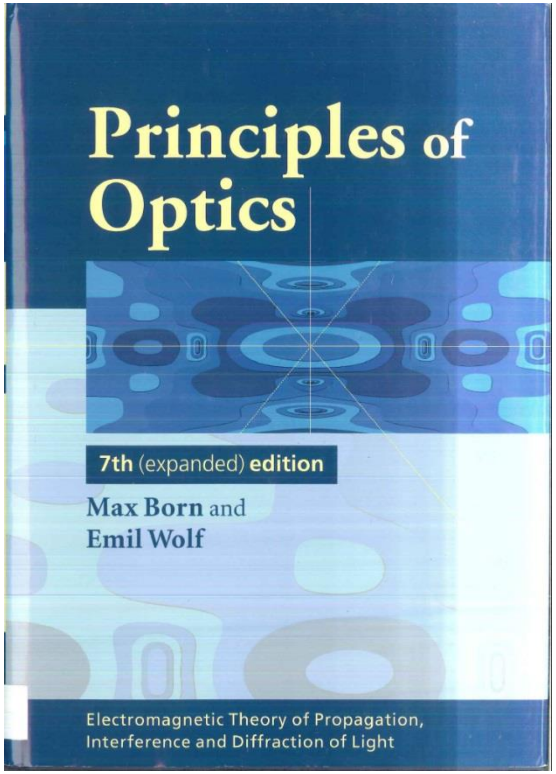

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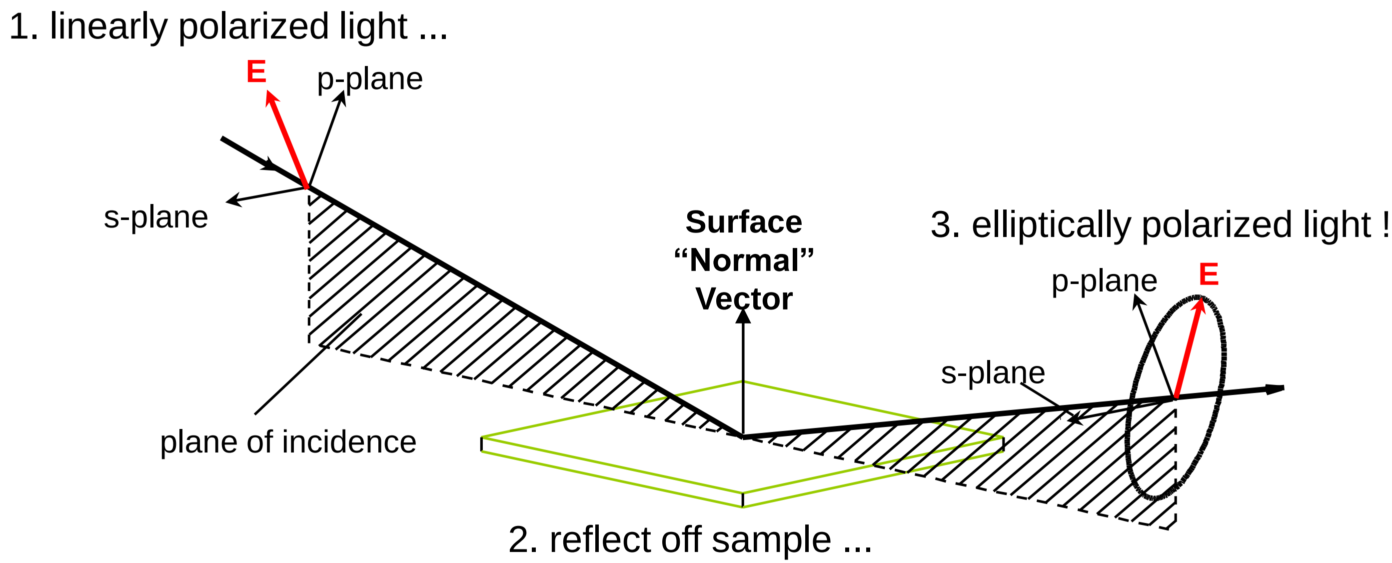
Ellipsometry: Angle & Plane of Incidence



1. Angle of Incidence.

Measured from Sample Normal.

2. Plane of Incidence.

Defined by incident beam, reflected beam, and sample normal.

3. Polarization Components

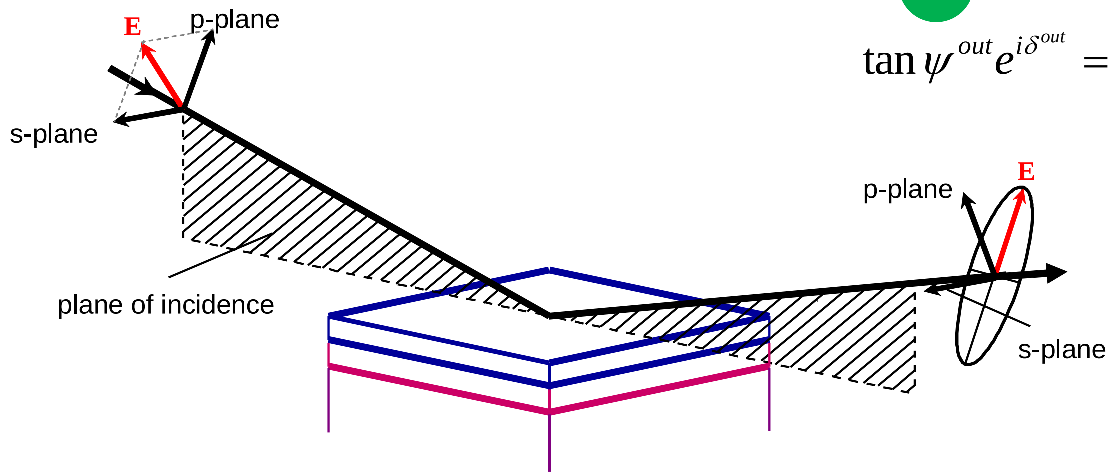
p- and *s*- are parallel and perpendicular to plane of incidence.

Ellipsometry Measurement

- **Measures <u>change</u> in polarization of reflected light.**

1

$$\tan\psi^{in} e^{i\delta^{in}} = \frac{\left|E_p^{in}\right|}{\left|E_s^{in}\right|} e^{i\left(\delta_p^{in}-\delta_s^{in}\right)}$$



2

$$\tan\psi^{out} e^{i\delta^{out}} = \frac{\left|E_p^{out}\right|}{\left|E_s^{out}\right|} e^{i\left(\delta_p^{out}-\delta_s^{out}\right)}$$

Change in Polarization represented as <u>Ratio</u> of Light-Out to Light-In

3

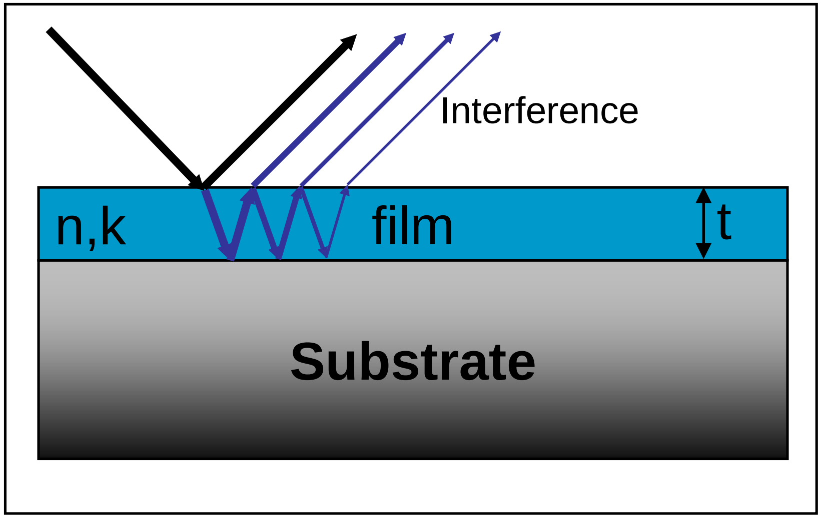
$$\rho \equiv \frac{\dfrac{\left|E_p^{out}\right|}{\left|E_s^{out}\right|}}{\dfrac{\left|E_p^{in}\right|}{\left|E_s^{in}\right|}} \frac{e^{i\left(\delta_p^{out}-\delta_s^{out}\right)}}{e^{i\left(\delta_p^{in}-\delta_s^{in}\right)}} = \frac{\left|E_p^{out}\right|}{\left|E_s^{out}\right|}\frac{\left|E_s^{in}\right|}{\left|E_p^{in}\right|} e^{i\left(\delta_p^{out}-\delta_s^{out}-\delta_p^{in}+\delta_s^{in}\right)}$$

Ellipsometry Equation

For Reflection, use the following Definitions:

$$r_p = \frac{\left|E_p^{out}\right|}{\left|E_p^{in}\right|} \qquad \Delta_p = \delta_p^{refl} - \delta_p^{in}$$

$$r_s = \frac{\left|E_s^{out}\right|}{\left|E_s^{in}\right|} \qquad \Delta_s = \delta_s^{refl} - \delta_s^{in}$$



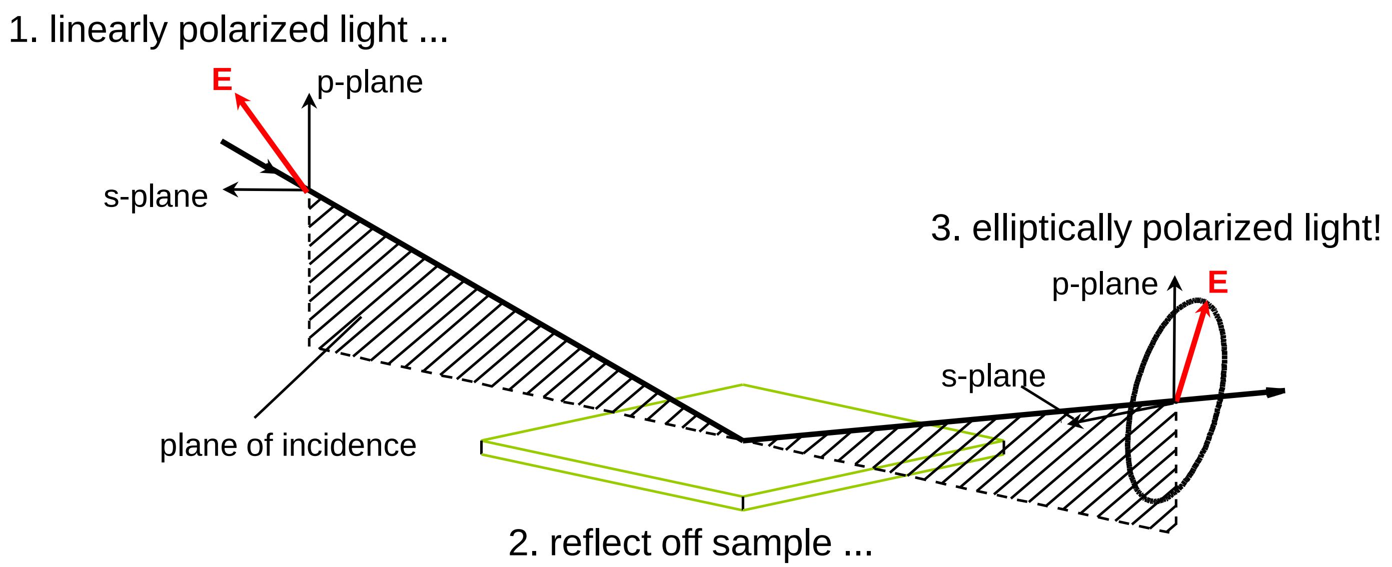
Rewriting, we get the <u>Ellipsometry</u> Equation:

$$\rho = \frac{r_p}{r_s} e^{i(\Delta_p - \Delta_s)} = \tan(\Psi) e^{i\Delta} = \frac{\tilde{r}_p}{\tilde{r}_s}$$

- **Can determine Optical constants & Film Thickness**

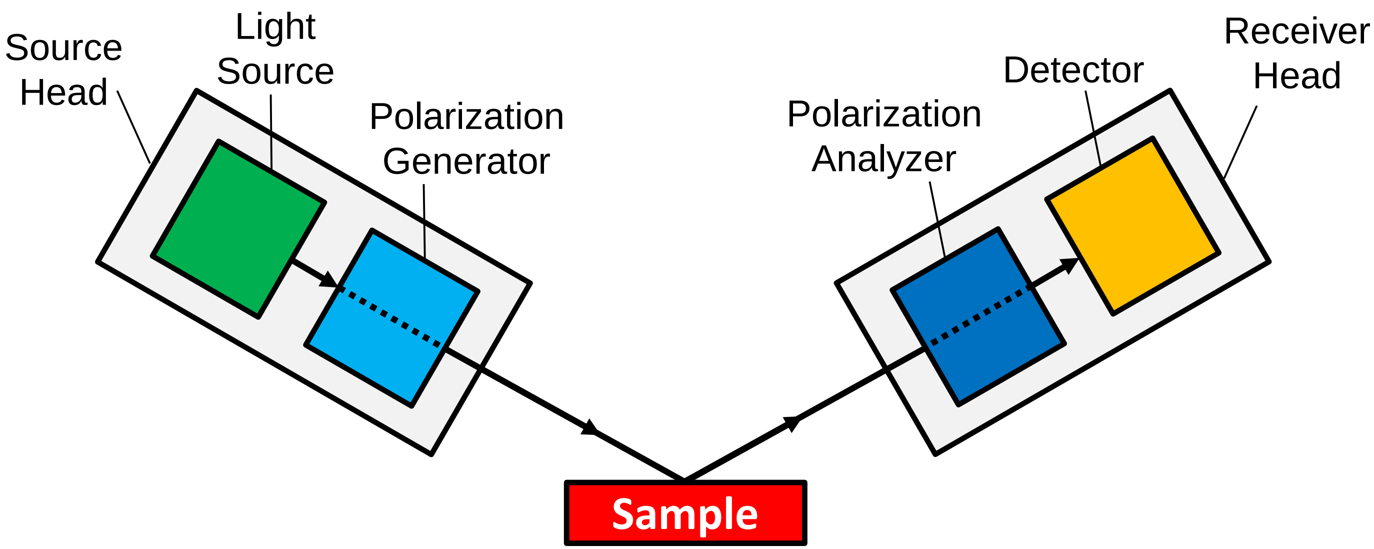
Summary: Ellipsometry Experiment

- Light is reflected from a surface of interest.
- The polarization state of incident light is known.
- The polarization state of reflected/transmitted light is measured.
- An ellipsometer determines the change in polarization from the sample. Ψ and Δ values.



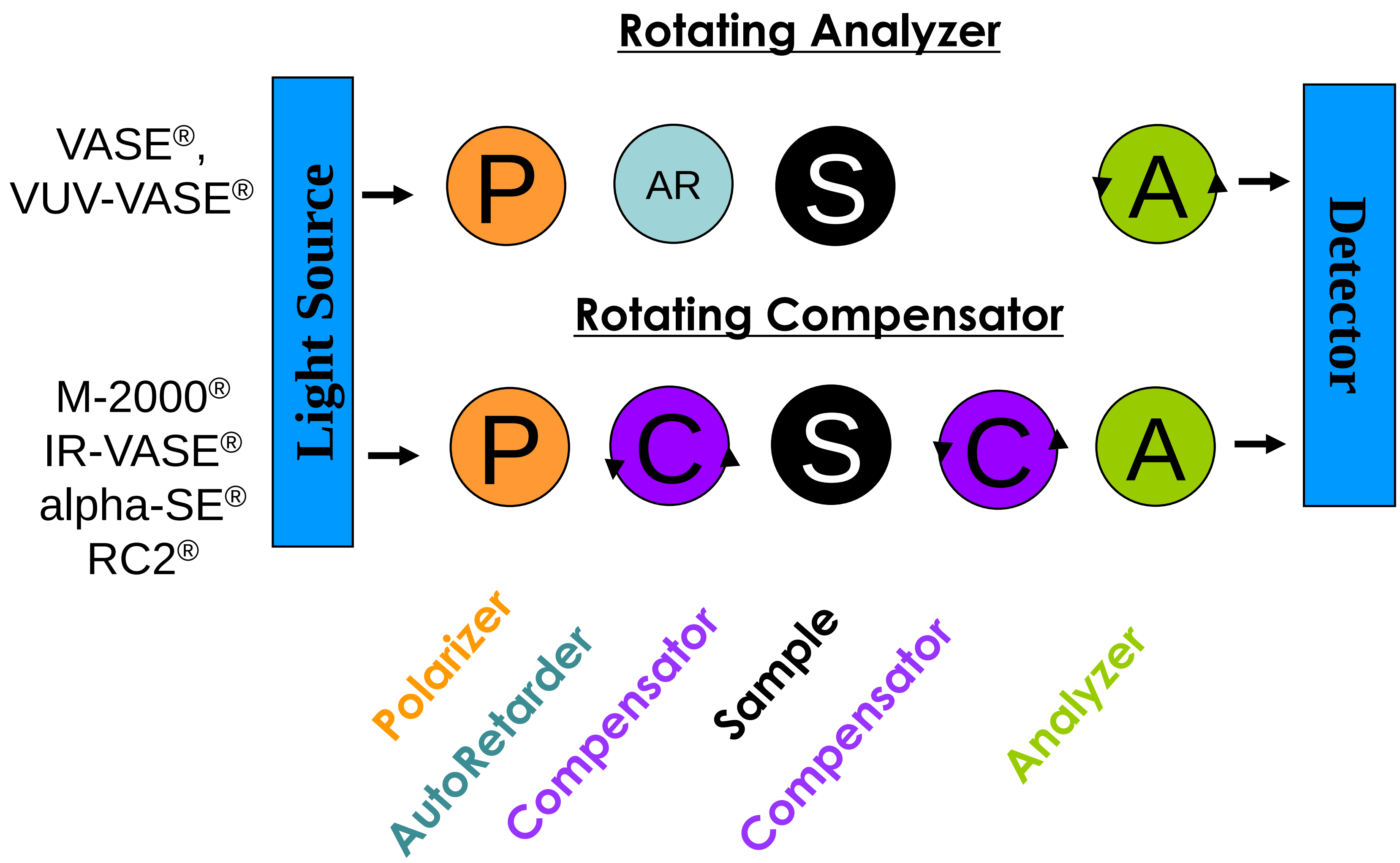
Ellipsometer: Block Diagram

- Every Ellipsometer contains the following components



- SE also needs wavelength selection.

Woollam Ellipsometers: Configurations



General SE References

Beginner:

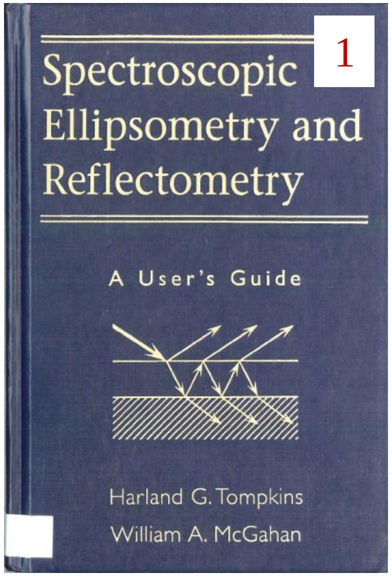
1. H.G. Tompkins, and W.A. McGahan, Spectroscopic Ellipsometry and Reflectometry, John Wiley & Sons, 1999.

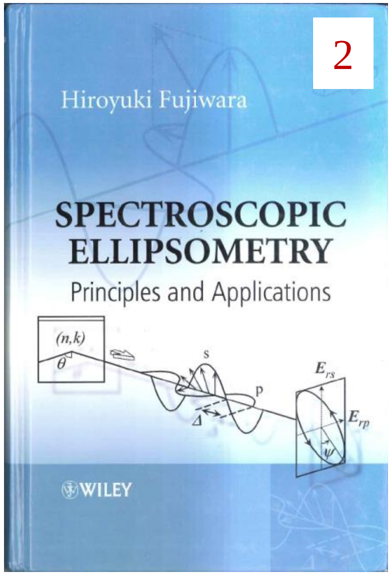
Intermediate:

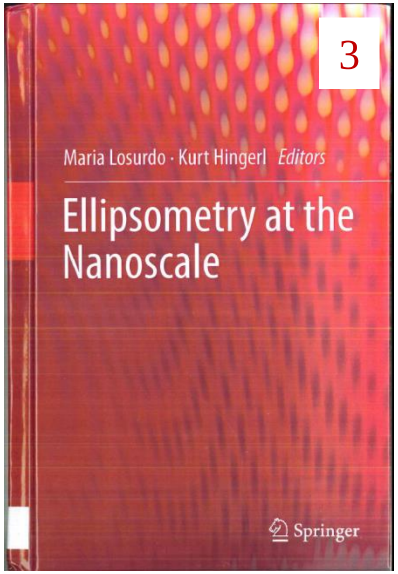
2. Hiroyuki Fujiwara, Spectroscopic Ellipsometry: Principles and Applications, John Wiley & Sons, 2007.

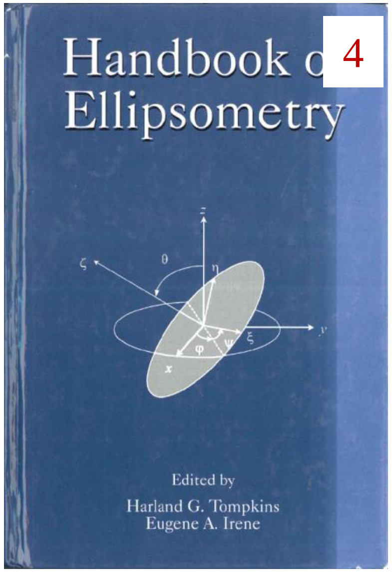
Advanced:

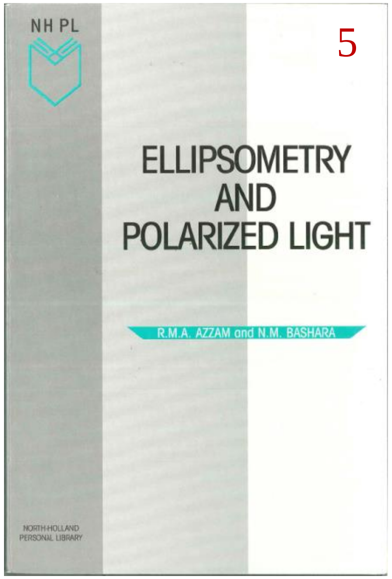
3. Ellipsometry at the Nanoscale, Lasurdo and Hingerl, eds., Springer-Verlag, 2013
4. Handbook of Ellipsometry, Tompkins and Irene, eds., William Andrew Publishing, 2005.
5. R.M.A. Azzam and N.M. Bashara, Ellipsometry and Polarized Light, Elsevier, 1977.





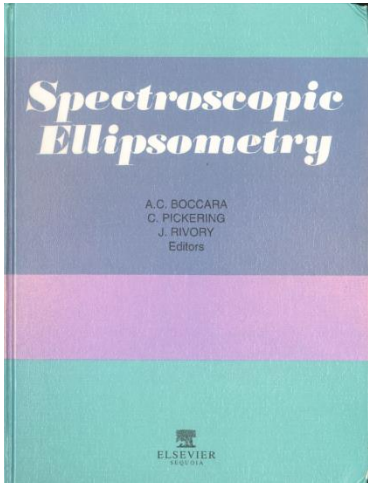


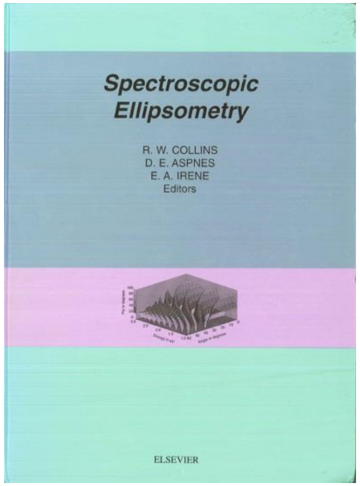


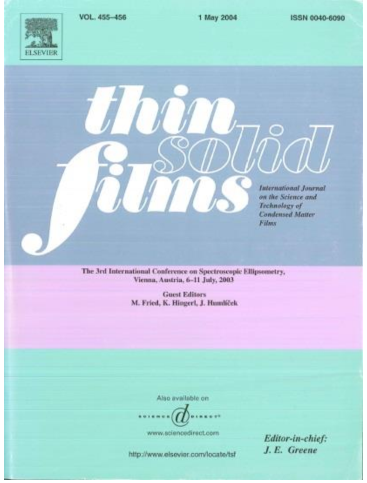


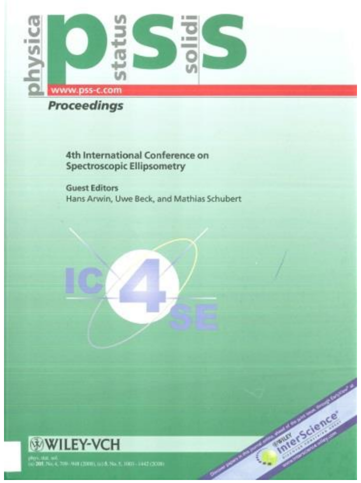
Ellipsometry Conference Proceedings

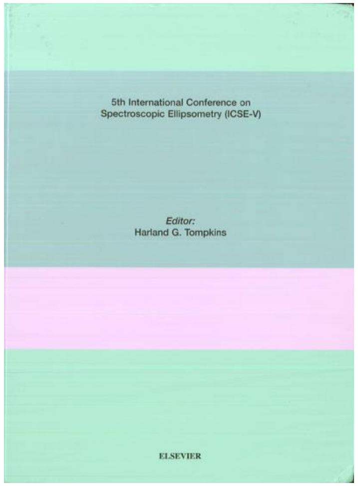
1. Spectroscopic Ellipsometry, (1993) A.C.Boccara, C.Pickering, J.Rivory, Editors, Elsevier Publishing.
2. Thin Solid Films Vol. 313-314 (1998). R.W.Collins, D.E.Aspnes, and E.A. Irene, Editors, Elsevier Science.
3. Thin Solid Films Vol. 455-456, (2004). M. Fried, K. Hingerl, and J. Humlicek, Editors, Elsevier Science.
4. Phys. Stat. Sol. (c) 5, No. 5, (2008). M. Schubert, H. Arwin, U. Beck, Editors, Wiley-VCH.
5. Thin Solid Films Vol. 519, Issue 9, (2011). H. G. Tompkins, Editor, Elsevier Science.











2 | 2_BK7_SE.dat, Append Transmission.

Step 1:

- Select Experimental Data Window.
- Open data file: 2_BK7_SE.dat.
- Append Data 2_BK7_T.dat

Step 2:

Select Graph Window

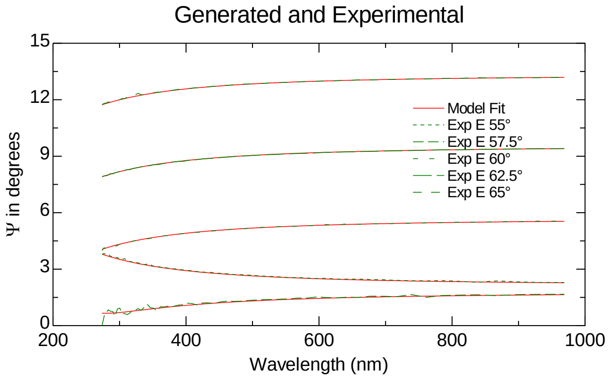
- Plot Ψ and Δ data.
- Plot Transmission data.
- What do they mean? (Describe polarization ellipse).
- What is each sensitive to? (Interpret the spectrum).

Learning Outcomes:

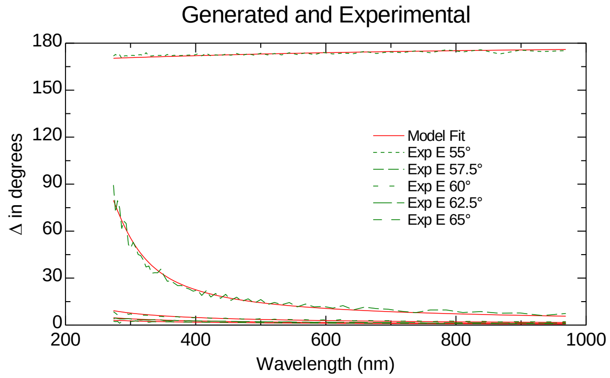
- Appending different types of data.
- Graphing different data types.
- Sensitivity of different data types to sample properties

Example 2: Uncoated BK7 Glass Substrate

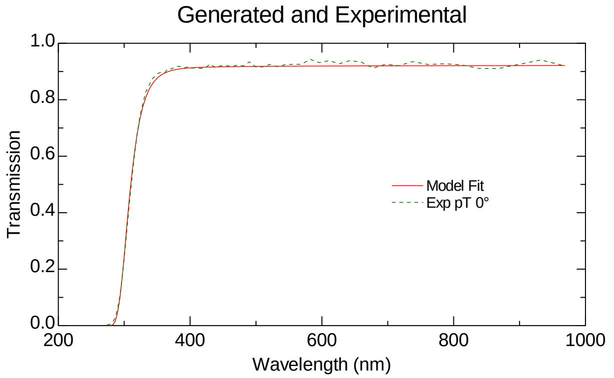
- 3 data types.
- Each sensitive to different sample properties (index, roughness, absorption).



Ψ: index



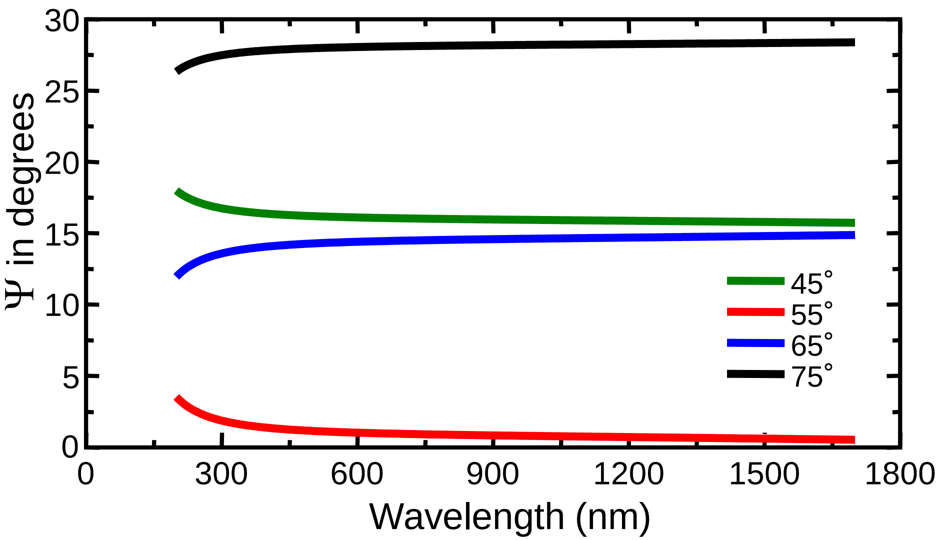
Δ: Roughness

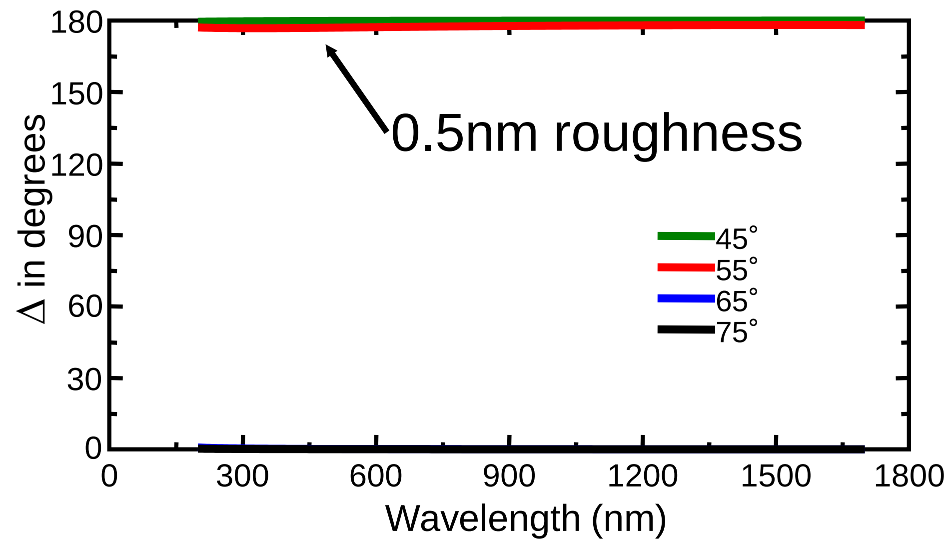


Transmission: Absorption

Spectral Features: Transparent Substrate

- Psi flat and smooth - follows shape of index
- Delta = 0° or 180° - except for surface films





3_nb.dat.

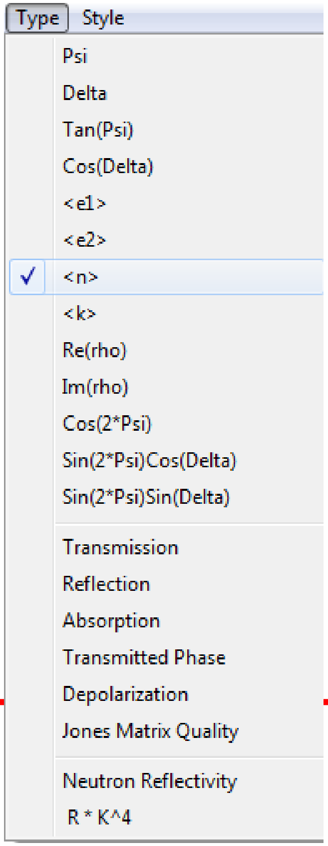
Step 1:

- ➢ Select Experimental Data Window.
- ➢ Open data file: 3_Nb.dat.

Step 2:

Select Graph Window

- ➢ Plot Ψ and Δ data.
- ➢ Plot <n> & <k>. <u>NOTE THE <> BRACKETS!</u>
- ➢ "Pseudo"-values. What do they mean?

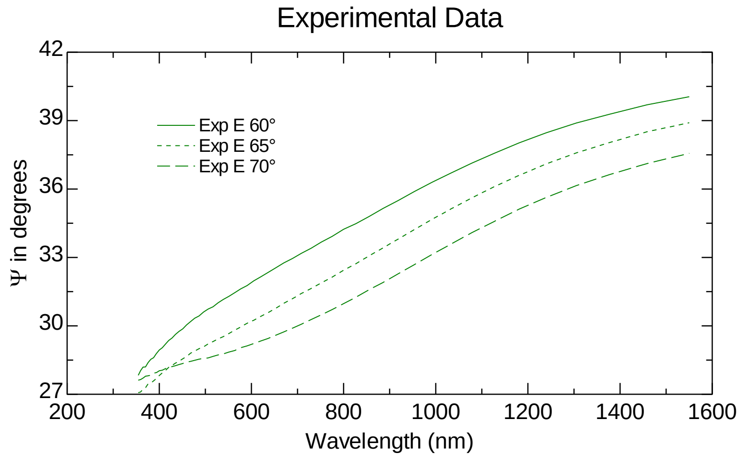


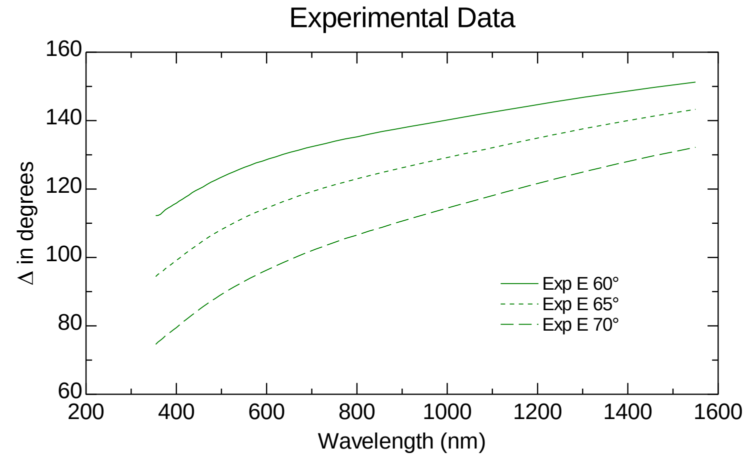
Learning Outcomes:

- Study spectrum of opaque material.
- Introduction to "pseudo" <n> & <k>.
- Sample properties causing change in polarization state.

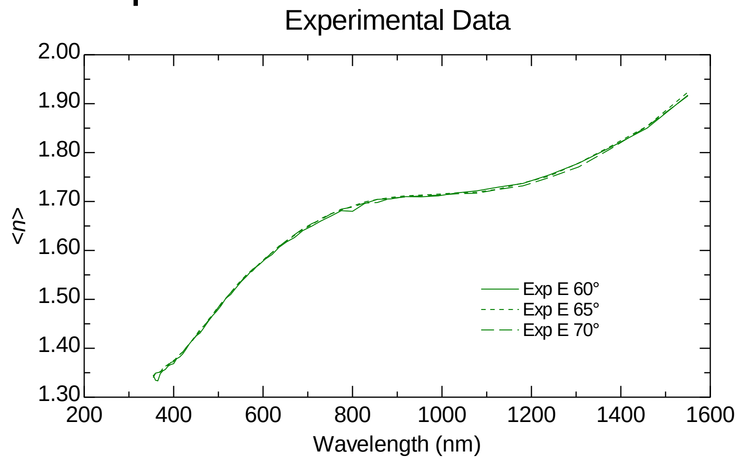
Opaque Sample: Metals

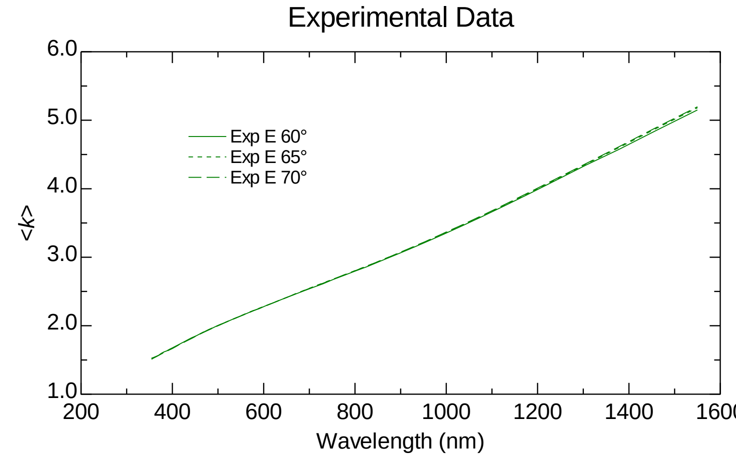
- Niobium: Psi and Delta





- Re-plotted as Pseudo <n>&<k>

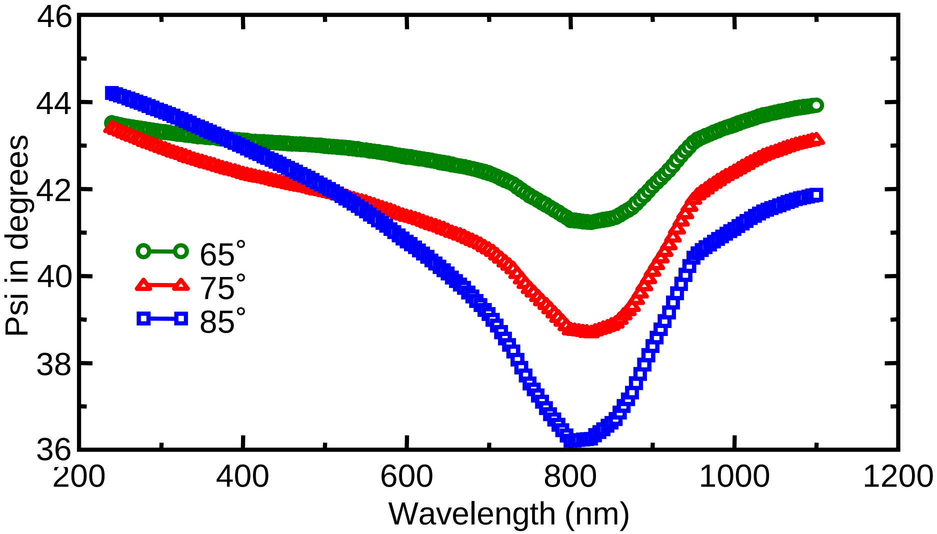


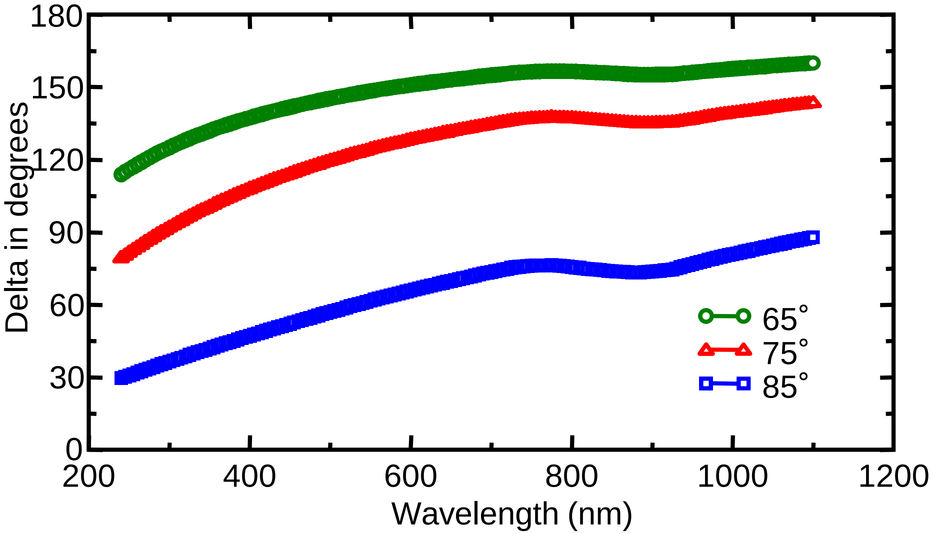


- Opaque Sample. All <n>&<k> angles the same.

Spectral Features: Opaque Metals

- Psi stays near 45
- Delta away from 0° or 180°
- Pseudo <n>&<k> same at all angles.





Substrate Identification

	Transparent	Absorbing
Psi	▪Flat ▪Approaches 0° at Brewster's angle	▪Shows features of n&k ▪Remains closer to 45° for all angles
Delta	▪Flat ▪Close to 0° or 180°.	▪Shows features of n&k ▪Stays between 0° and 180°
<Pseudo n&k>	▪<n> has Cauchy shape ▪<k> close to zero	▪<n&k> follow actual n&k.

<u>Transparent Substrate Exceptions:</u>

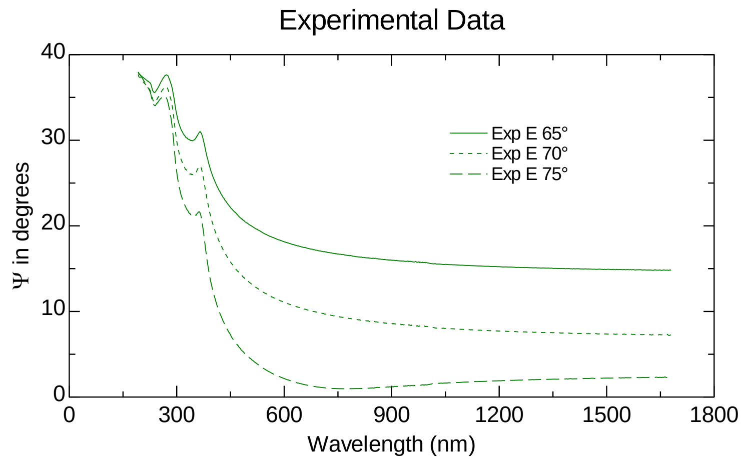
1. <n> separation for variable angle when backside reflections are present.
2. <k> non-zero and Delta away from 0,180° if surface layer (e.g. roughness).

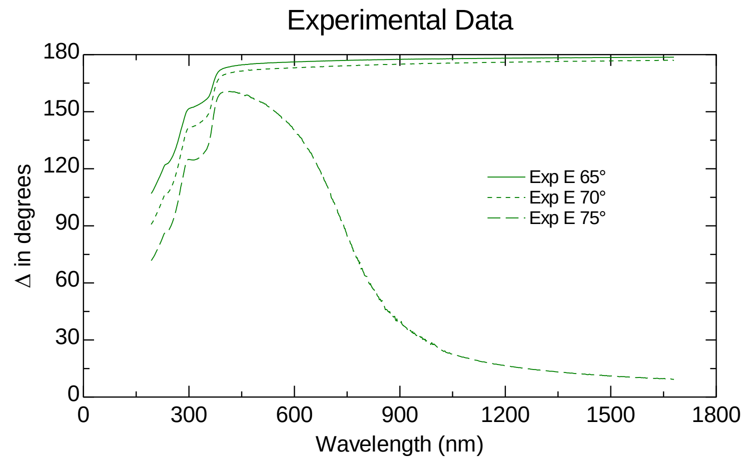
What about Semi-Absorbing?

4_Si wafer.dat

Step 1:

- Select Experimental Data Window.
- Open data file: 4_Si wafer.dat.



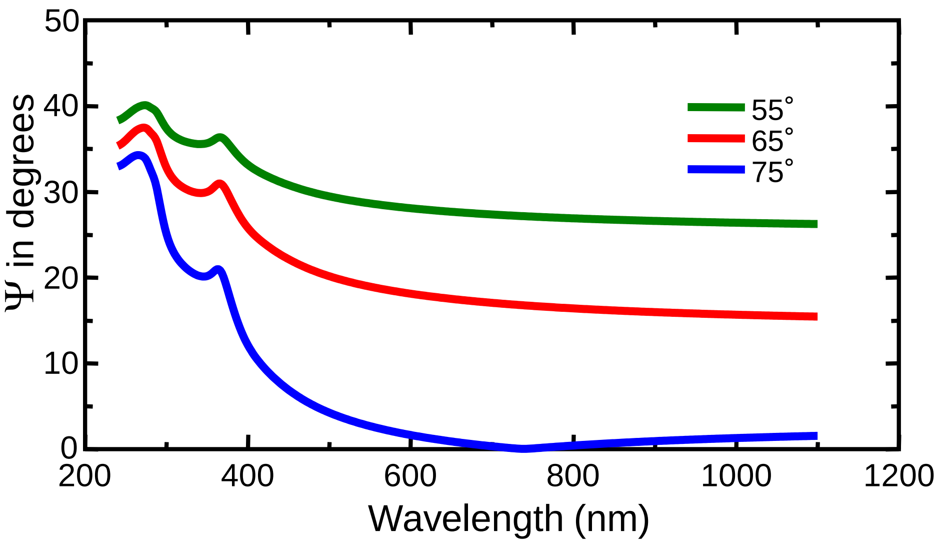


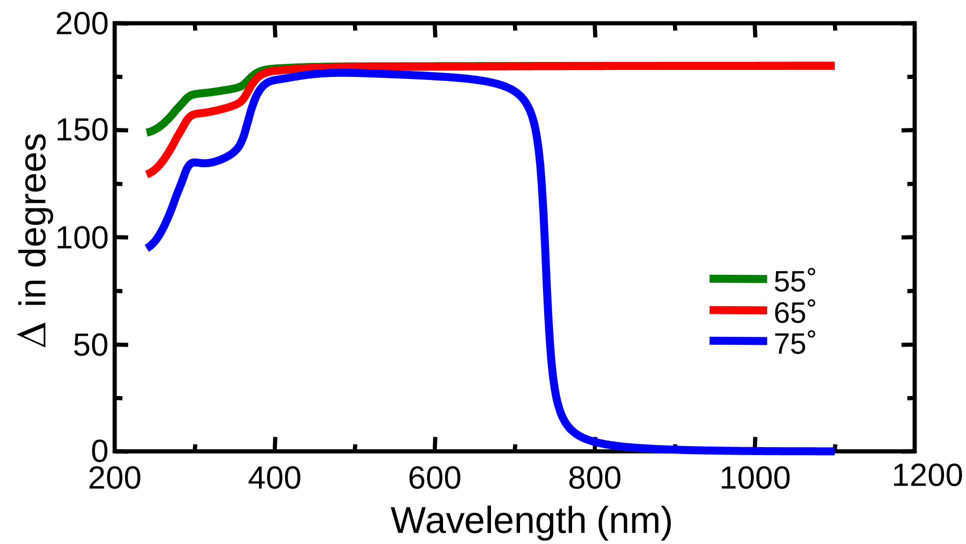
Learning Outcomes:

- Study spectrum of crystalline material.
- Note sharp structure below 450 nm. Why? Why so sharp?
- Identify transparent and absorbing regions.

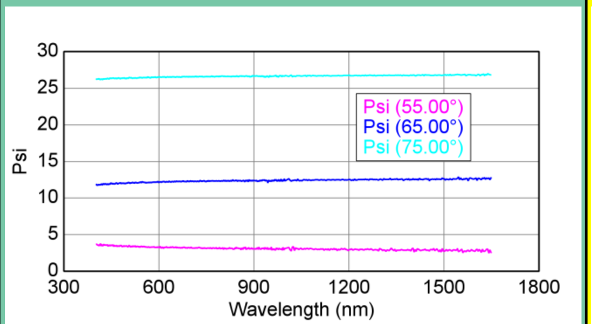
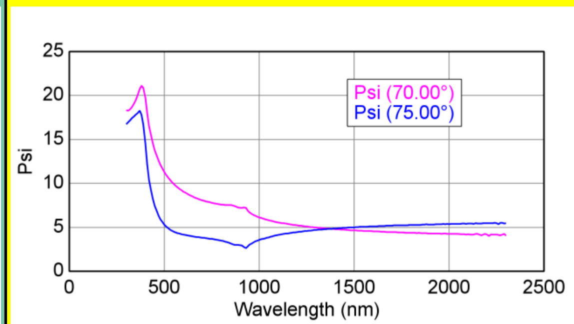
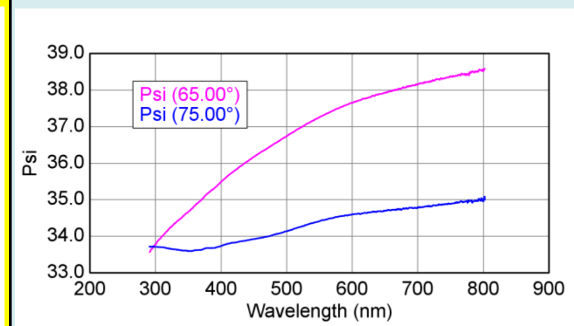
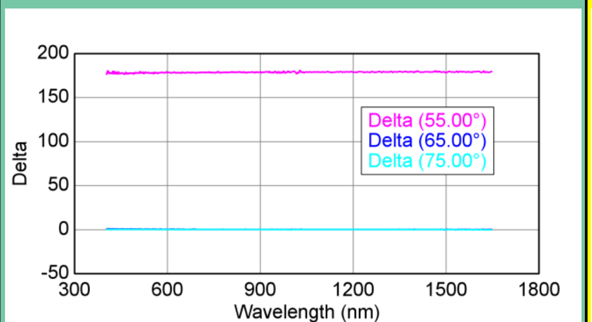
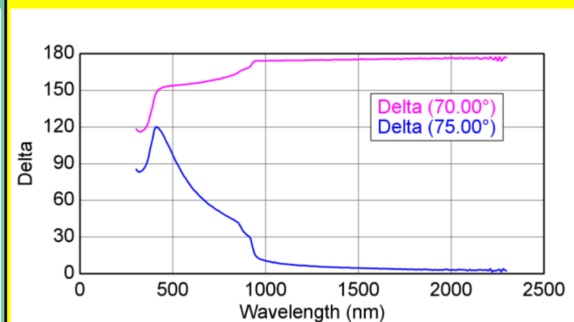
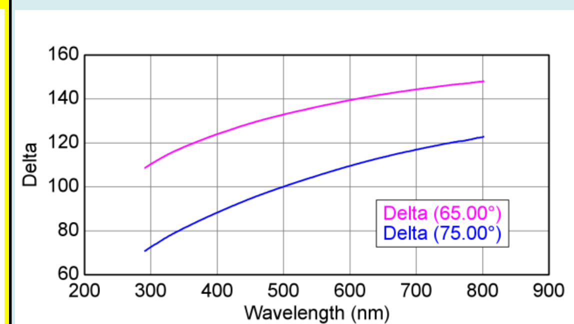
Substrate - Semiconductors

- Psi follows shape of absorption.
- Delta away from 0° or 180° when absorbing.
- Sharp features due to absorption.





Review: Substrate Types, Spectral Features.

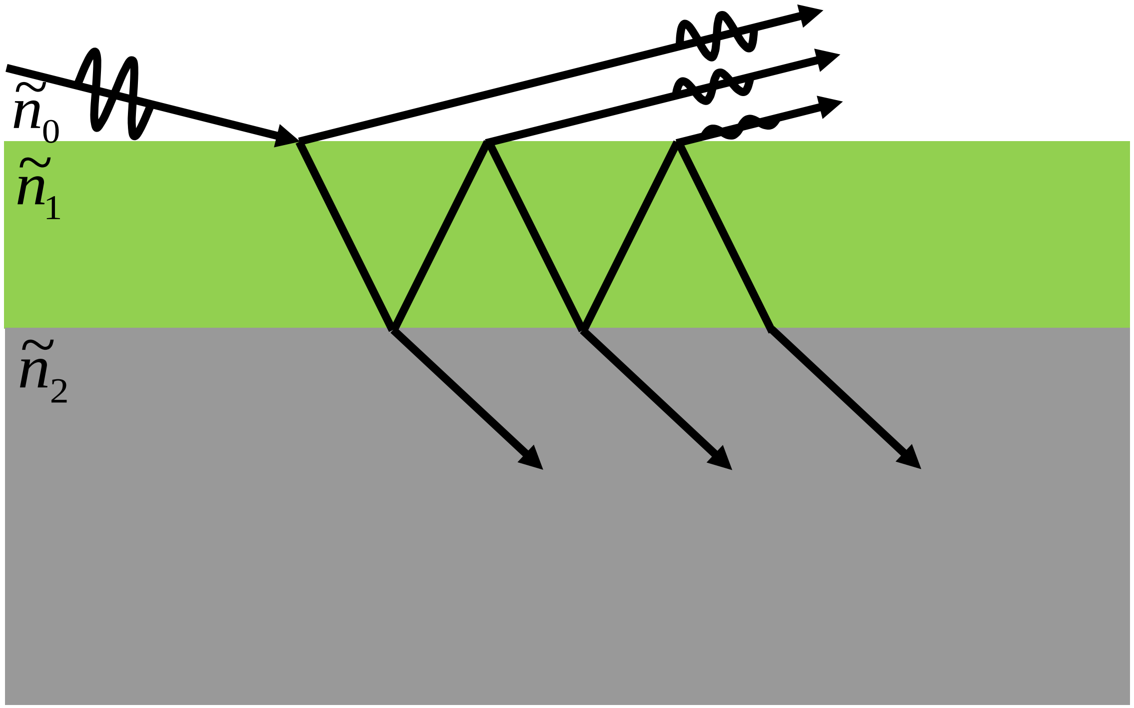
	Transparent	Semi-Absorbing	Absorbing
Ψ			
Δ			

Describe unique features of each spectrum.

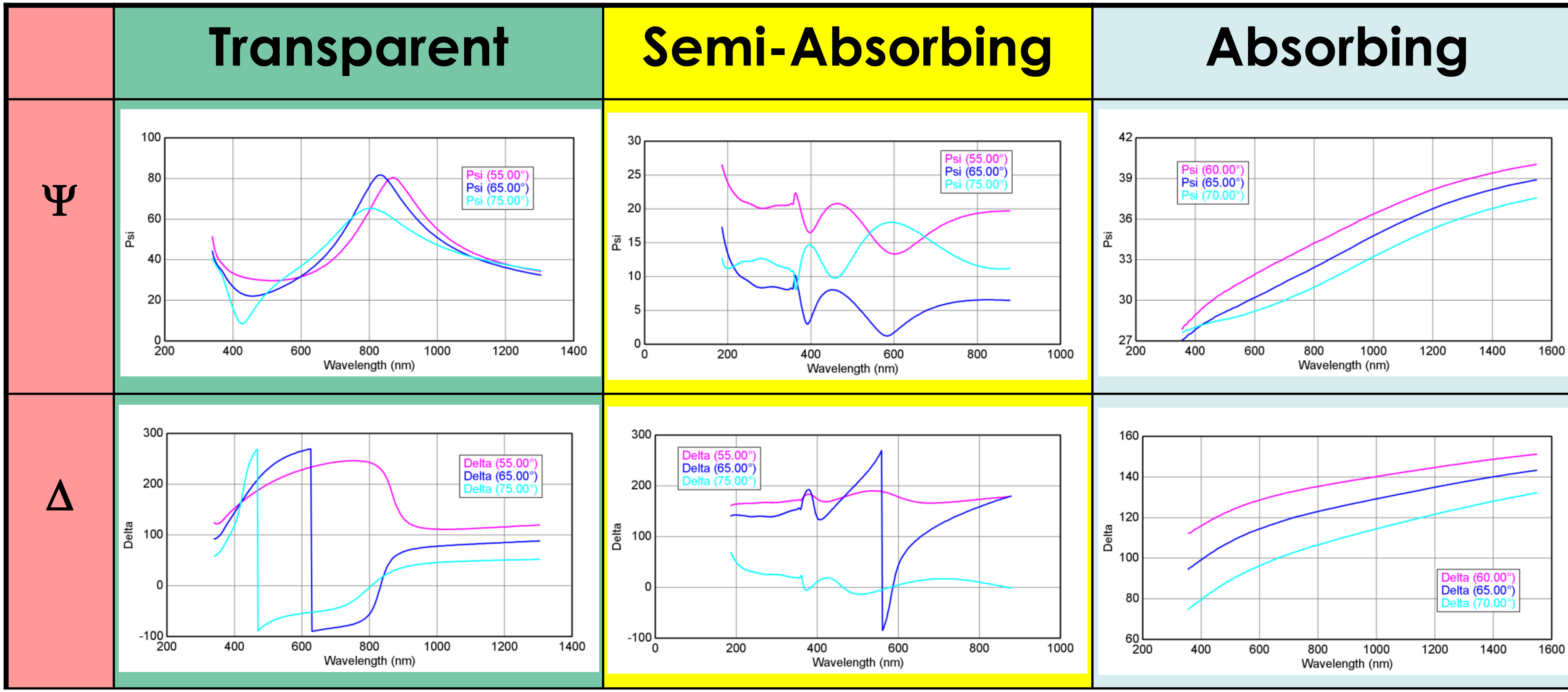
Coated Samples!

Thin Film Identification

- Multiple Reflections at interfaces.
- Use to estimate film thickness and Index.
- Can be transparent, Absorbing, or Semi-Absorbing.



Coated Thin Film Examples



Coatings add interference effects in transparent regions.

Transparent Film on Silicon

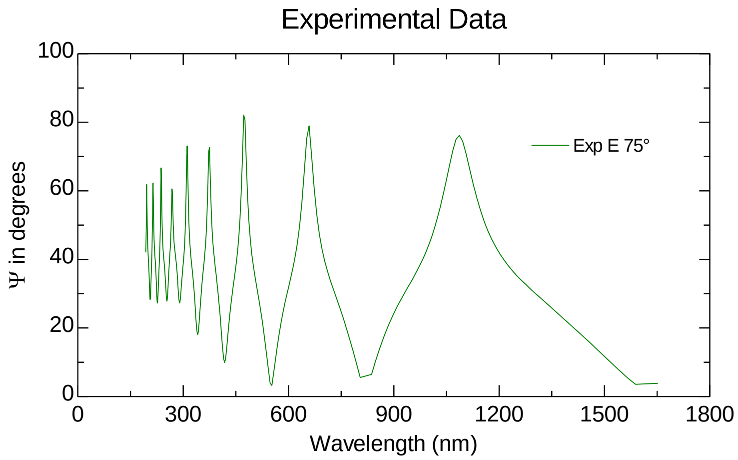
Step 1:

- ➢ Open data file: 5_SiO2 on Si.dat.

Step 2:

Select Graph Window

- ➢ Plot Ψ and Δ data.
- ➢ **Note the interference effects.**
- ➢ What Causes these oscillations?



Learning Outcomes:

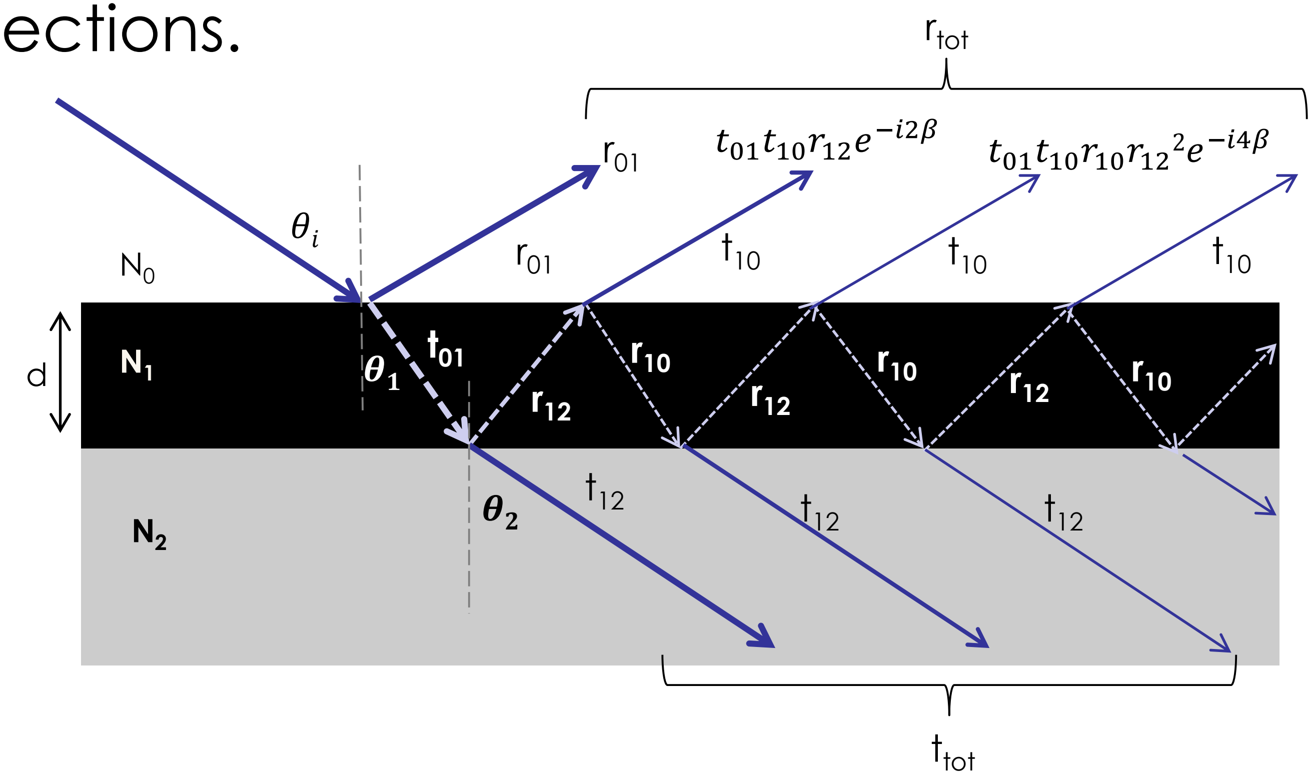
- Identify spectrum of a coated substrate with transparent film.
- Observe thin-film interference effects from transparent Film.

Thin Film on Substrate

- Multiple reflections in single film lead to an infinite series of reflections.

Phase from different optical paths is tracked by film phase thickness (β)

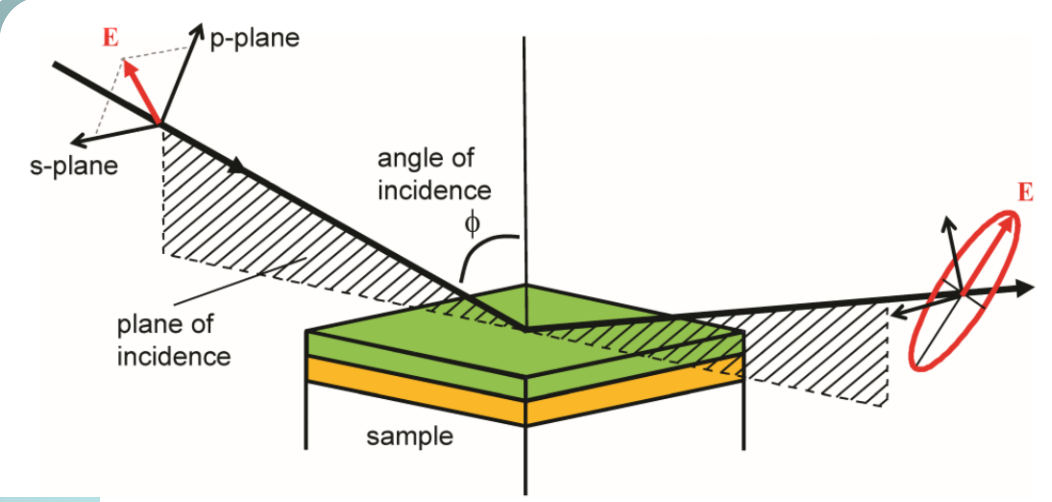
$$\beta = 2\pi\left(\frac{d}{\lambda}\right)N_1\cos\theta_1$$

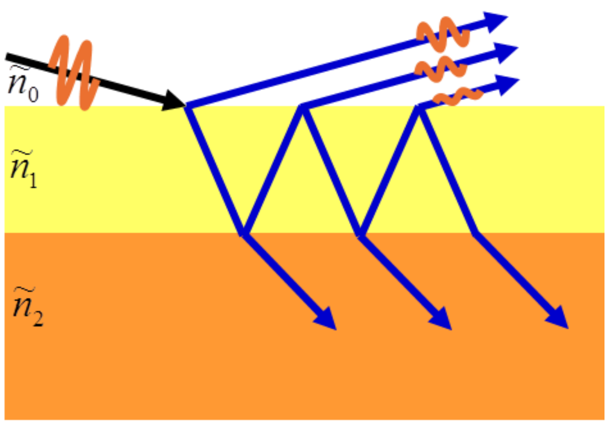


$$r_{tot} = r_{01} + t_{01}r_{12}t_{10}e^{-2i\beta} + t_{01}r_{12}{}^2r_{10}t_{10}e^{-4i\beta} + \ldots$$

Thin-Film Interference Effects

- SE measures polarization change as light interacts with sample.

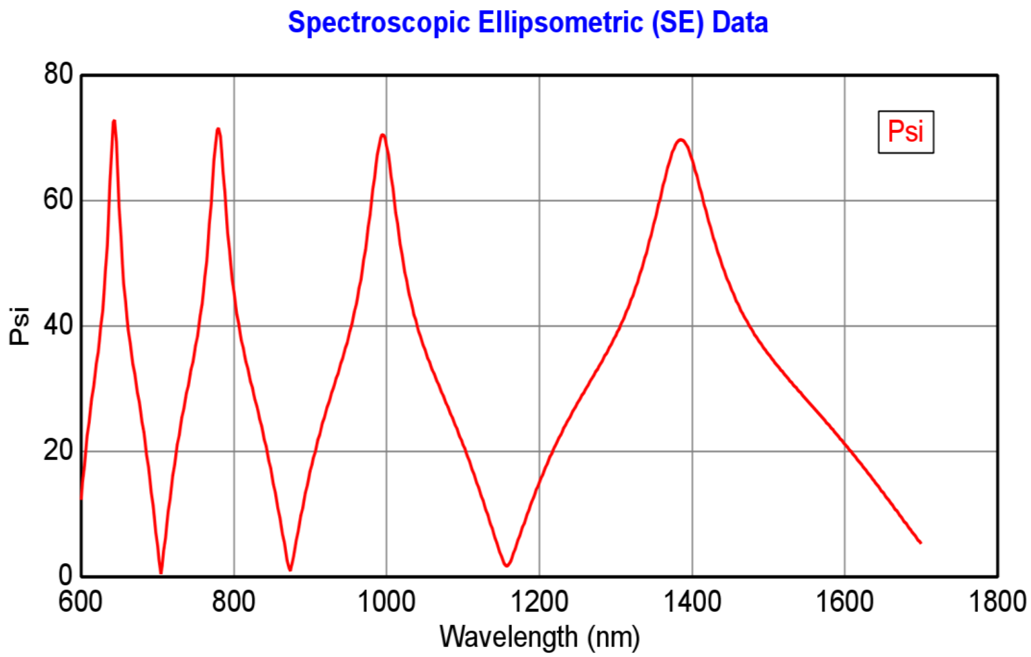


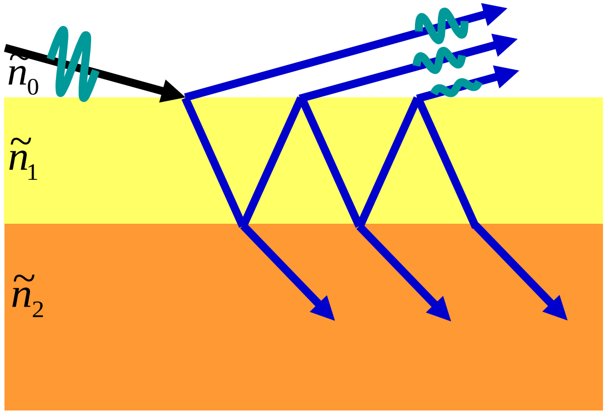


- Interference occurs as light recombines after traveling different paths through thin film.

SE features – Transparent Films

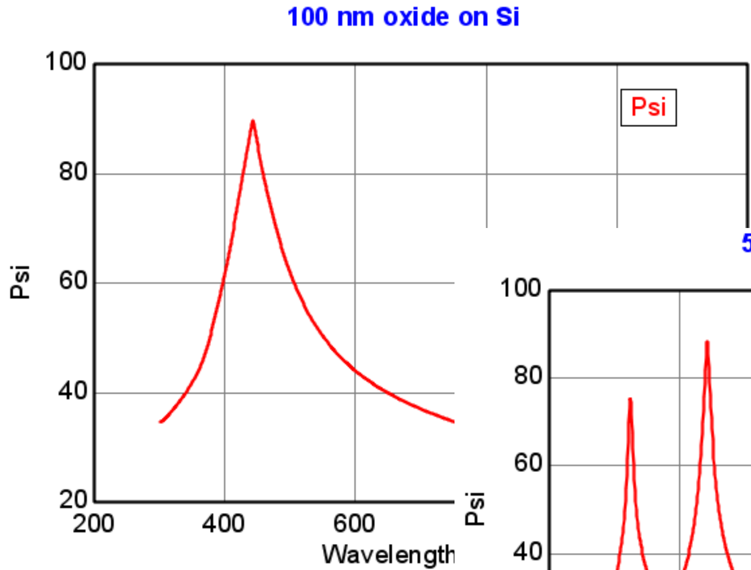
- Oscillation patterns in ellipsometry data due to thin film interference.
- Pattern affected by thickness and index.

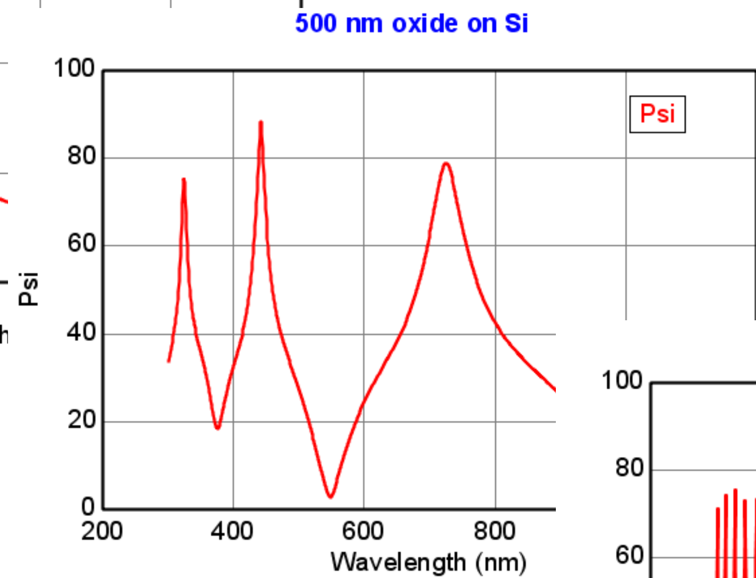


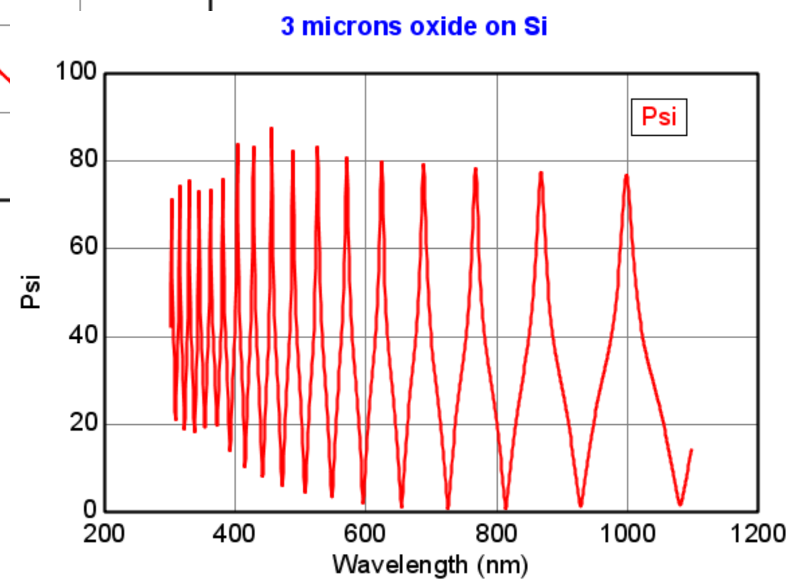


Transparent - oscillations

Thickness Effects







Thicker films have more interference oscillations

6 6_Dielectric on Glass.dat

Very Thick Transparent Film on Glass

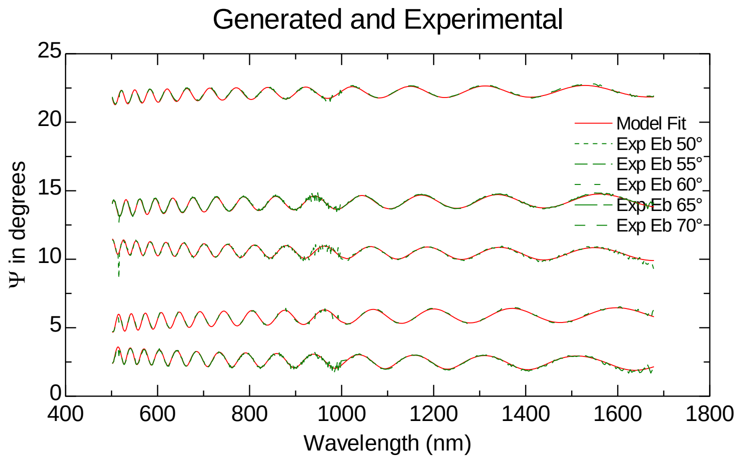
Step 1:

- Open data file: 6_Dielectric on Glass.dat.

Step 2:

Select Graph Window

- Plot Ψ and Δ data.
- Thick or thin film?
- Why small amplitudes?



Learning Outcomes:

- Identify spectrum of thick versus thin transparent film.
- Note small amplitude of oscillations. Why?

Thin Film Identification

	Transparent	Absorbing
Psi	▪Oscillates ▪Size of oscillations signify index difference between substrate and thin film ▪Number of oscillations indicate thickness	▪No oscillations. ▪Shows features of n&k. ▪Looks like opaque substrate.
Delta	▪Oscillates ▪Number of oscillations indicate thickness	▪Shows features of n&k. ▪Stays between 0° and 180°.
<Pseudo n&k>	▪May separate for multi-angles.	▪Overlapping at multi-angles.

VERY THIN LAYER Exceptions:

1. Oscillations will not appear until about 25-50 nm thickness.
2. Psi may go above 45° for thin coatings.

What about Semi-Absorbing?

Break!

7_SiNx on Si.dat

Semi-Absorbing Film on Silicon

Step 1:

➢ Open data file: 7_SiNx on Si.dat.

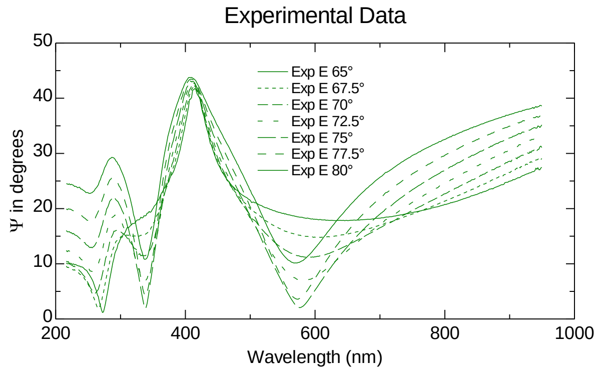
Step 2:

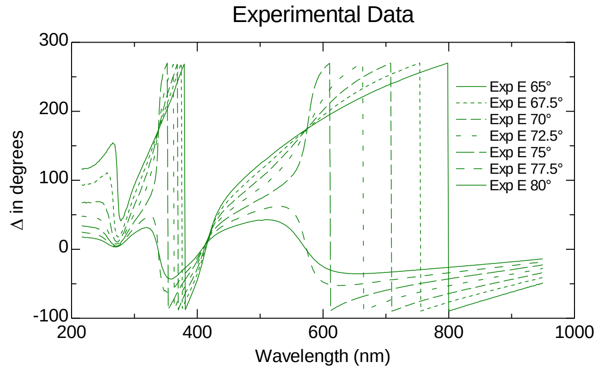
Select Graph Window

➢ Plot Ψ and Δ data.

➢ Note the interference effects.

➢ **Discuss IR and UV behavior.**





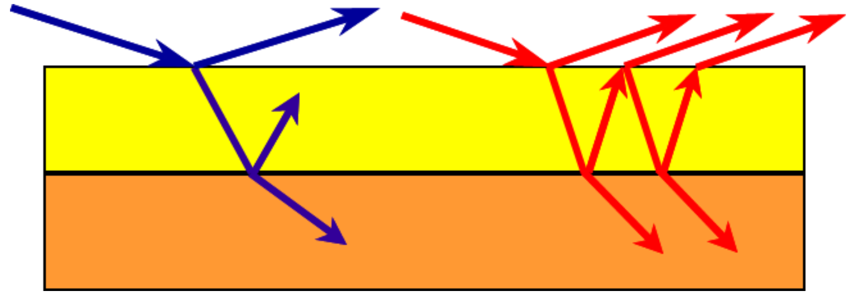
Learning Outcomes:

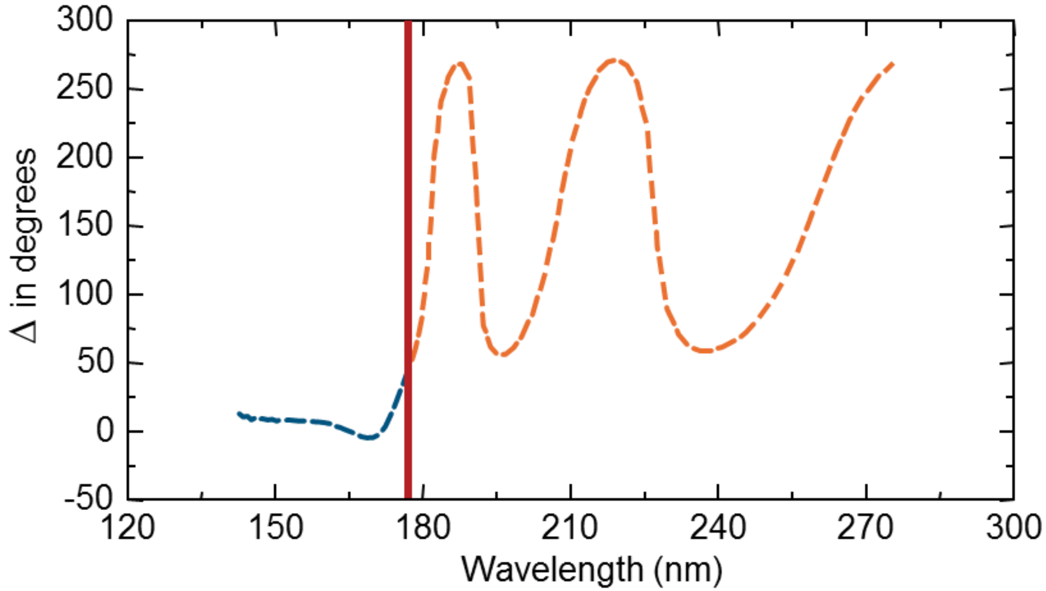
- Identify spectrum of a UV absorbing film.
- Observe thin-film interference effects and absorption effects.

Semi-Absorbing Films

Spectral Identification: What to expect?

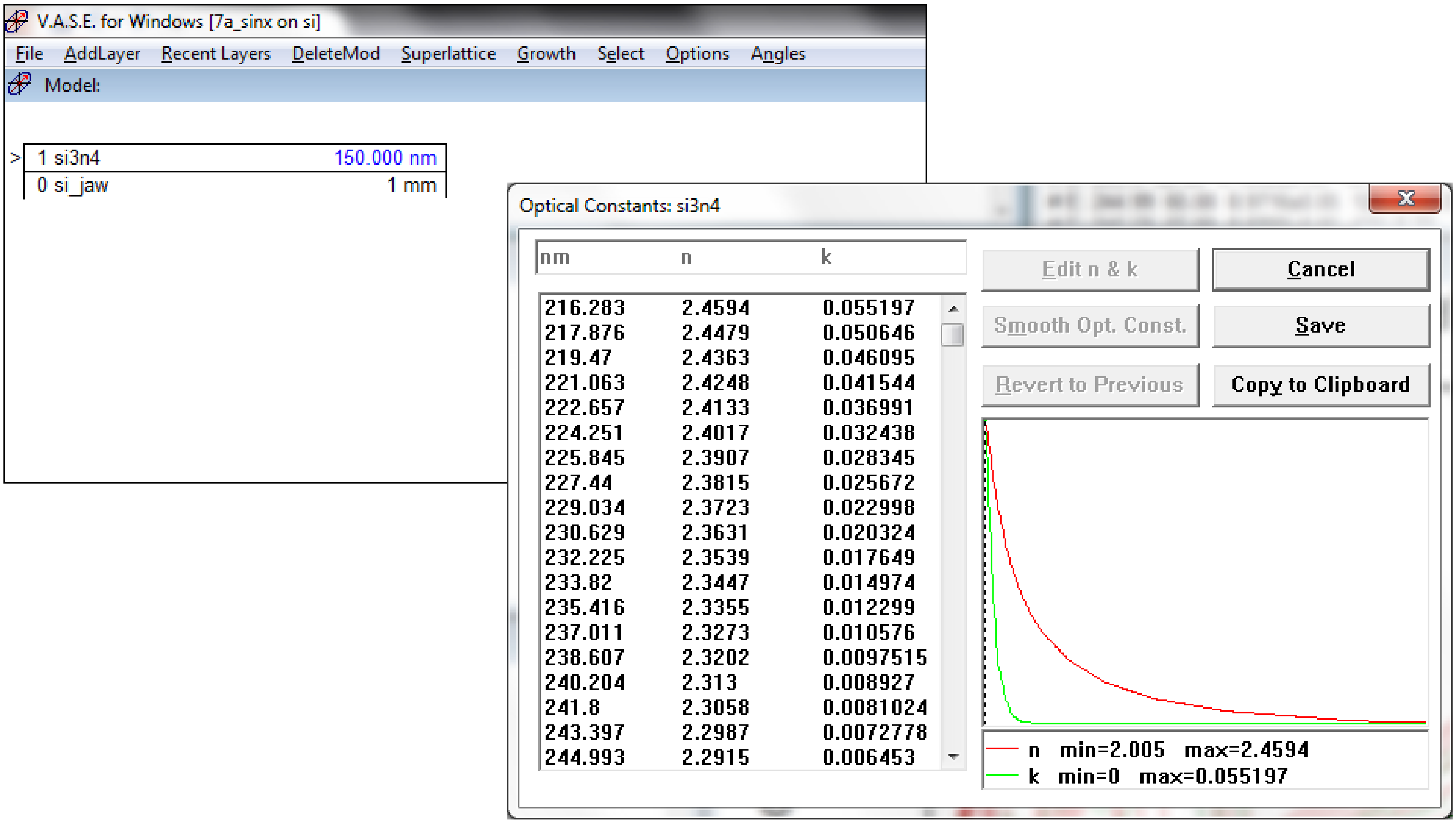
- If light is absorbed before returning to surface, only top reflection is 'seen' (Film appears as opaque substrate).





WVASE Model Window

Add layers. Define fit parameters.



Contains optical constants of each layer.

What are "Optical Constants"?

7_SiNx on Si.dat

Build Model For Silicon Nitride on Silicon

Step 1:

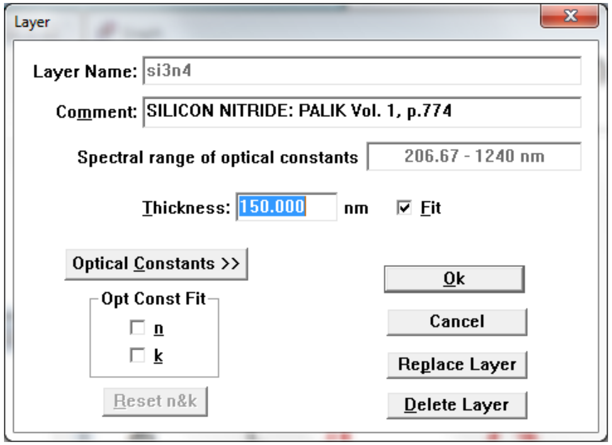
- Open data file: 7_SiNx on Si.dat.

1	si3n4	150.000 nm
0	si_jaw	1 mm

Step 2:

Select Model Window.

- Add Layer: Si_jaw.mat.
- Add Layer: Si3N4.mat.
- Add fit Parameter: Film Thickness.
- Show table of optical constants.

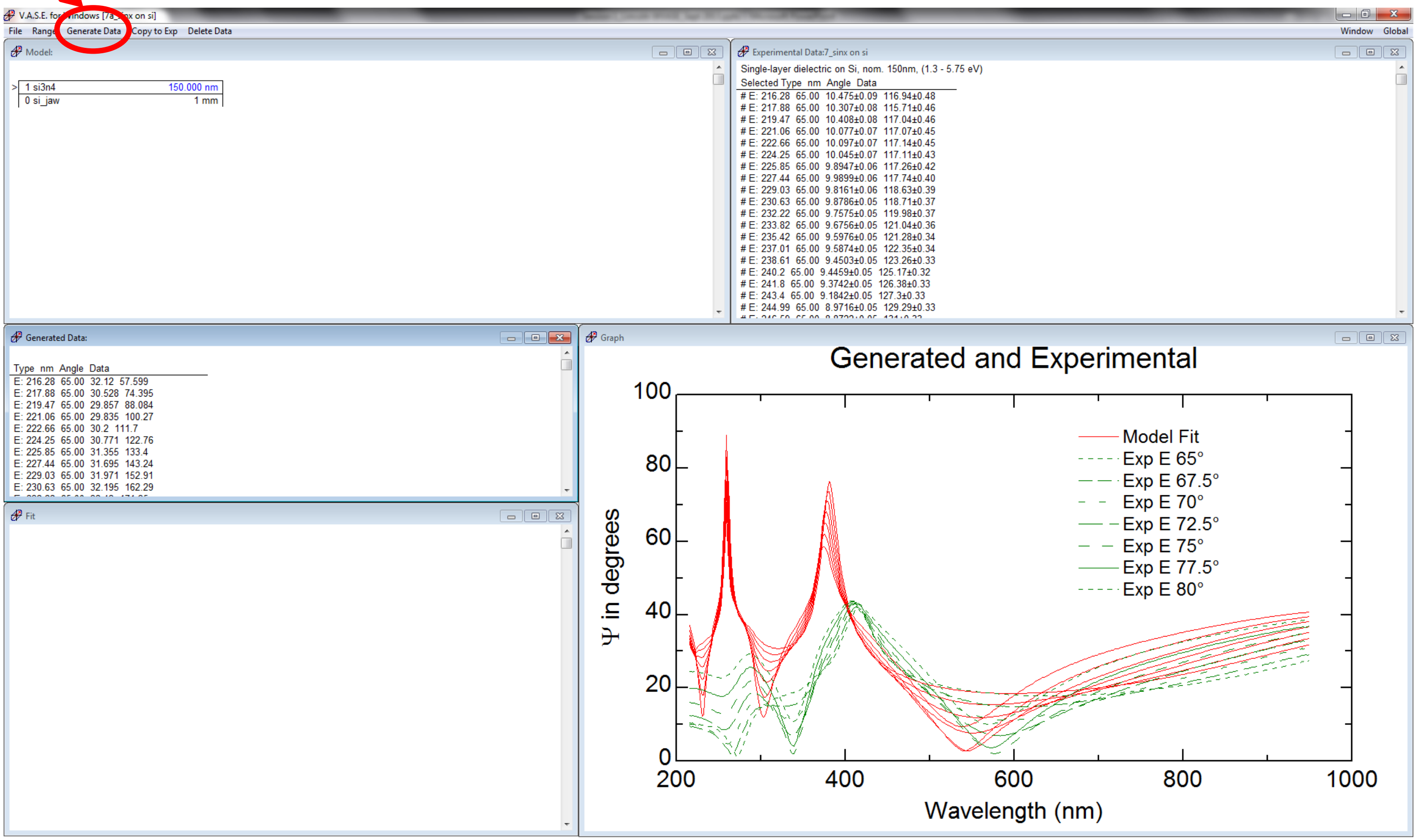


Learning Outcomes:

- Building a model. Adding layers.
- Adding fit parameters.

Generate Data Window

Generates data from the Model



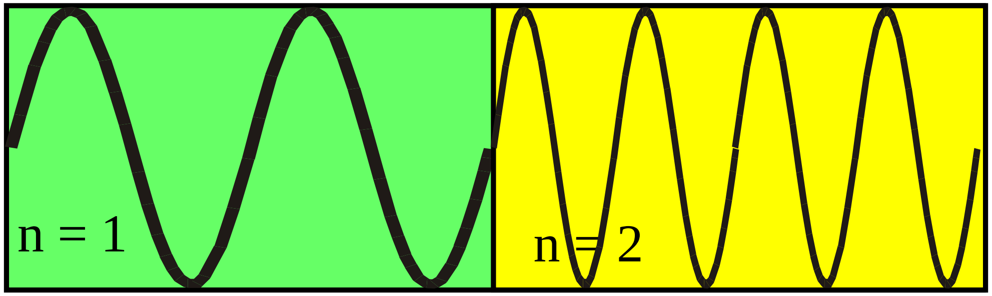
Graphs compare Model Generated and Experimental Data.

Thickness is close, so why not a perfect match?

Optical Constants, Refractive Index, n

Light in Different Media:

Velocity and wavelength vary in different materials.



$$v = \frac{c}{n}$$

speed of light (c)

Frequency (color) of wave remains the same!

$$f = \frac{v}{\lambda}$$

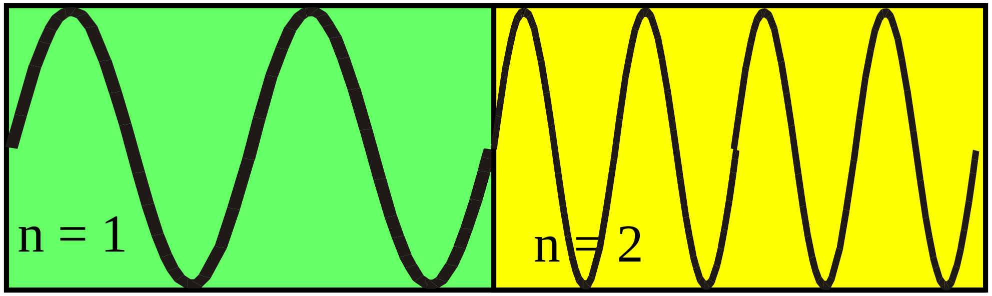
Energy of photon remains the same:

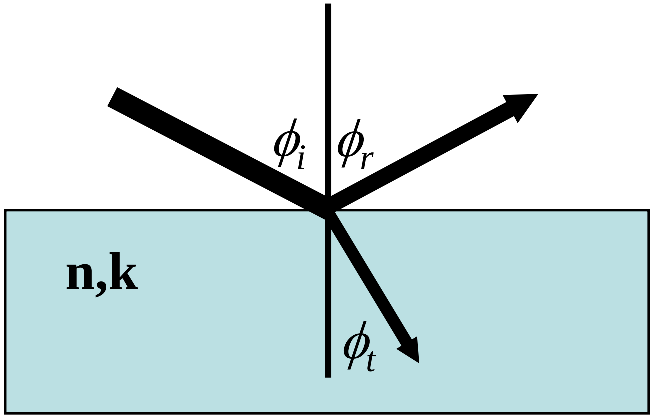
$$E(eV) = h\upsilon \cong \frac{1{,}240}{\lambda(nm)}$$

Planck's constant (h)

Index of Refraction, n

- **Index of Refraction (*n*)**
- **Describes How Light is affected by Materials:** reflection, refraction, phase velocity, absorption





$$\upsilon = \frac{\mathrm{v}}{\lambda} = \frac{c}{n\lambda}$$

Frequency constant

Refractive Index, n

- Determines **Wave speed**.

$$v = c/n$$

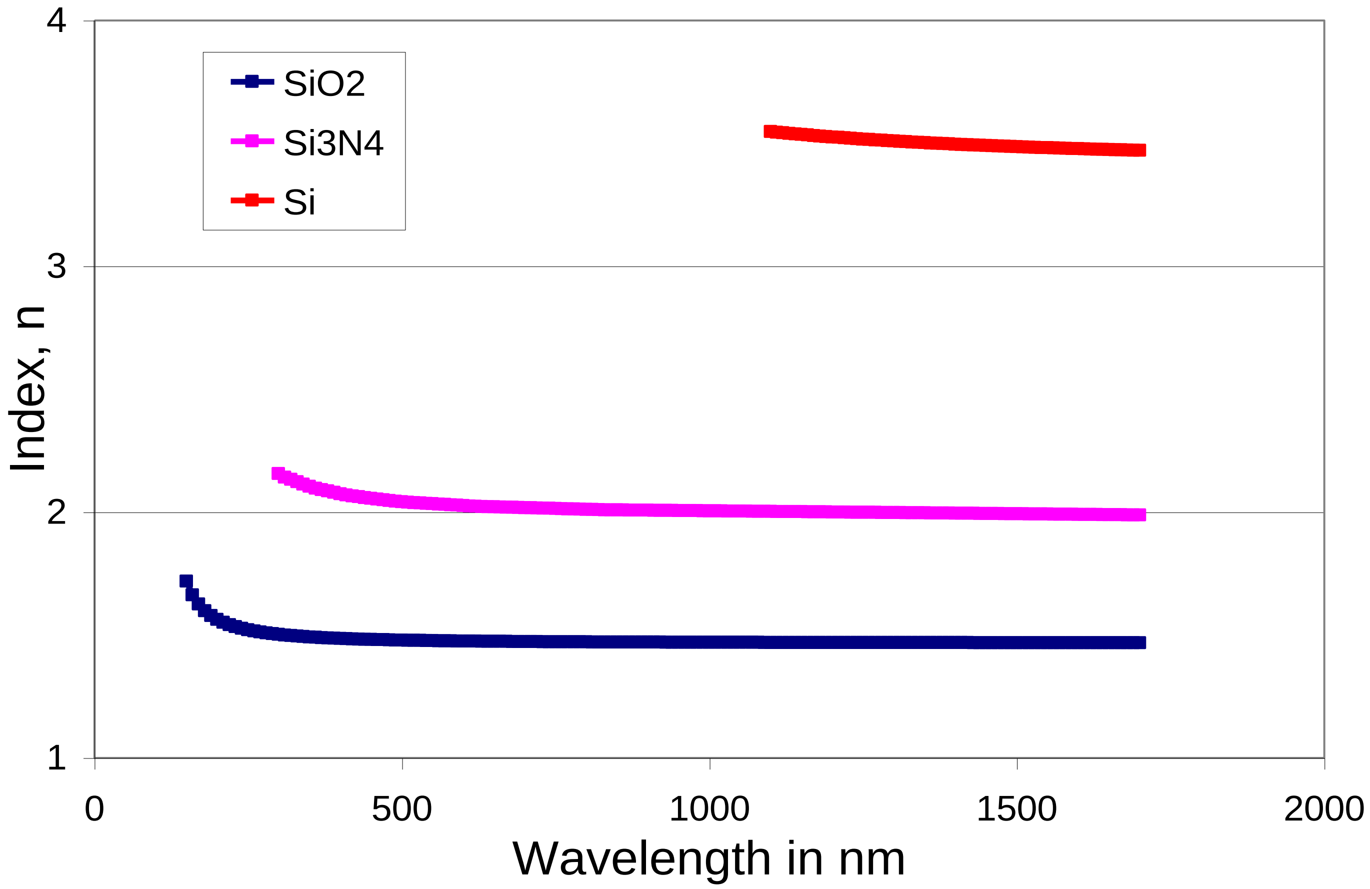
- Determines **Angle of Propagation**.
  - Snell's Law of Refraction:

$$n_1 \sin\theta_1 = n_2 \sin\theta_2$$

  - Example: Pencil in glass of water appears "Bent", or "Broken". Caused by refraction.

Refractive Index: Transparent Materials

- Index decreases for longer wavelengths.
- Higher index for stronger UV absorption.



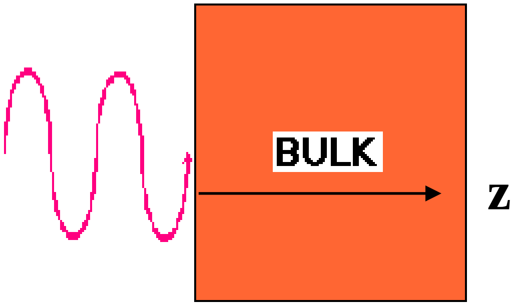
Absorption and Extinction

$$I = I_o e^{-\alpha z}$$

$$\alpha = \frac{4\pi k}{\lambda}$$

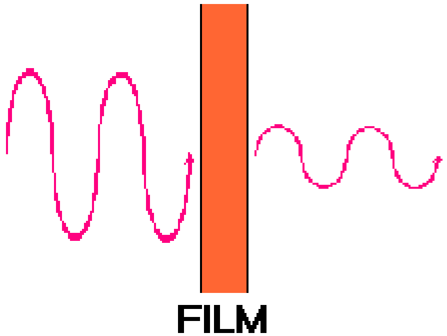
Bulk Material Absorption:

Deeper propagation gives:
= more energy loss.
= complete extinction.



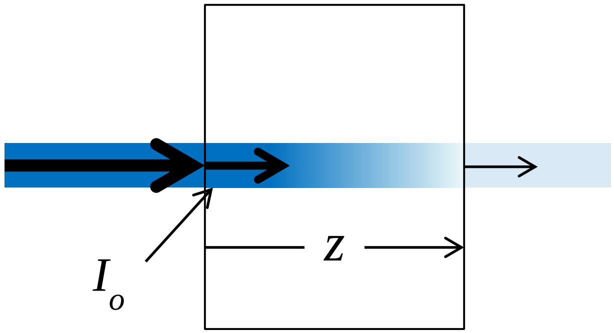
Absorbing films:

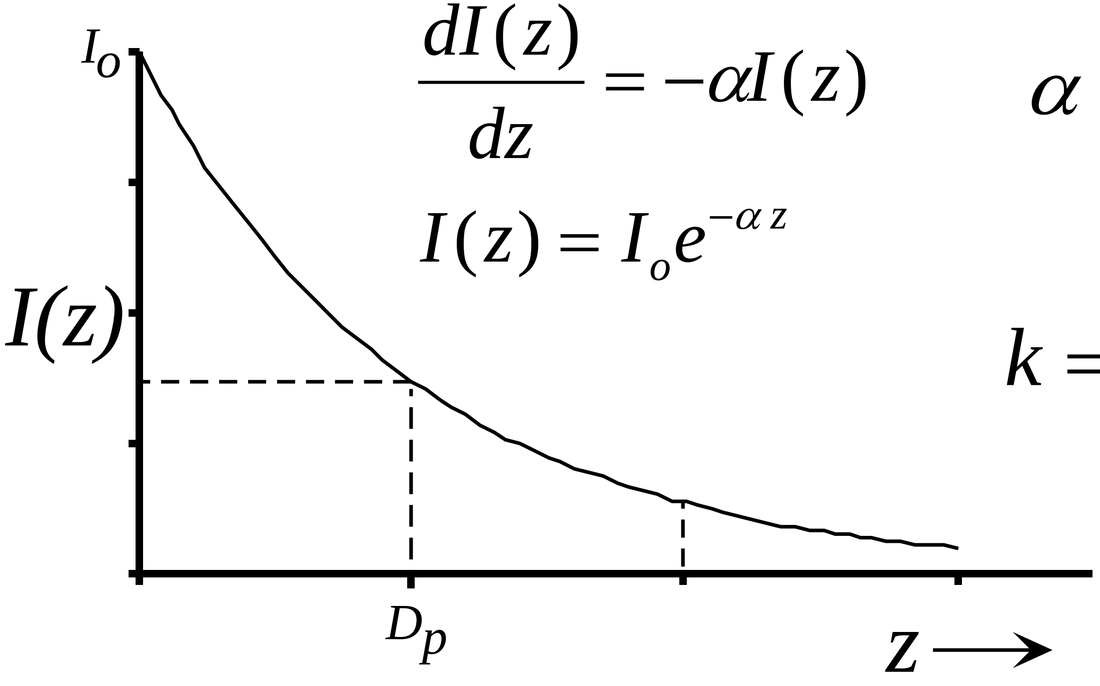
Increasing thickness gives:
= longer propagation path in film.
= wave spends longer time in film.
= more absorption by material.
= more extinction of wave.



Absorption: Beer-Lambert-Bouguer Law

- Absorption coefficient (**α**)
- Extinction coefficient (*k*)
  - Loss of wave energy to the material.





$$\frac{dI(z)}{dz} = -\alpha I(z)$$

$$I(z) = I_o e^{-\alpha z}$$

$$\alpha = \frac{4\pi k}{\lambda}$$

$$k = \frac{\lambda}{4\pi}\alpha$$

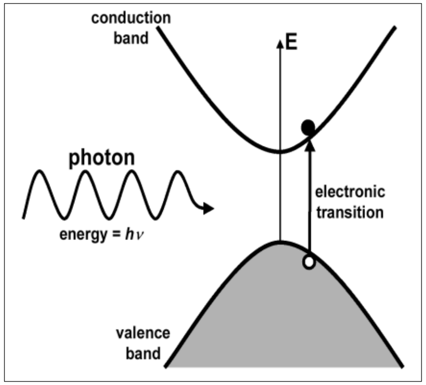
Pierre Bouguer
(1698-1758)

Johann Heinrich Lambert
(1728-1777)

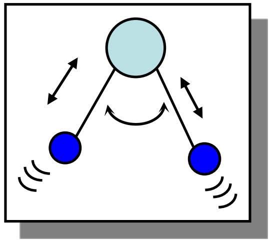
Multiple types of optical absorption

- Common absorption of EM waves:

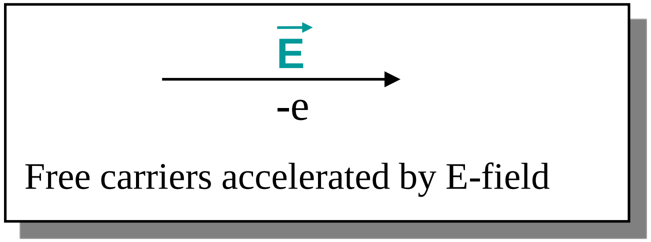
Electronic
UV-visible-near IR frequencies



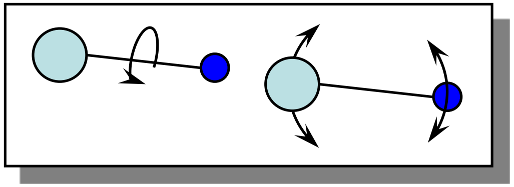
Vibrational
mid-IR freq



Free carriers
(conductivity)
mostly IR

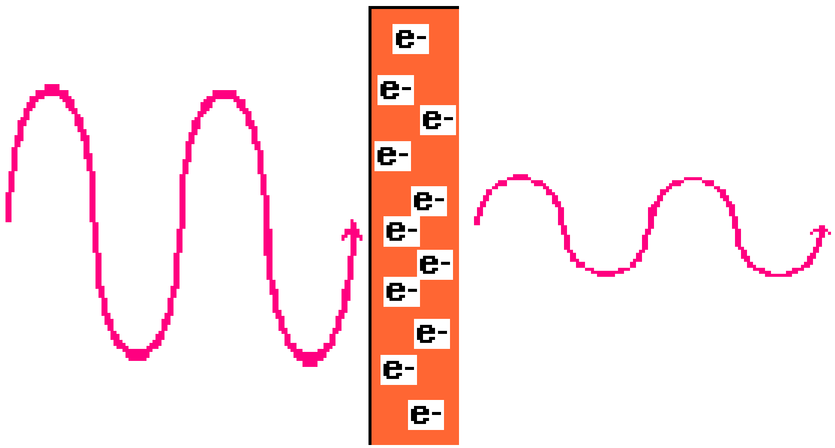


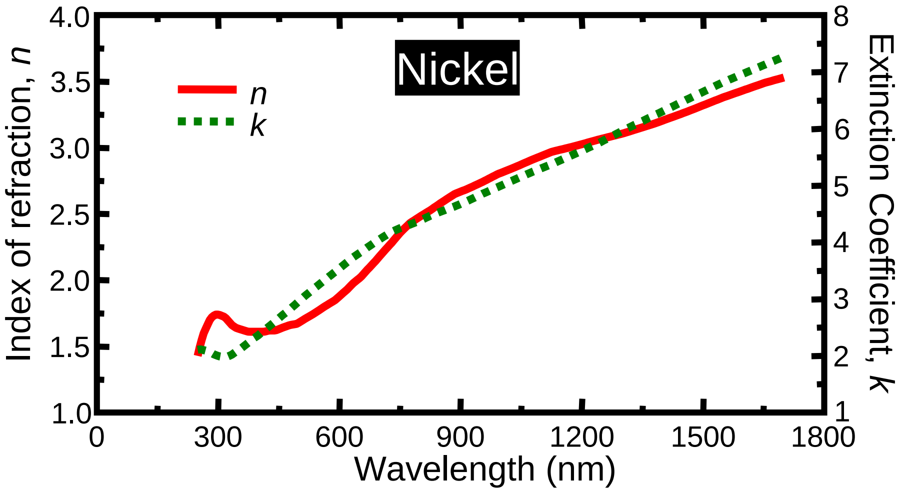
Rotational
(microwave oven)



Metals: Free-carrier Absorption

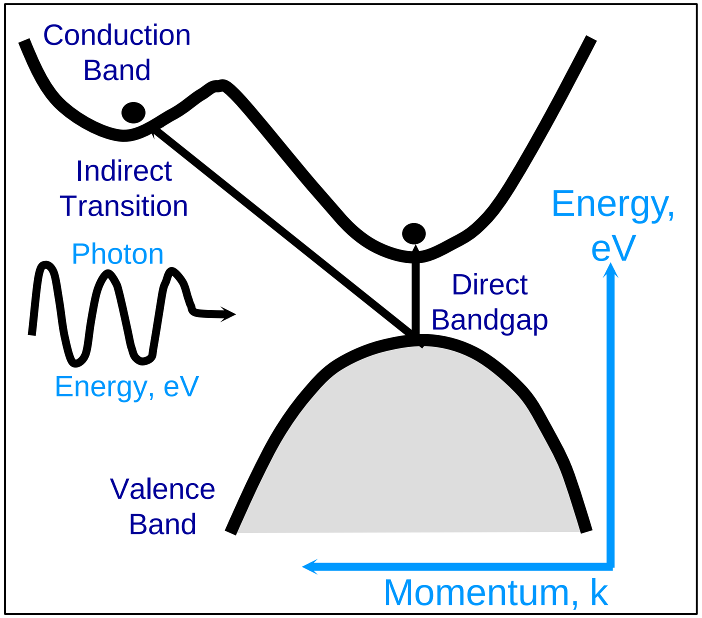
- Metals have more electrons than needed for bonding (covalent bonds = sharing electrons).
- Electric wave causes “free” electrons to move.
- When electrons collide with nearby atoms wave energy is lost as heat.

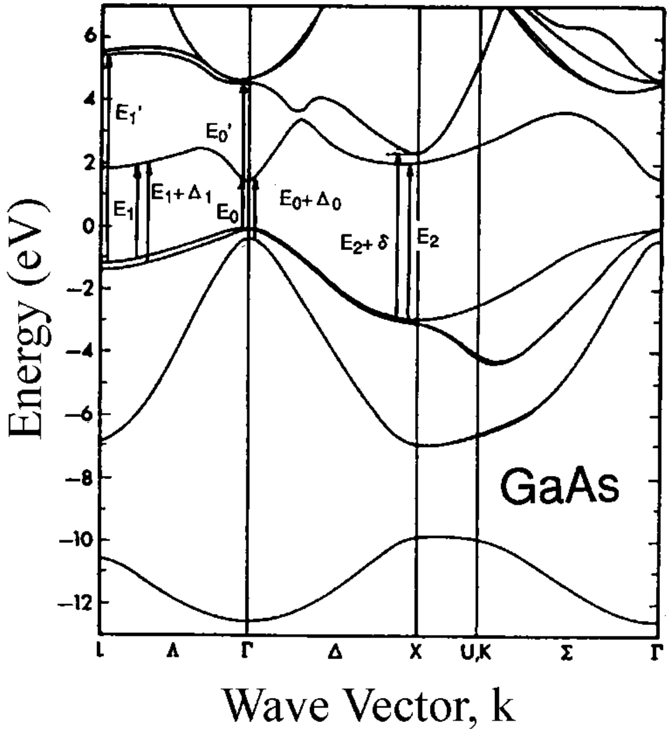




Semiconductors: Electronic Transitions

- Electrons in energy bands.
- Gap between valence-conduction band.
- If light (photon) provides enough energy electron may excite to higher state.



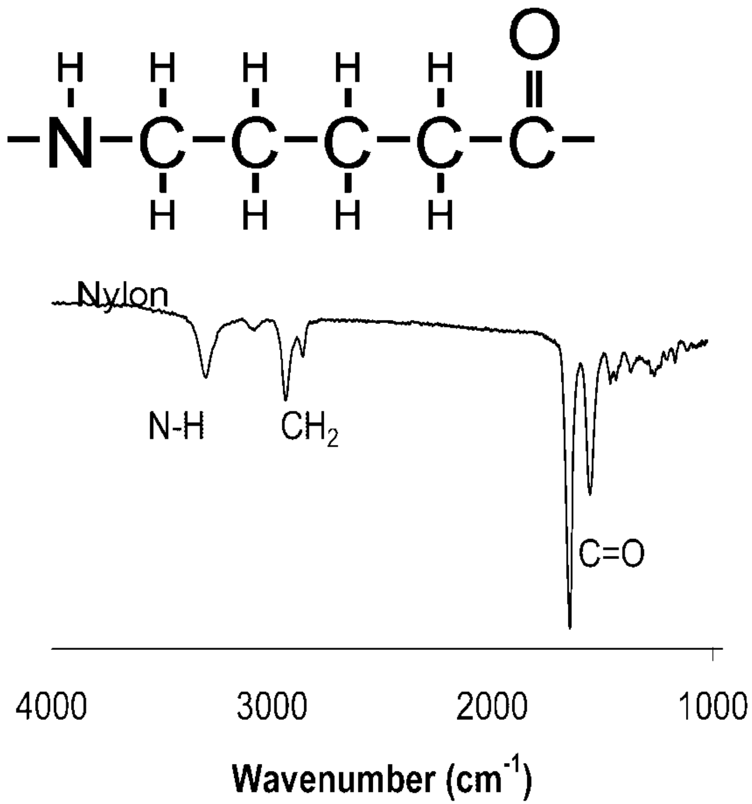


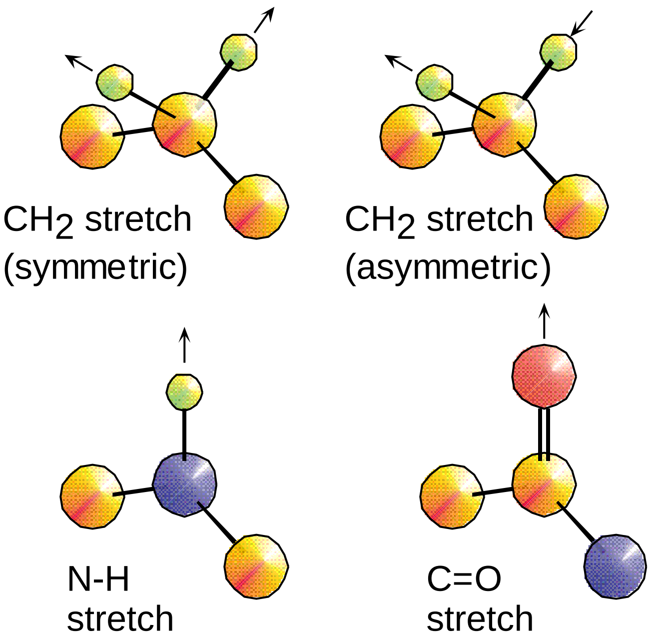
- Real materials have complicated energy bands.
- See lots of sharp structures in optical constants.

S. Adachi, *Optical properties of crystalline and amorphous semiconductors*, Kluwer Academic Publishers, Boston (1999).

Infrared Absorption: Molecular Vibrations

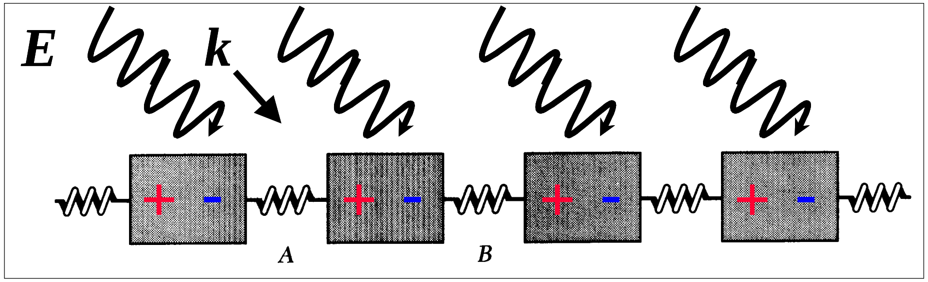
- Infrared light has low energy. Can vibrate molecules (stretching, bending, twisting, rotating).



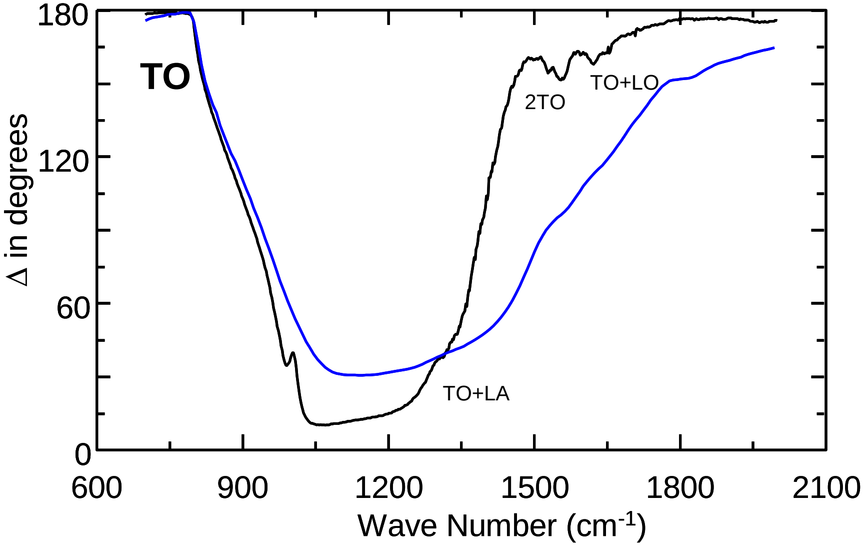


Infrared Absorption: Crystal Lattice Vibrations

- Electric Field causes crystal lattice to vibrate.
  - Longitudinal (LO) or Transverse (TO) Optical "Phonons".



M. Schubert, 2002



T.E. Tiwald et al., *Thin Solid Films*, 313-314 (1998) 661.

Optical Constants

- **Complex Refractive Index:**

$$\tilde{n}(\lambda) = n(\lambda) \pm ik(\lambda)$$

$$E(z,t) = E_0 \exp[i(wt - \mathbf{K}z + \delta)]$$
$$\boldsymbol{K} = \frac{2\pi}{\lambda}(n - ik)$$

Describes what material does to light wave.

- Slows down, wavelength changes, refraction, extinction.

Alternatively…

- **Complex Dielectric Function:**

$$\varepsilon(\lambda) = \varepsilon_1(\lambda) \pm i\varepsilon_2(\lambda)$$

$$\boldsymbol{D} = \varepsilon \boldsymbol{E}$$
$$\varepsilon = \varepsilon_0(1+\chi), \quad \varepsilon_r = \frac{\varepsilon}{\varepsilon_0}$$

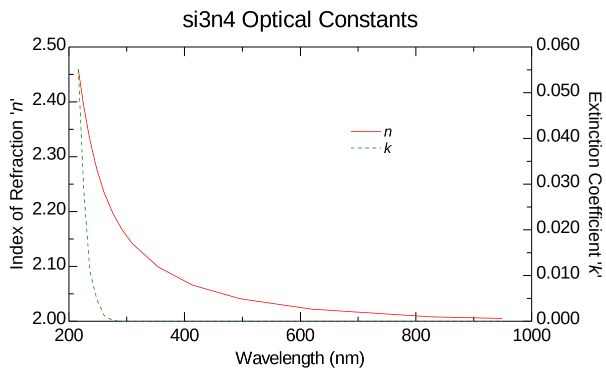
Describes what wave does to material.

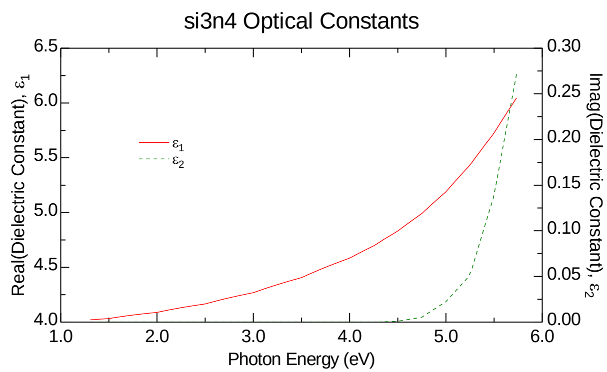
Graphing Optical Constants in WVASE.

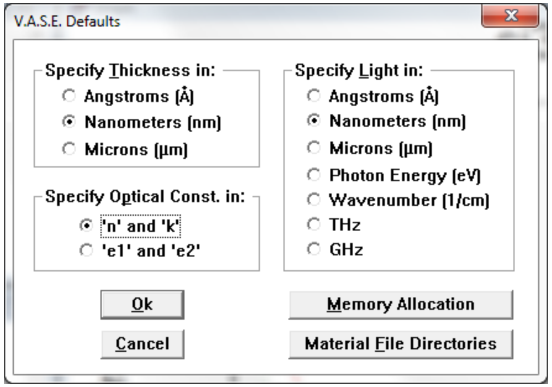
Using **Graph Window.**

- **Select** **Data: "Current Layer (Opt. Const.)"**
- Note position of current layer arrow ">" next to layer.

- Select **Global, then "Defaults"**
- Change plot to "e1 & e2" vs eV.





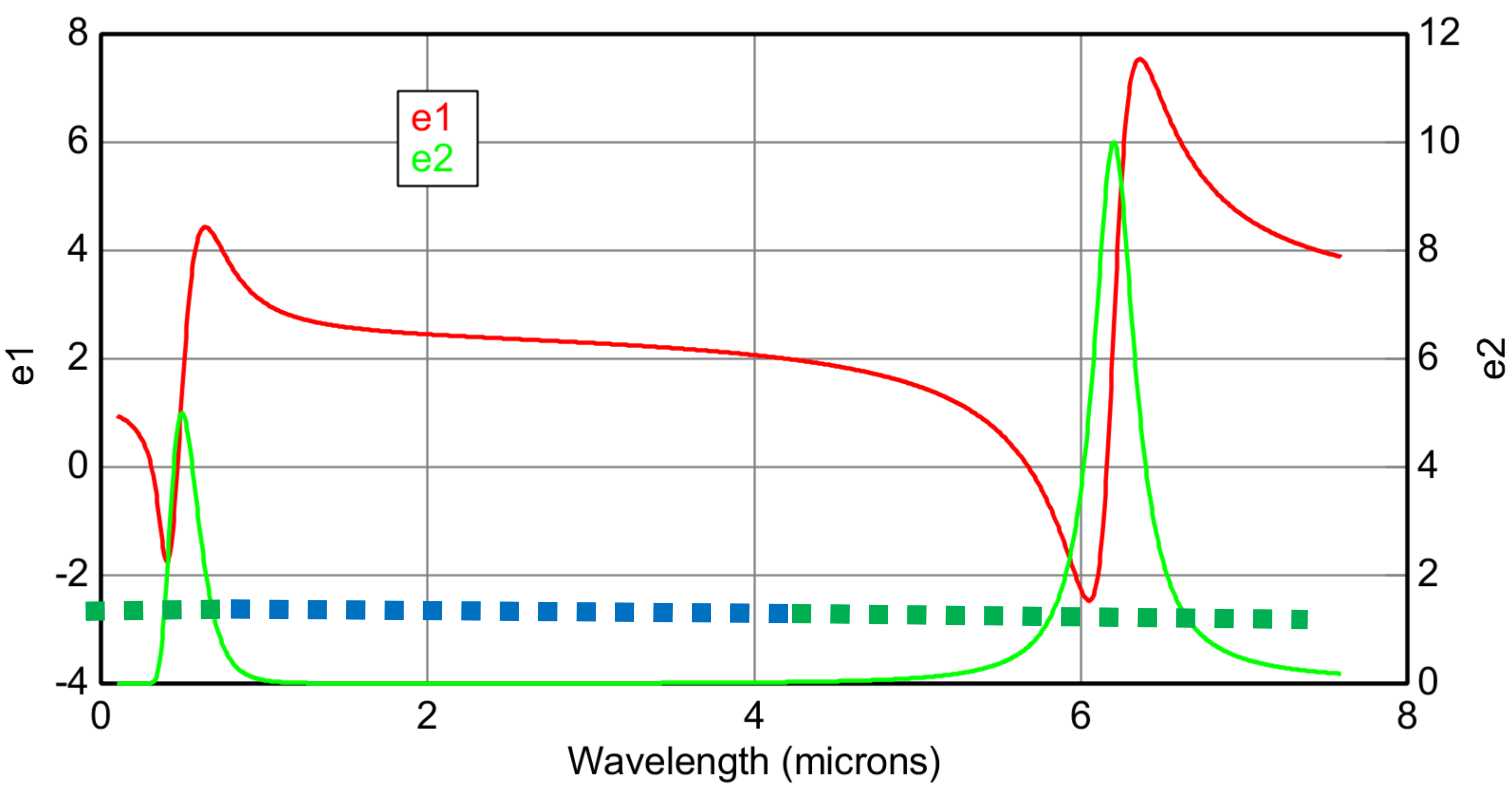


Learning Outcomes:

- Graphing layer optical constants in WVASE.
- Understand "Current layer".
- Changing defaults settings.

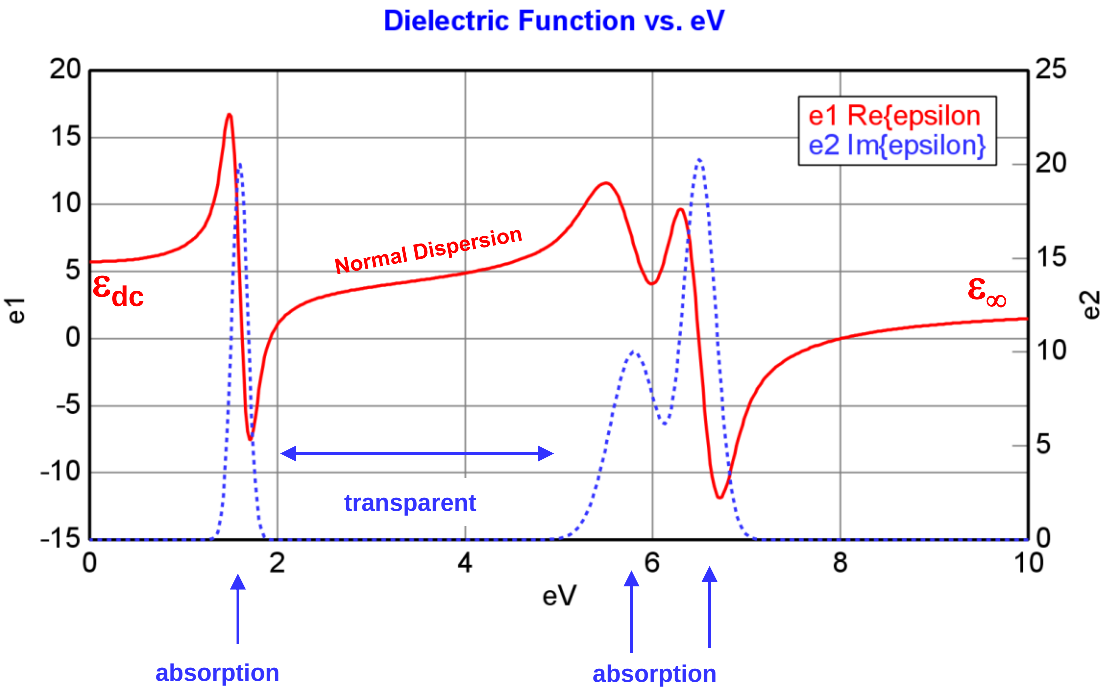
Dispersion: Wavelength Dependence

- Optical Properties vary with wavelength.
- Transparent regions (**normal** dispersion).
- Absorbing regions (**anomalous** dispersion).



The Dielectric Function ε(ω)

- The Dielectric Function ε(E) or ε(ω), is the Dielectric Polarization as a function of Energy (or Frequency).



- Regions of transparency, and regions of absorption.
- **Where do these features come from?**

Kramers-Kronig Relation

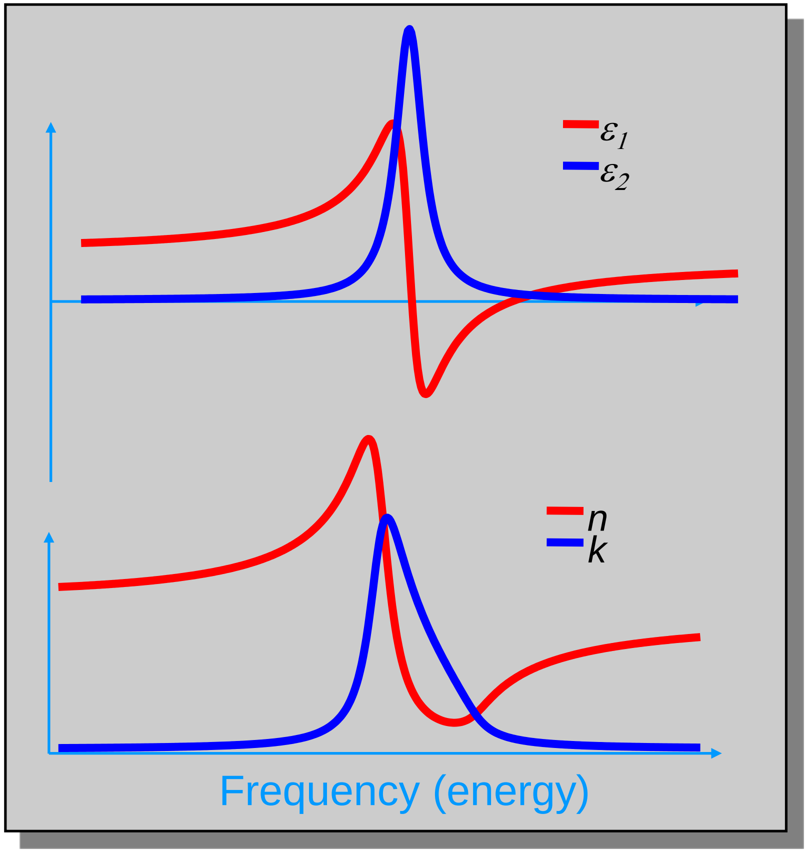
- Real and imaginary parts depend on each other.

- Optical constants **must** satisfy KK-relation to be physical.
- "Bumps make wiggles"…the shape of n & k curves are related.

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{\omega' \varepsilon_2(\omega')}{\omega'^2 - \omega^2} d\omega'$$

$$\varepsilon_2(\omega) = -\frac{2\omega}{\pi} P \int_0^\infty \frac{\varepsilon_1(\omega') - 1}{\omega'^2 - \omega^2} d\omega'$$

P means "principal part"



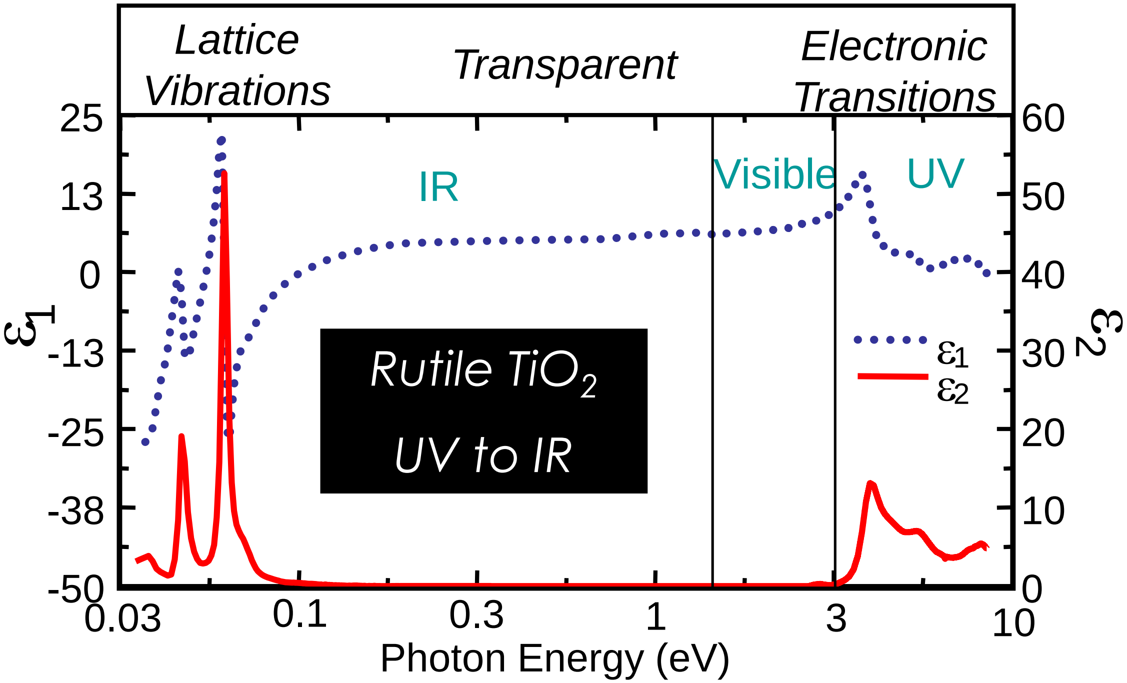
Integral equation relates area under ε_2 to shape of ε_1 and vice-versa.

Absorbing Regions

Absorbing regions occur in different parts of the spectrum.

Absorptions have different shapes, depending on cause.

- Free-carriers
- Electronic Transitions
- Molecular Vibrations
- Lattice Vibrations



Dispersion Models: Practical Use.

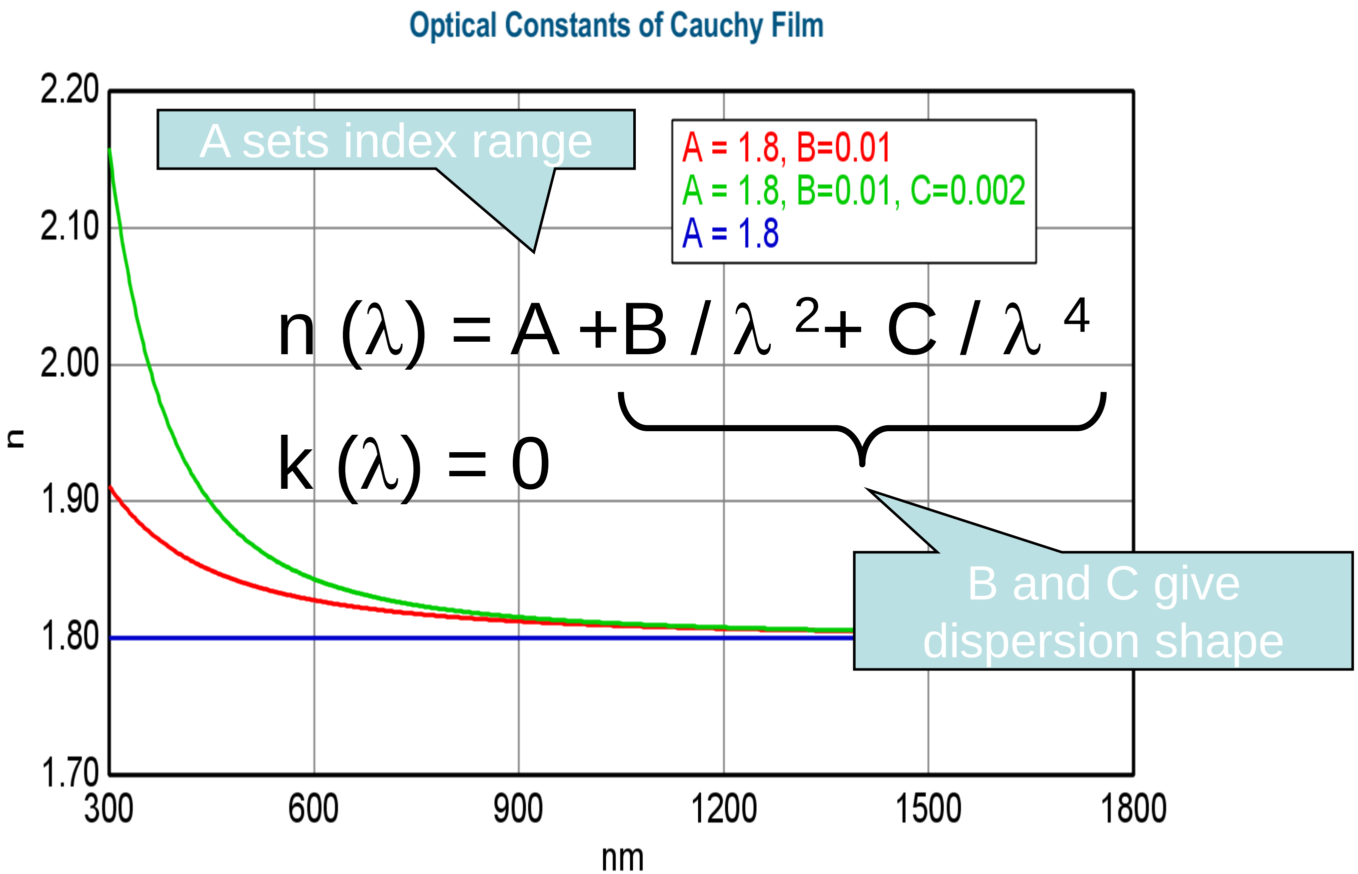
- Equations used to describe the optical functions versus wavelength.

- Transparent Materials:
  - Cauchy, Sellmeier models.

- Absorbing Materials:
  - Large variety of Oscillator Models:
  - Lorentz, Drude, Gaussian, Tauc-Lorentz, etc.
  - All available within Genosc.mat layer!

Transparent Materials: Cauchy Dispersion Equation

- Describes index (n) as a function of wavelength n(λ).
- For transparent materials only (k=0 or very small).



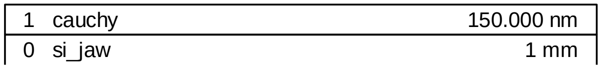
Augustin-Louis Cauchy (1789-1857)

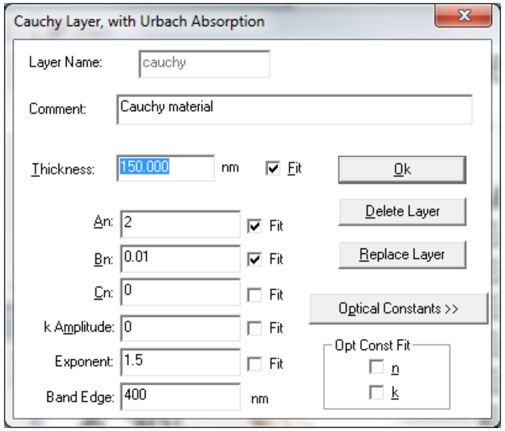
7_SiNx on Si.dat

Using Model For Silicon Nitride on Silicon

Select Model Window.

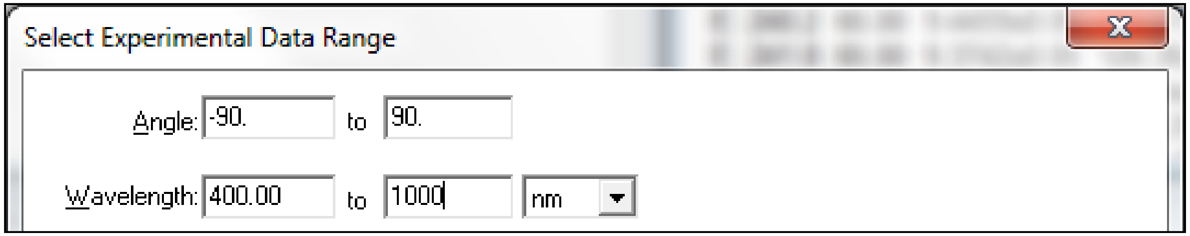
- Replace Si3N4 layer with Cauchy.mat
- Set An=2, Bn=0.01.





Select Experimental Data Window.

- Range Select 400-1000 nm.



- Generate data.

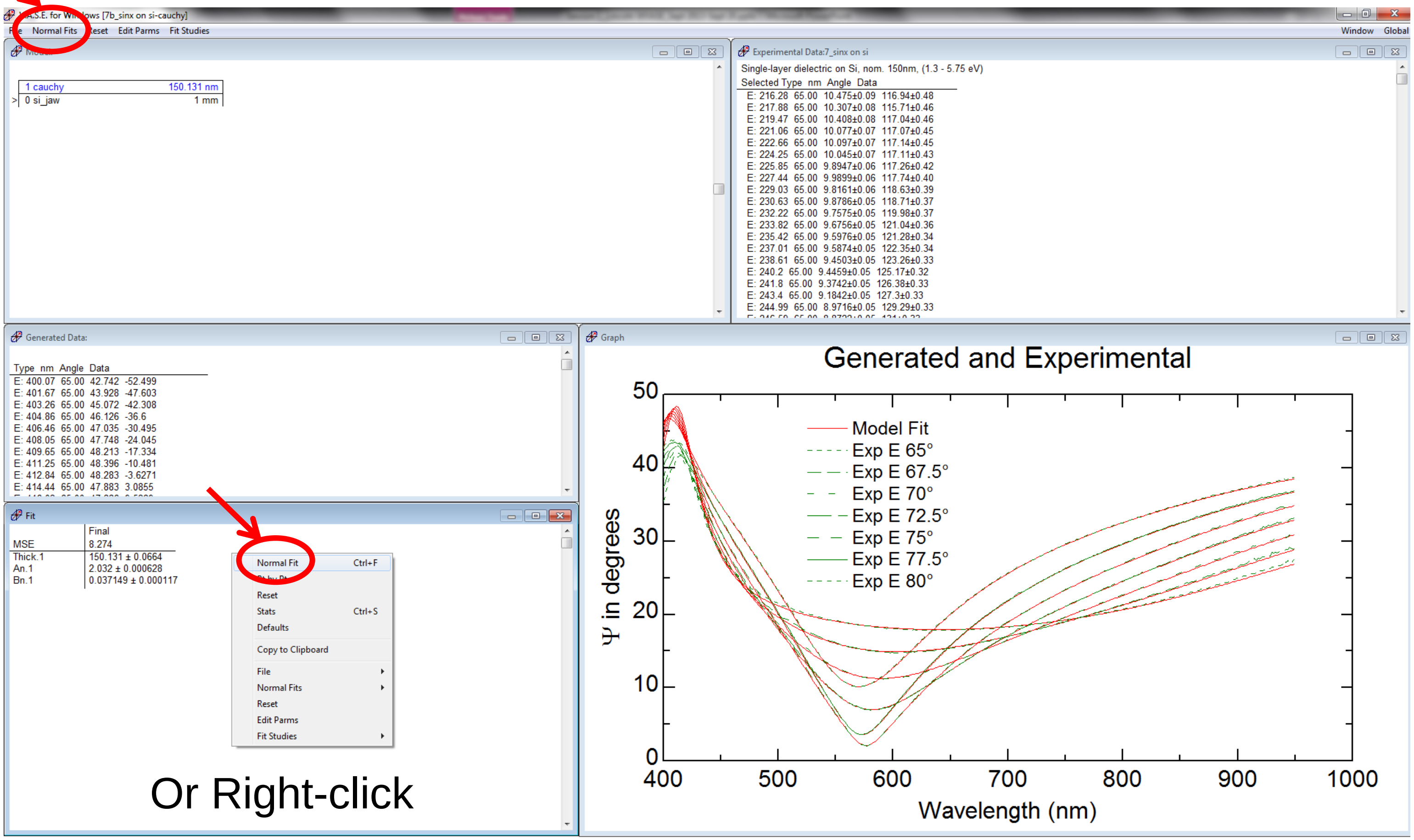
Learning Outcomes:

- Replacing layers.
- Define Fit parameters. Cauchy model for index.
- Select Experimental data range.

WVASE Fit Window

Used to optimize model by adjusting fit parameters

"Normal" fit



Perform a "Normal Fit" to start.
What's going on below 450 nm? Beyond 850 nm?
How to improve this fit?

Dispersion Models: Practical Use.

- Equations used to describe the optical functions versus wavelength.

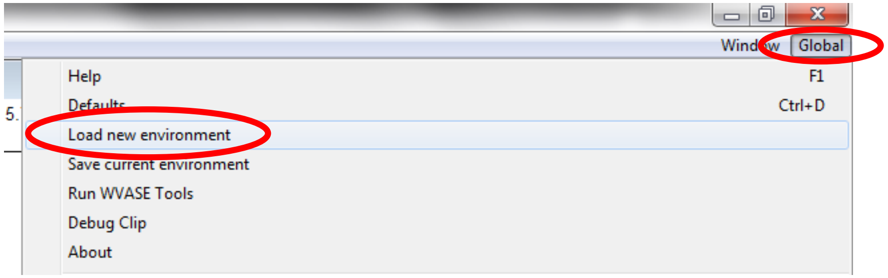
- Transparent Materials:
  - Cauchy, Sellmeier

- Absorbing Materials:
  - Large variety of Oscillator Models:
  - Lorentz, Drude, Gaussian, Tauc-Lorentz, etc.
  - All available within Genosc.mat layer!

7d_SiNx on Si-genosc.env

Silicon Nitride on Silicon
Final Model Using Genosc.mat

- Select **Global, then "Load New Environment".**



- **Open 7d_Sinx on Si-genosc.env**
- Examine Ψ and Δ data fits. Are the fits good?
- Click Genosc layer to open Window.
- Study oscillators and poles used for fit.

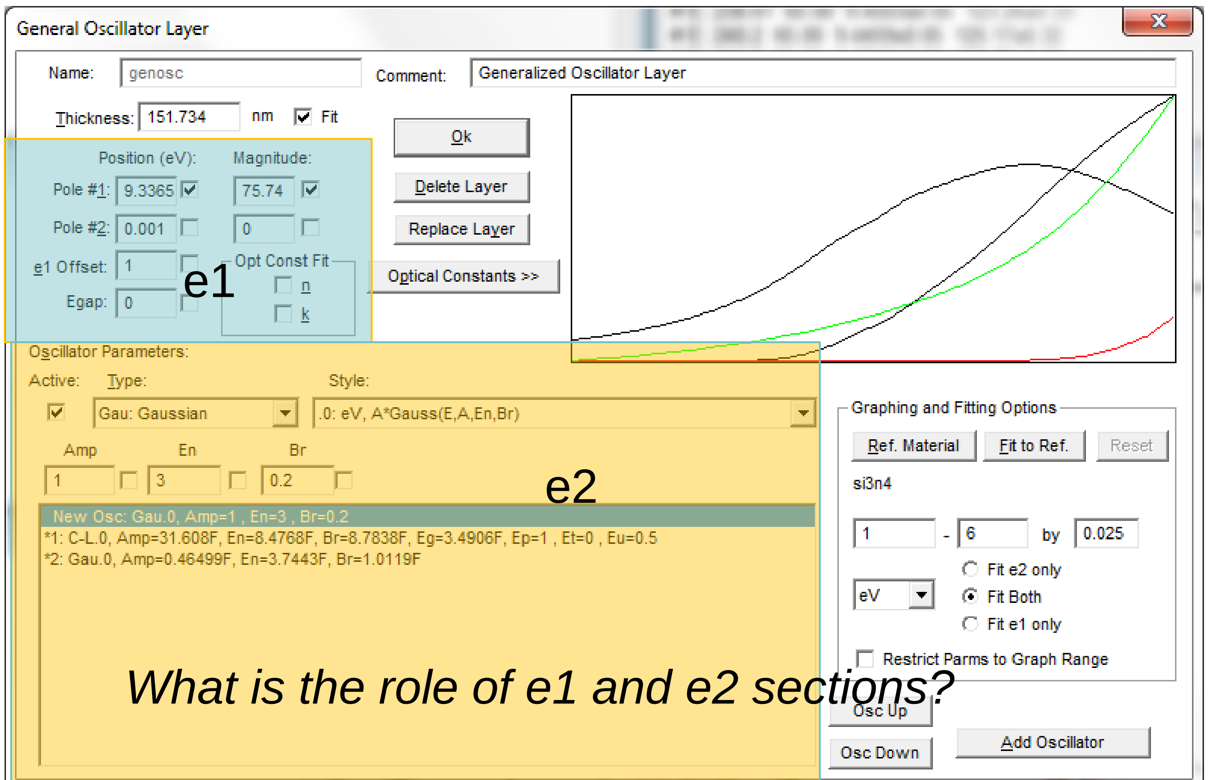
Learning Outcomes:

- Opening Environment Files.
- Study Genosc fit.

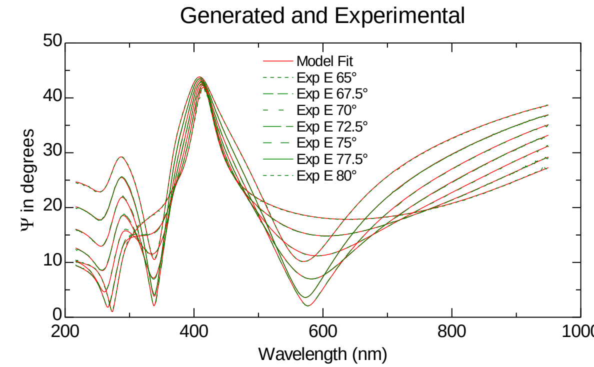
Silicon Nitride on Silicon

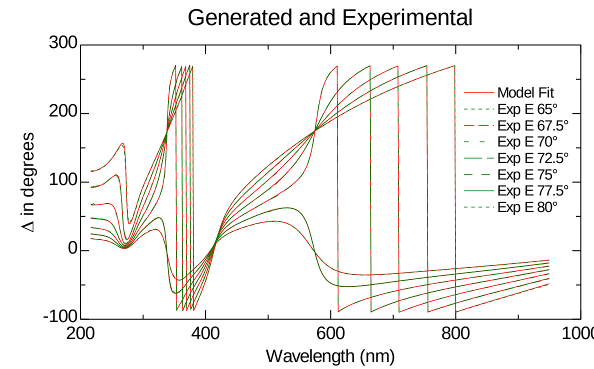
Final Results

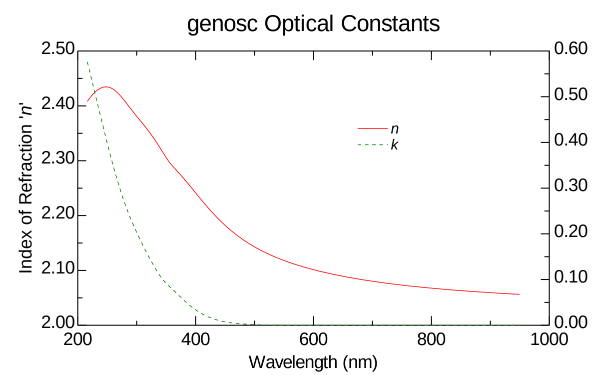
2	srough	1.877 nm
1	genosc	151.734 nm
0	si_jaw	1 mm



What is the role of e1 and e2 sections?





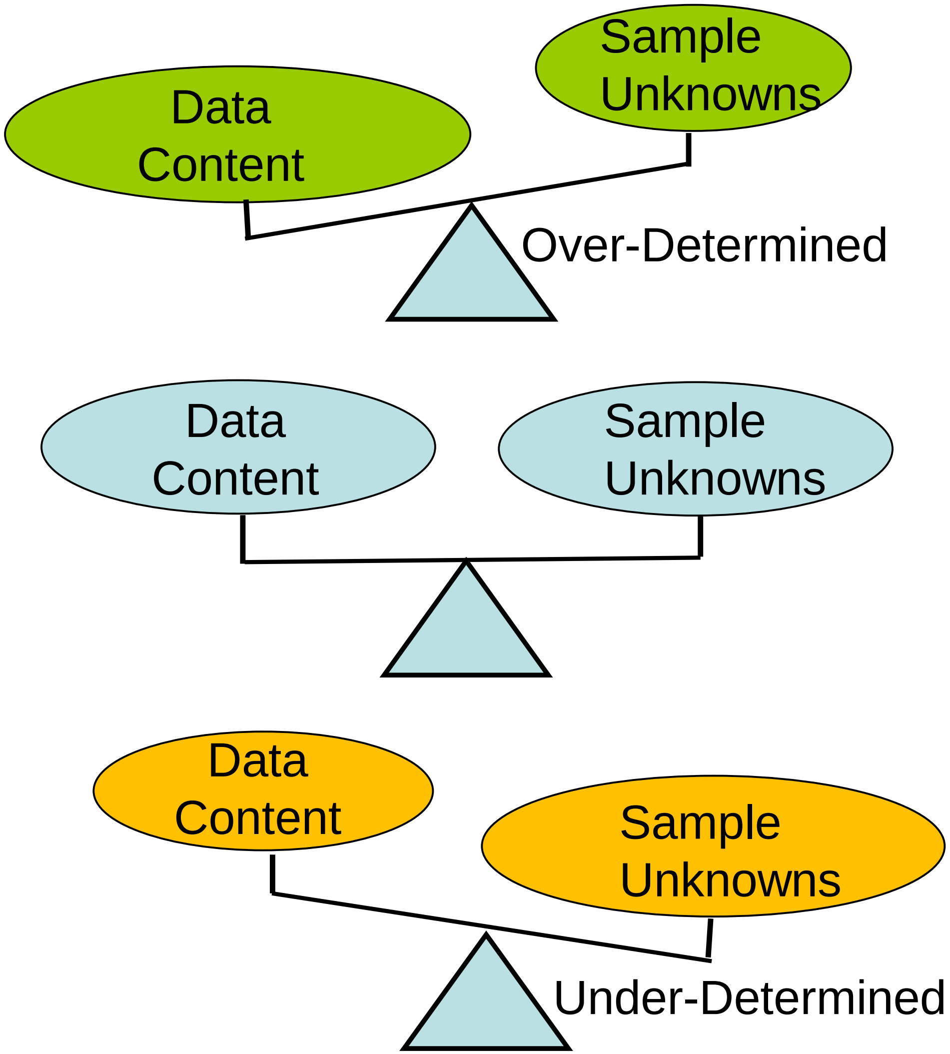


Ellipsometry Data Analysis

- Rest of this course…3 days.
- How to analyze data.
- Introduce some general concepts.

Data Content vs Sample Unknowns

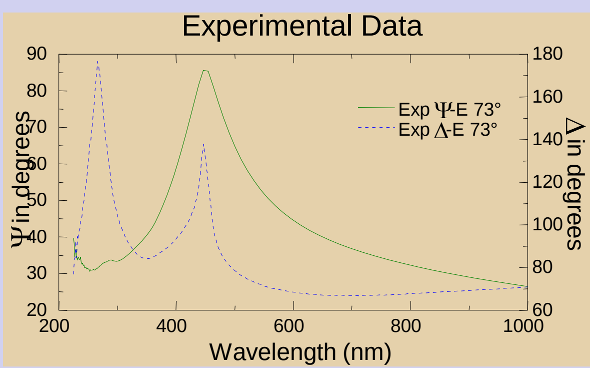
- **Ensure data contains information to solve all unknowns.**

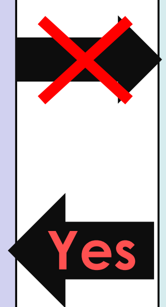


Why Analyze Data?

- Ellipsometry measures two parameters: **Ψ and Δ**.
- Ψ and Δ are a function of film thicknesses and optical constants of materials under study.
- Desired **information must be extracted through a model based analysis** using optical physics.
- Inverse Problem:
  - **Result** is known instead of **Cause**.
  - Ellipsometry measures the "resulting" polarization change rather than sample properties that are the "cause".

Ellipsometry Measurement



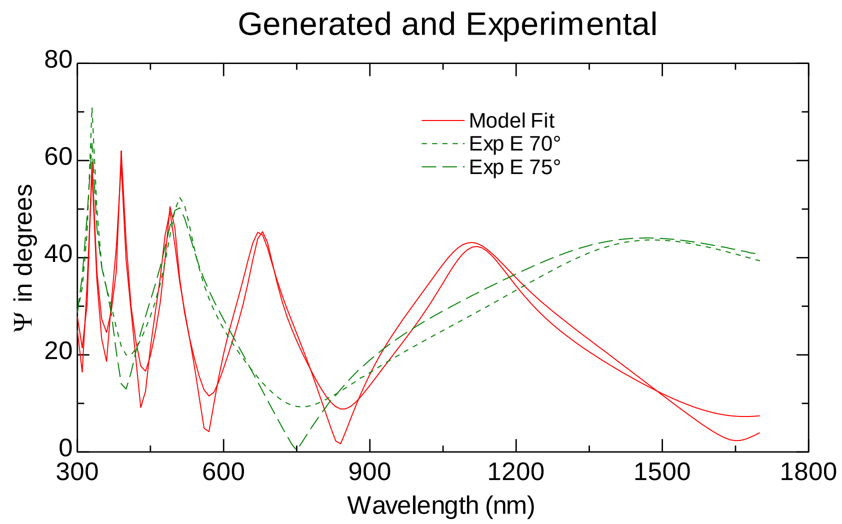


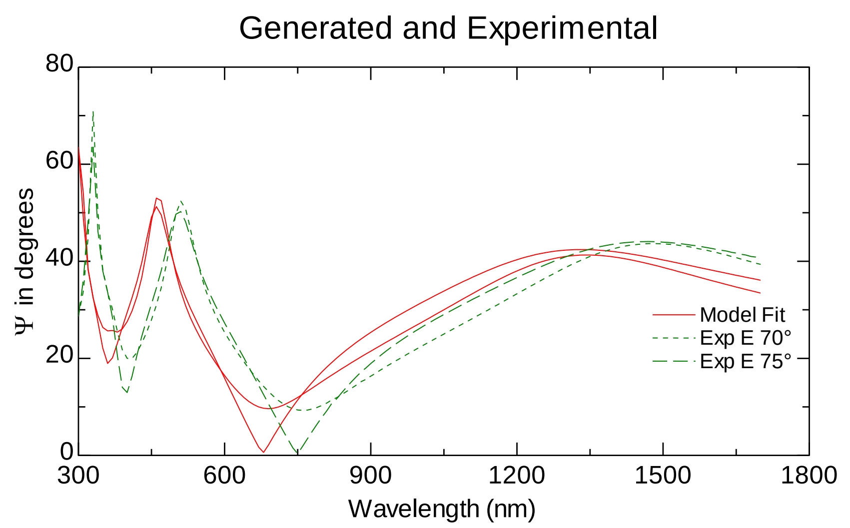
Sample Structure

2	srough	20.00 Å
1	film	1500.00 Å
0	silicon	1 mm

Generate Data From Model

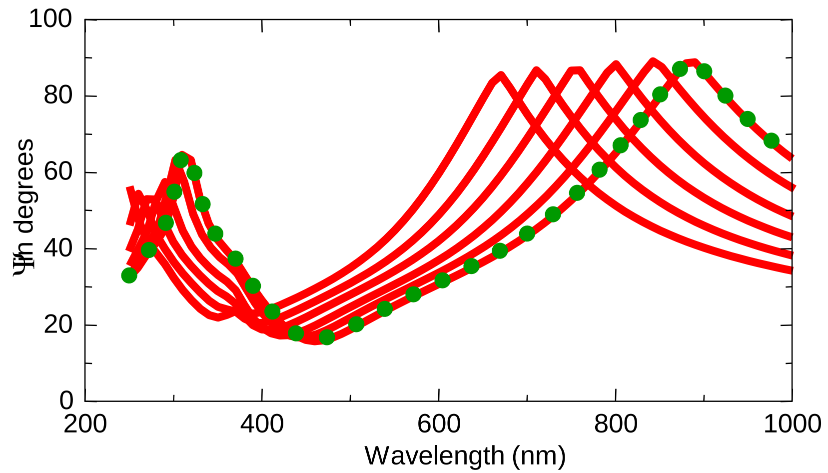
- Calculate psi & delta from model.
- Compare to Experimental data.
- Adjust unknown (fit) parameters to get close to solution.

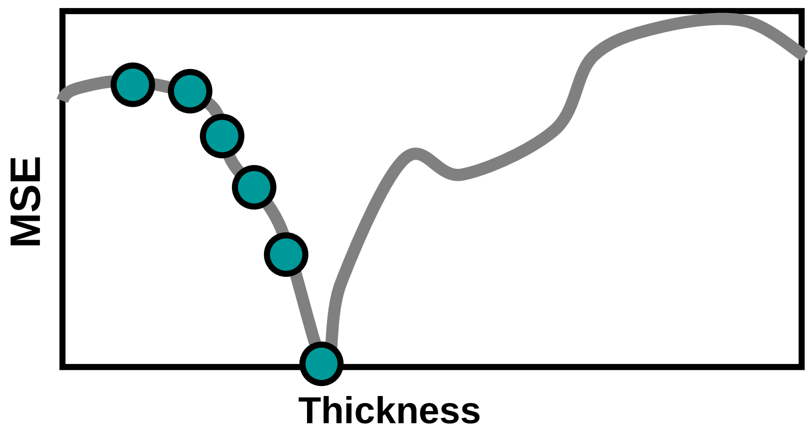




Data Fitting

- Software adjusts "fit" parameters to find best match between model and experiment.
- MSE is Difference.





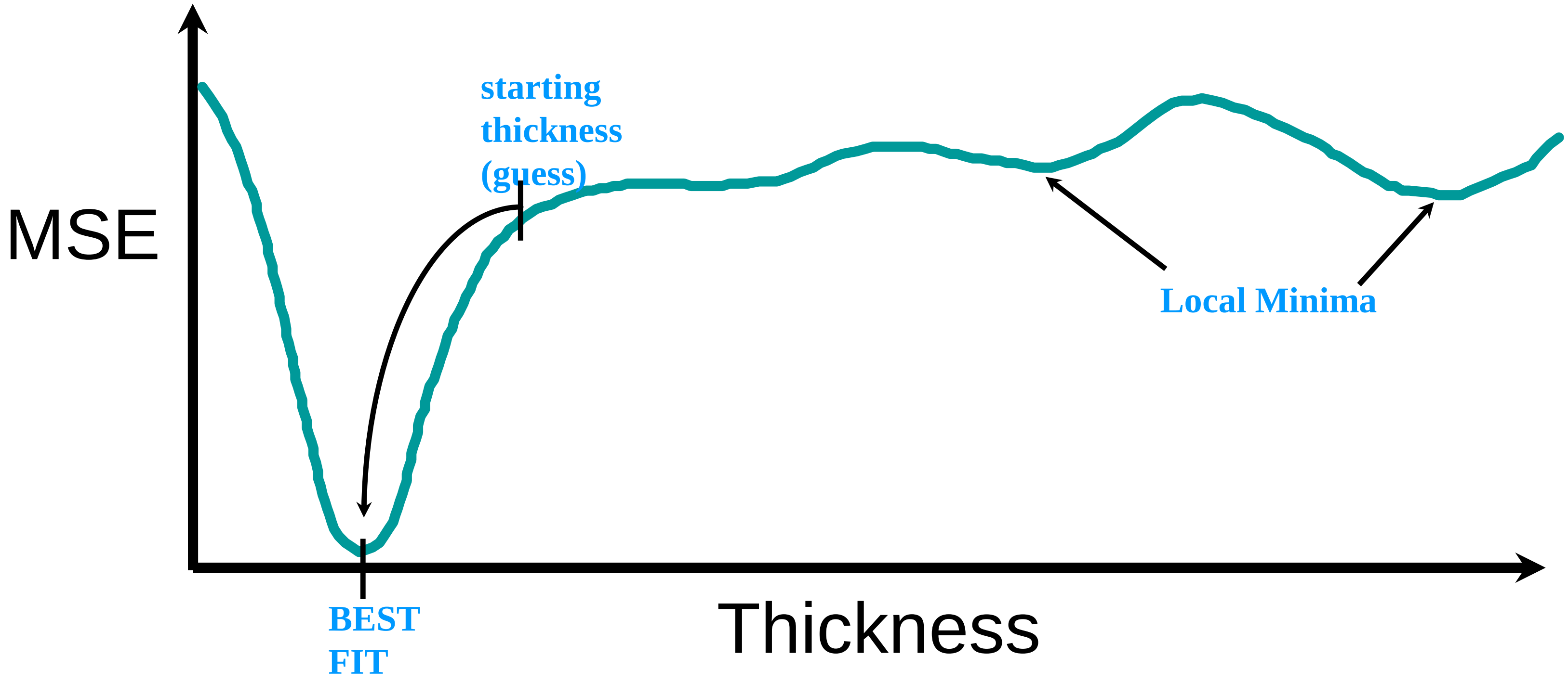
Data Fitting Algorithm

$$MSE = \frac{1}{2N-M}\sum_{i=1}^{N}\left[\left(\frac{\Psi_i^{\mathrm{mod}}-\Psi_i^{\mathrm{exp}}}{\sigma_{\Psi,i}^{\mathrm{exp}}}\right)^2+\left(\frac{\Delta_i^{\mathrm{mod}}-\Delta_i^{\mathrm{exp}}}{\sigma_{\Delta,i}^{\mathrm{exp}}}\right)^2\right]=\frac{1}{2N-M}\chi^2$$

- WVASE32 uses a Mean Squared Error (MSE) to quantify the difference between experimental and calculated model data.
- A smaller MSE implies a better fit.
- The MSE is weighted by the error bars on each measured data point, so noisy points are weighted less heavily.

Minimizing the MSE

- Levenberg-Marquardt algorithm used to quickly determine the minimum MSE (gives best fit to data).



Quality of Data Fit

Use our Physical Intuition!

When fit is complete resulting fit parameters must be evaluated for sensitivity and possible correlation.

- Compare experimental data with generated data.
- How low is MSE? Can it be reduced further by increasing model complexity?
- Are fit parameters physical?
- How large are 90% confidence limits?
- Check Correlation matrix. Are parameters correlated? Can some be turned off?

Correlation Matrix

- Example of Correlation Matrix
  - matrix of two-parameter correlation coefficients calculated from the covariance matrix

Any off diagonal elements near +/-1 are correlated.

Correlation Matrix

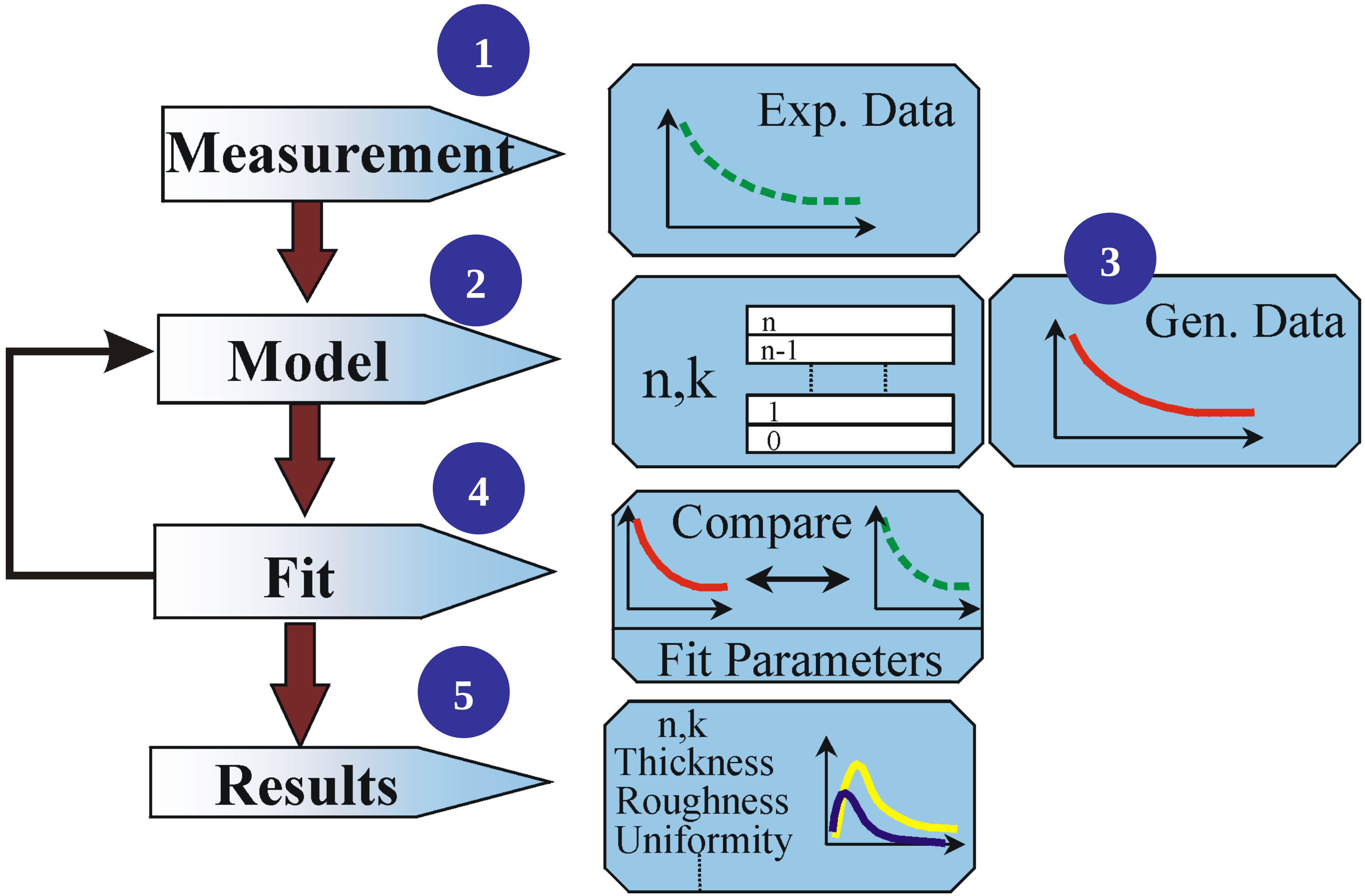
	ThkUni	Thick.2	An.2	Bn.2	Cn.2
ThkUni	1.000	0.065	-0.091	0.028	-0.022
Thick.2	0.065	1.000	-0.680	-0.117	0.054
An.2	-0.091	-0.680	1.000	-0.530	0.515
Bn.2	0.028	-0.117	-0.530	1.000	-0.965
Cn.2	-0.022	0.054	0.515	-0.965	1.000

Correlated Parameters: Cn.2 and Bn.2

General Rules for Data Analysis

- Find the **simplest optical model** that fits Experimental Data.
  - User fewest fit parameters.
- **Verify uniqueness** of the model.
  - Check correlation matrix, and error bars on parameters.
- Optical 'constants' for materials are not always constant, and **quality of fit can only be as good as the optical constants** assumed in the model.
  - May need to fit n & k.

Data Analysis Flowchart



Summary – Session #1

- **Introduction to Spectroscopic Ellipsometry**
  – Polarized light, Ellipsometry experiment.
- **Classification of Samples:**
  – Substrate, or coated,? Single-Layer, Multi-Layer?
  – Absorbing, Transparent, Semi-Absorbing?
  – Data Features: Spectral Interpretation.
- **Optical constants.**
  – Refraction, absorption, n & k. Dispersion.
  – Oscillator models, Cauchy, Lorentz, Gaussian, etc.
  – WVASE Genosc layer.
- **Fundamentals of WVASE.**
  – Basic software operation.

Lunch!