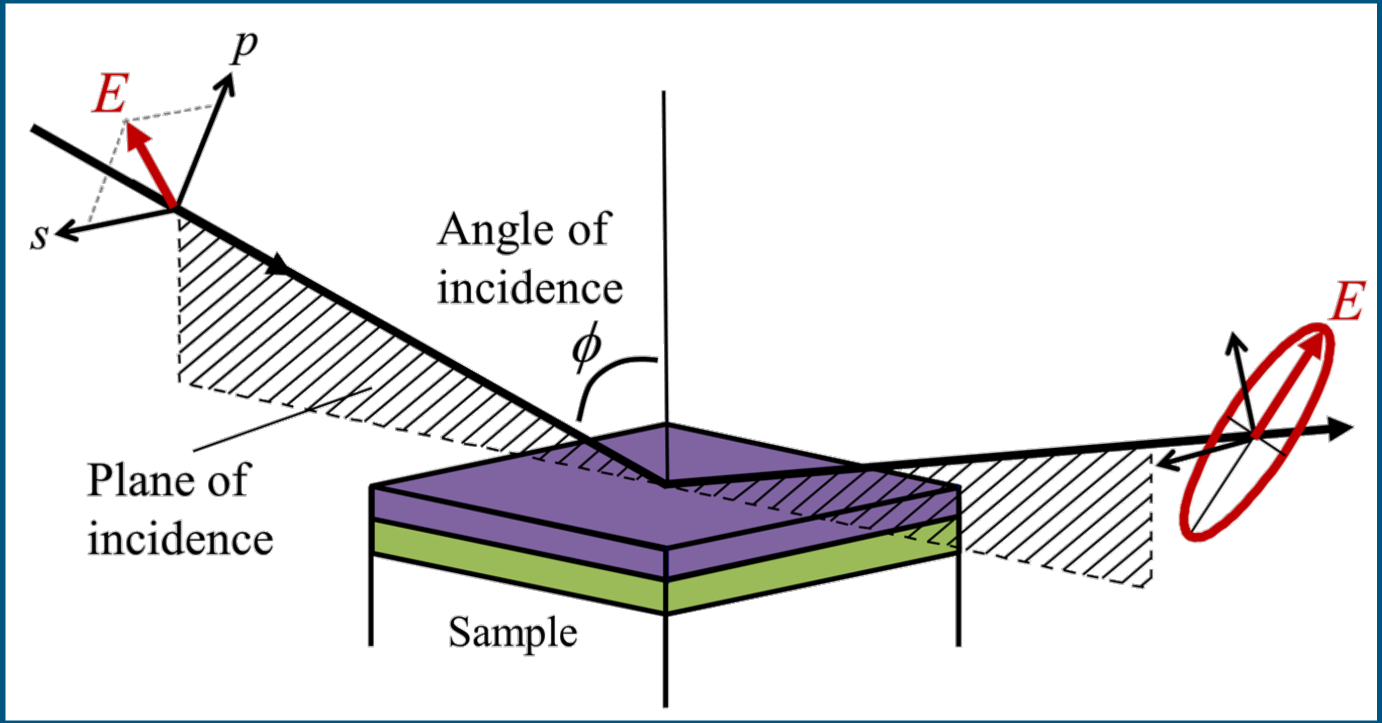
J.A. Woollam
Ellipsometry Solutions

Theory and Basic Substrates

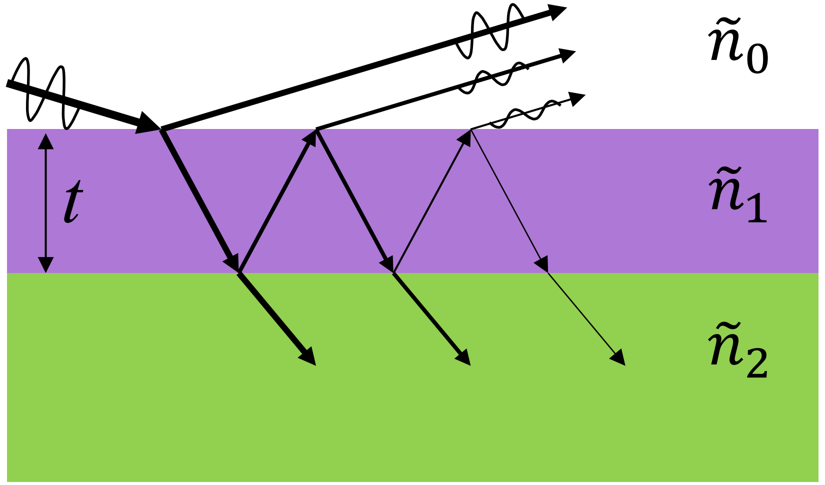


James N. Hilfiker

March 2025

Course Outline

- **Session 1: Theory & Substrates (Semiconductors and Glass)**
- Session 2: Transparent Films
- Session 3: Absorbing & Semi-Absorbing Films (B-Spline)
- Session 4: Semi-Absorbing Films (Gen-Osc)
- Session 5: Thin Absorbing Films and Multilayers
- Session 6: Advanced Topics

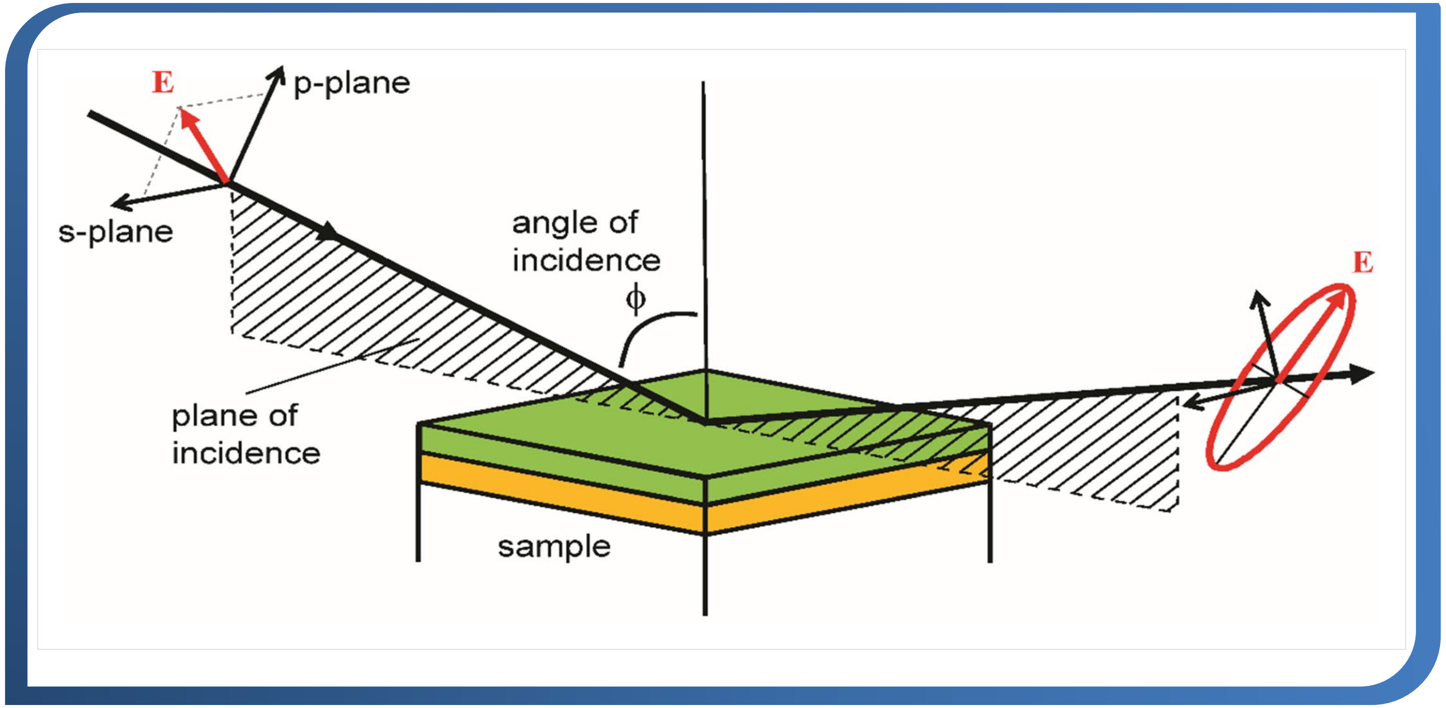


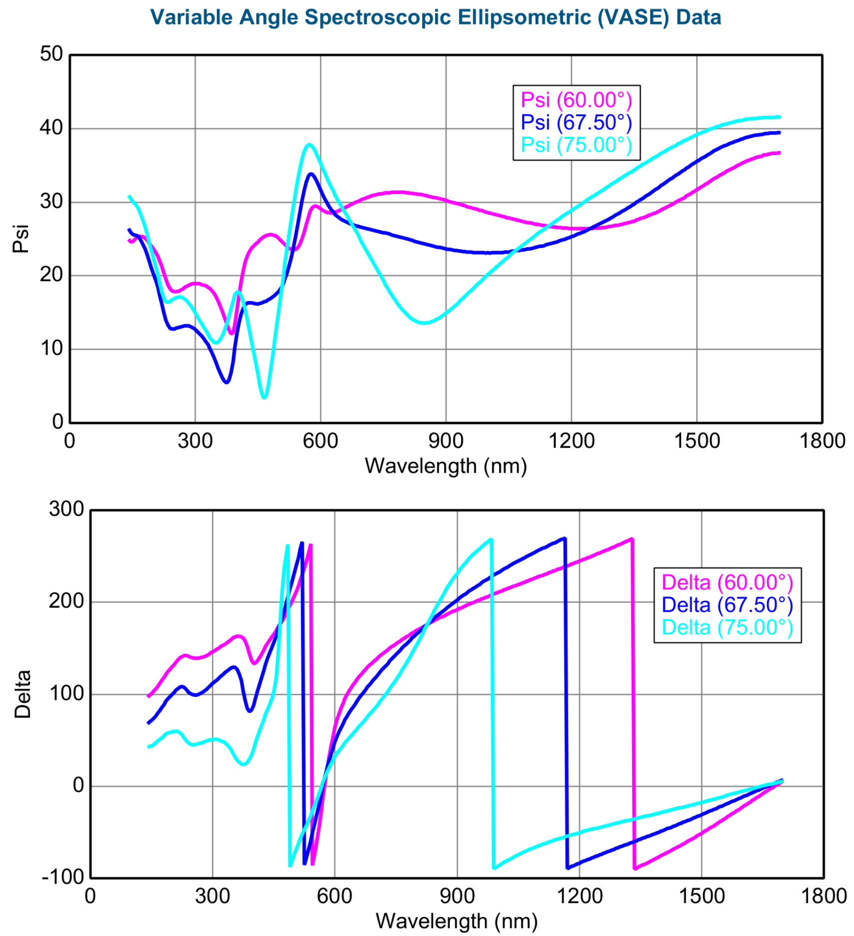
Session 1 Outline

- Theory and Fundamentals of Ellipsometry
- Modeling Overview
- Semiconductor Substrates
- Transparent Glass Substrates

What is Ellipsometry?

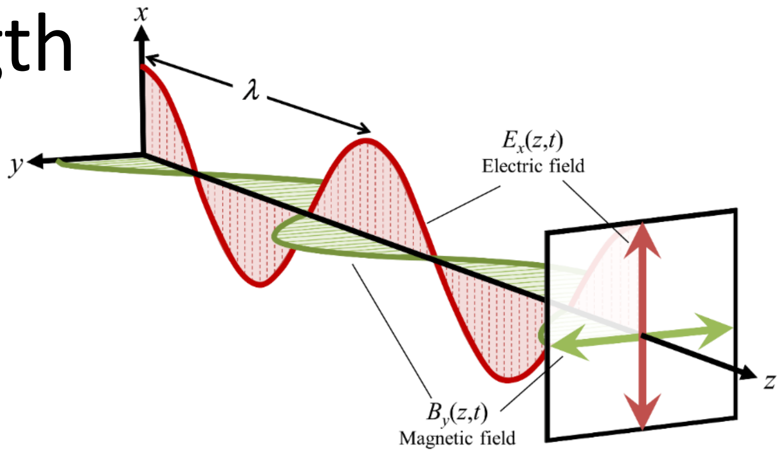
- Ellipsometry measures the change in polarization of light that reflects from or transmits through a sample.

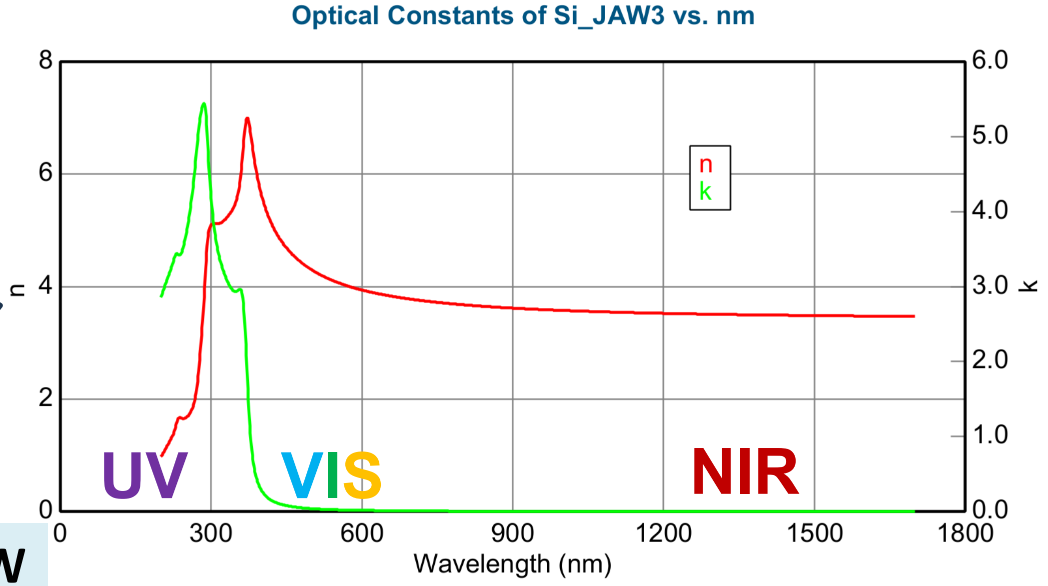




Light

- Wavelength





- Photon Energy

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

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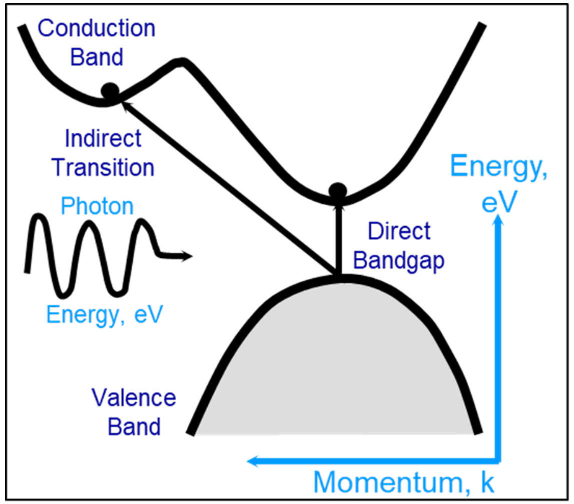
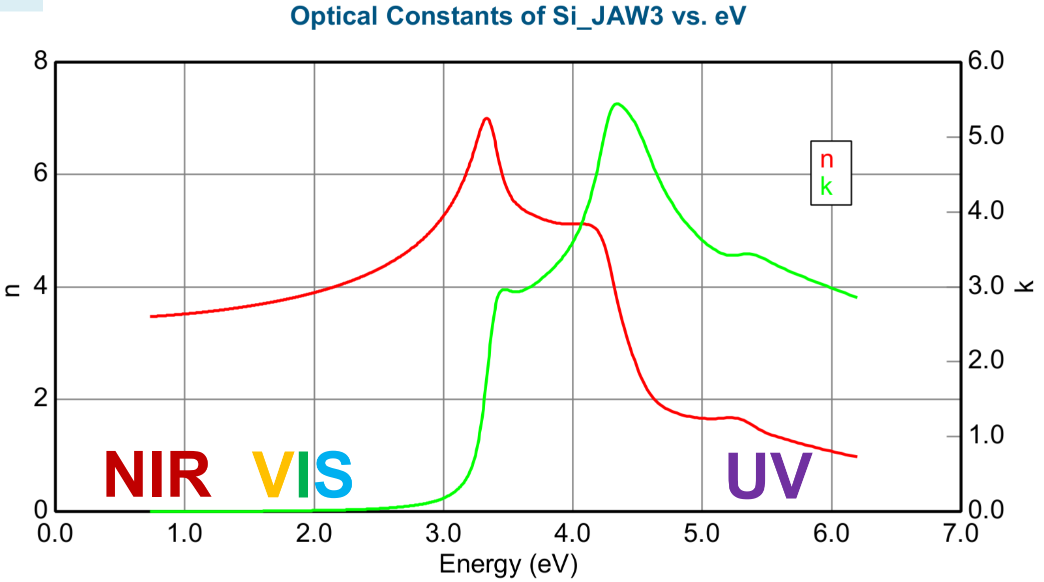
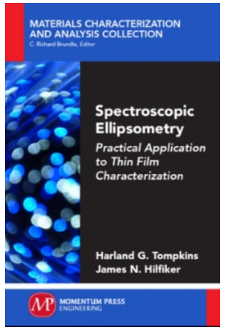


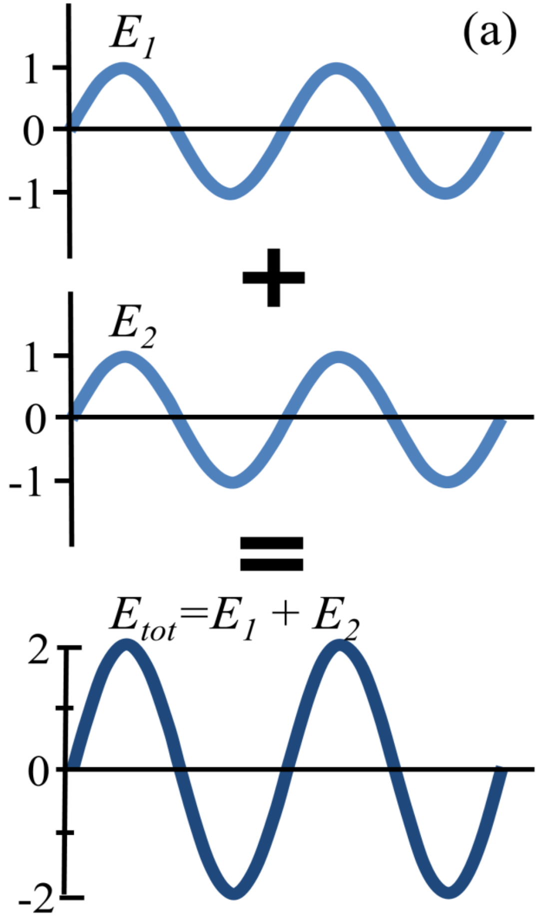




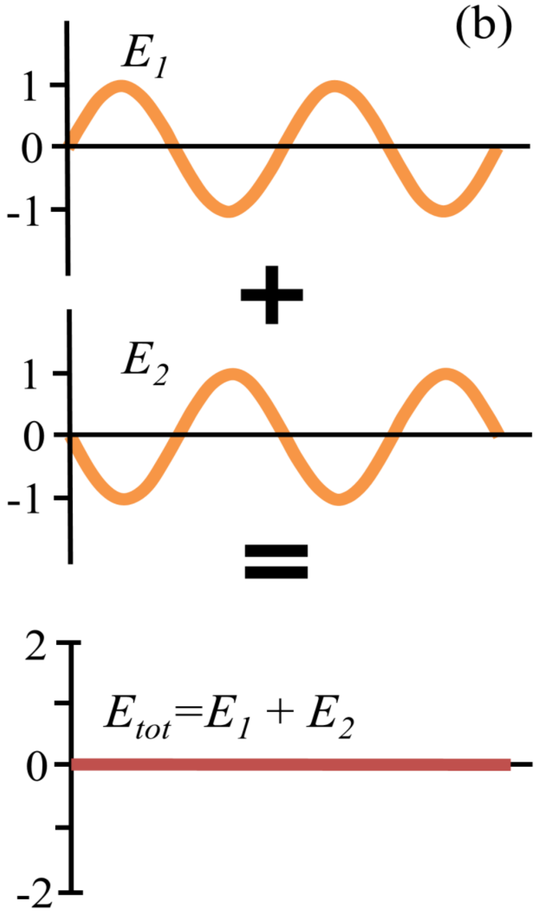
Combining Waves

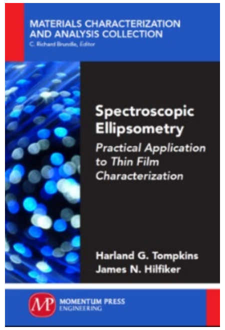
- "Coherent" waves with <u>same frequency</u> and <u>traveling/vibrating</u> in the <u>same direction</u> combine into a single wave.

Constructive Interference



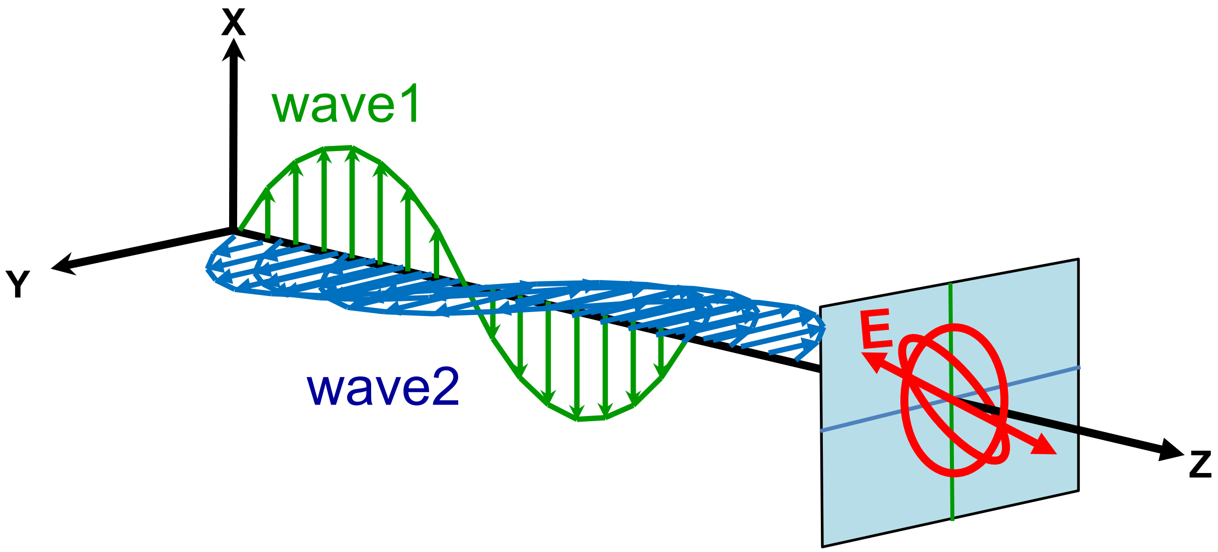
Destructive Interference





What is Polarization?

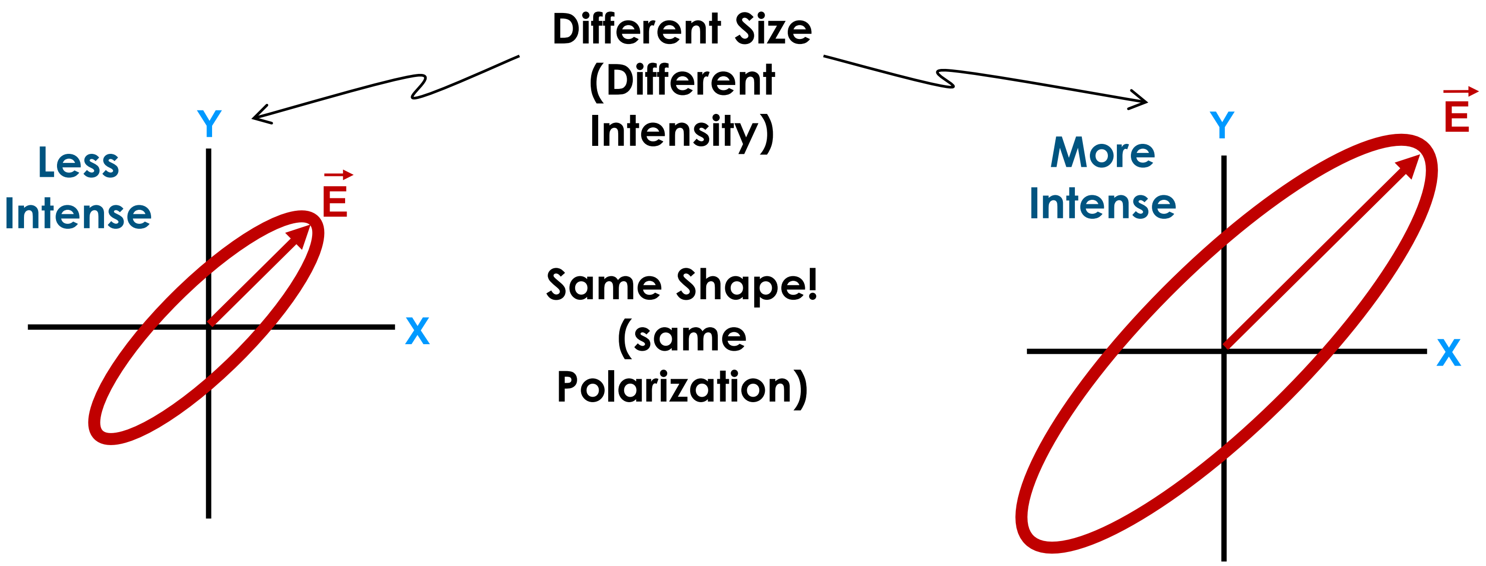
- Describes <u>shape</u> of Electric Field oscillations.



- <u>Linear</u>: arbitrary amplitudes, in-phase
- <u>Circular</u>: equal amplitudes, 90° phase difference
- <u>Elliptical</u>: arbitrary amplitudes, arbitrary phases

Characteristics of Light

- Energy = Color (frequency of E-field oscillation)
- Intensity = time-averaged "Size" of E-field $I \propto E^2$
- Polarization = "Shape" of Electric field.



Describing Polarization: Jones Vector

- Polarization described by 2 amplitudes and 2 phases
- Can be written as <u>Jones Vector</u>:

$$\begin{bmatrix} E_x \\ E_y \end{bmatrix} = \begin{bmatrix} E_{x0} e^{i\delta_x} \\ E_{y0} e^{i\delta_y} \end{bmatrix}$$

$$\vec{E}(z,t) = \vec{E}_x + \vec{E}_y = \hat{x} E_{x0} e^{i\delta_x} + \hat{y} E_{y0} e^{i\delta_y}$$

Jones Vector has 4 degrees of freedom to define polarization:
2 amplitudes and 2 phases

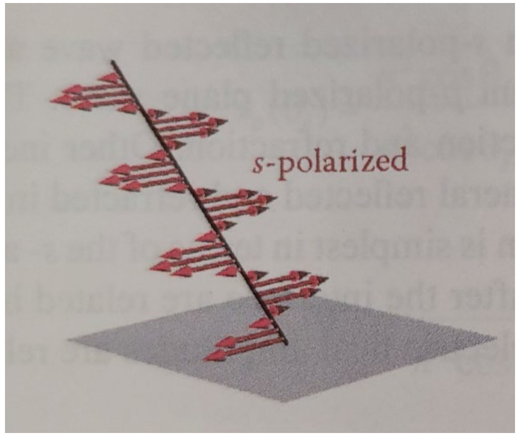
Ellipsometry reduces the 4 degrees of freedom for Jones Vector to 2: amplitude ratio and relative phase

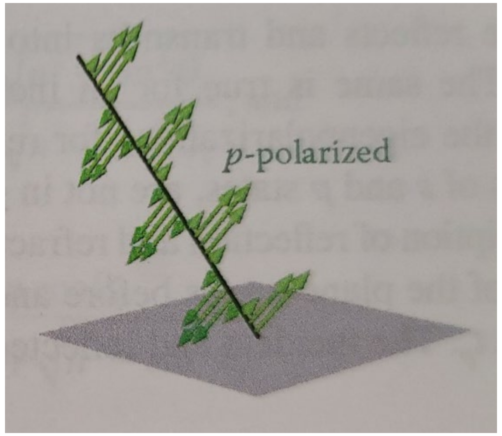
$$\frac{\widetilde{E}_x}{\widetilde{E}_y} = \frac{|E_{0x}|}{|E_{0y}|} e^{i(\delta_x - \delta_y)} = \tan\psi_{xy} e^{i\delta_{xy}}$$

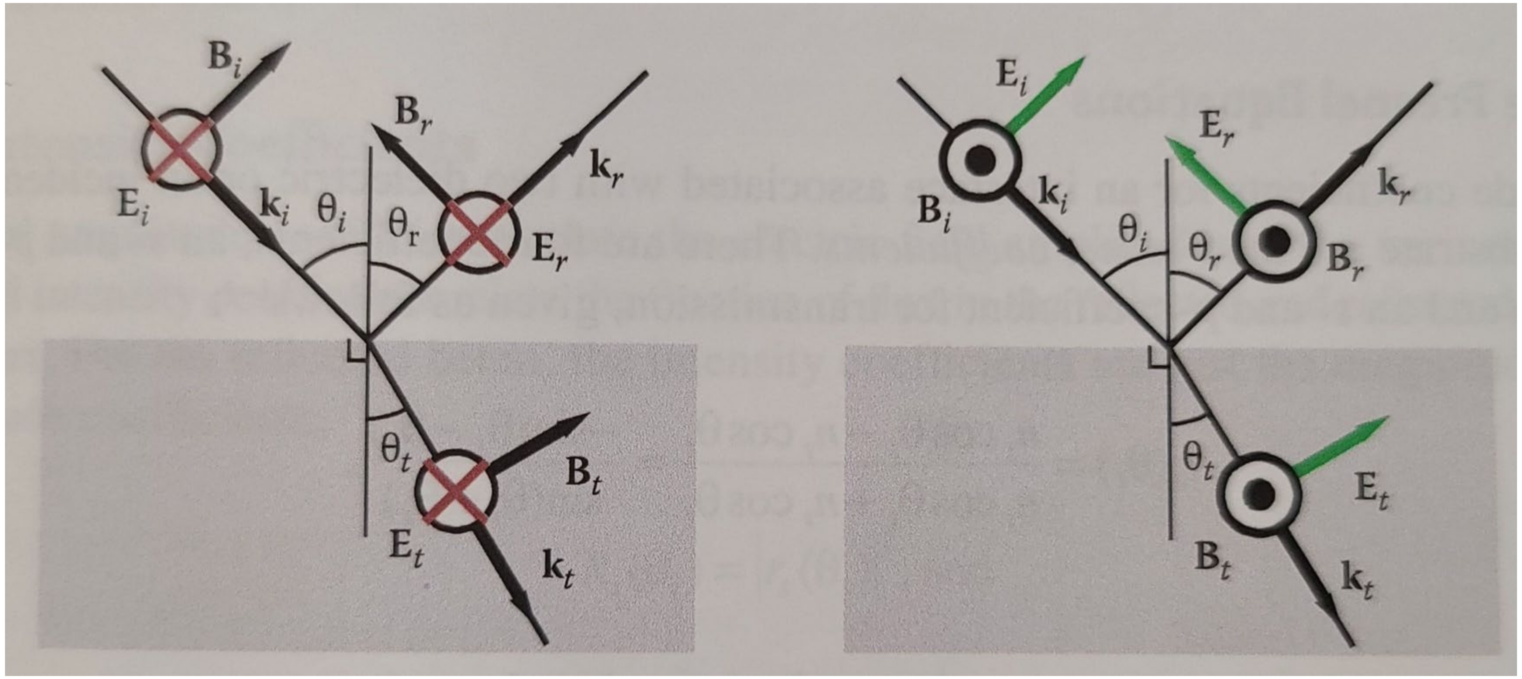
$$e^{im} e^{in} = e^{i(m+n)}$$
$$e^{im} / e^{in} = e^{i(m-n)}$$

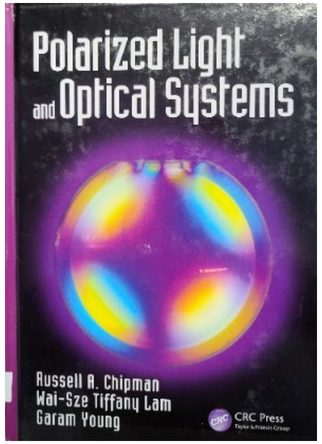
p- and s- polarizations

- p-polarized electric field is parallel to the plane of incidence
- s-polarized electric field is perpendicular to the plane of incidence



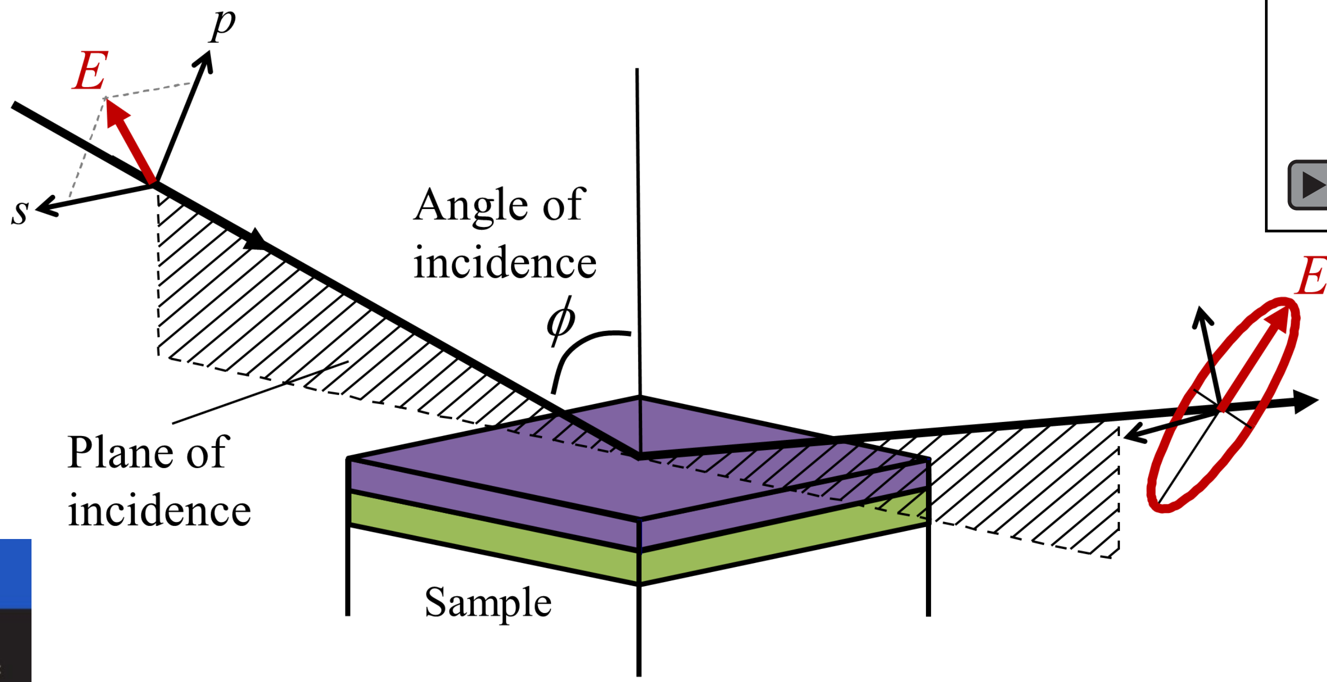




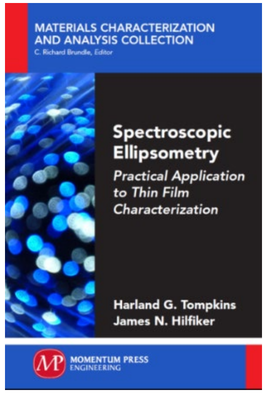


Spectroscopic Ellipsometry (SE)

- Measures change in polarization that occurs when light reflects from a surface at oblique angles.



$$\frac{\tilde{E}_p}{\tilde{E}_s}$$



$$\frac{\tilde{r}_p}{\tilde{r}_s} = \frac{\tilde{E}_p^{out} / \tilde{E}_p^{in}}{\tilde{E}_s^{out} / \tilde{E}_s^{in}} = \frac{\left|E_{out\,p}\right| / \left|E_{in\,p}\right|}{\left|E_{out\,s}\right| / \left|E_{in\,s}\right|} e^{i(\delta_p - \delta_s)} = \tan(\psi) e^{i\Delta}$$

Optical Constants

Refractive Index

$$\tilde{n} = n - ik$$

- n = "refractive index"
- k = "extinction coefficient"
  - Describe phase velocity
  - Describe reflection and refraction
  - Describe light absorption

$$\tilde{n}^2 = \tilde{\varepsilon}$$

Dielectric Function

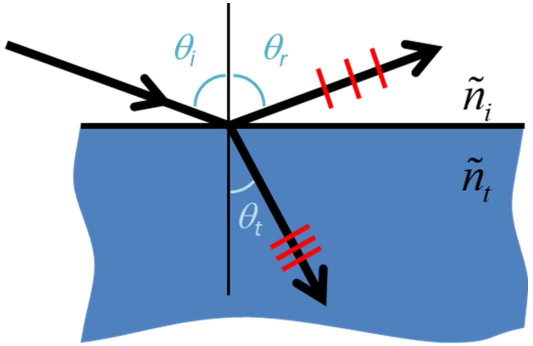
$$\tilde{\varepsilon} = \varepsilon_1 - i\varepsilon_2$$

- ε_1 = volume polarizability
- ε_2 = volume absorption
  - Describe the interaction of light and the dipoles within the material

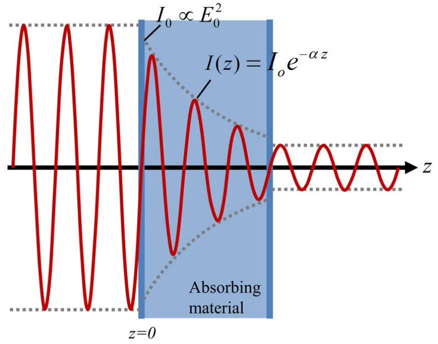
$$\vec{D} = \varepsilon_0\vec{E} + \vec{P} = \tilde{\varepsilon}(\omega)\varepsilon_0\vec{E}$$

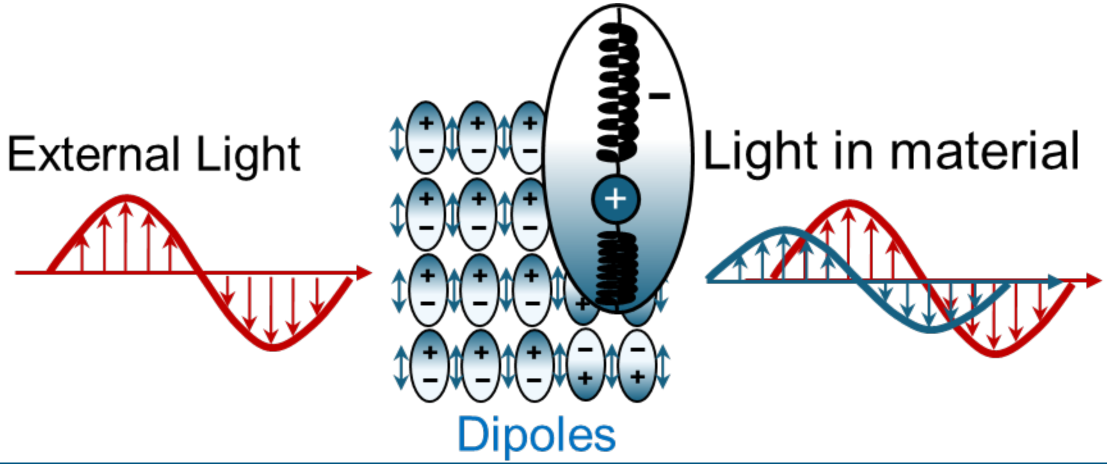
$$\mathrm{v} = \frac{c}{n}$$

$$\tilde{n}_i \sin\theta_i = \tilde{n}_t \sin\theta_t$$



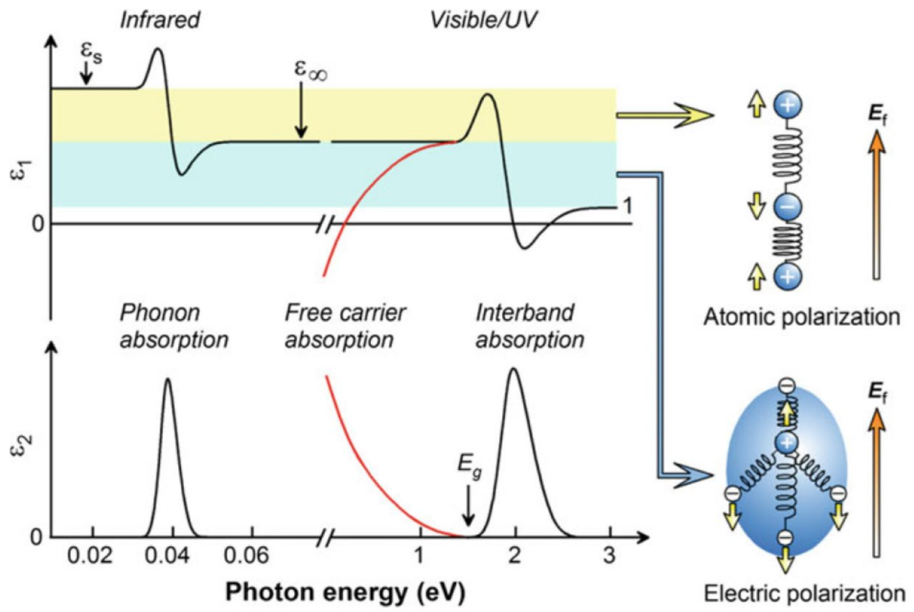
$$\alpha(\lambda) = \frac{4\pi k(\lambda)}{\lambda}$$

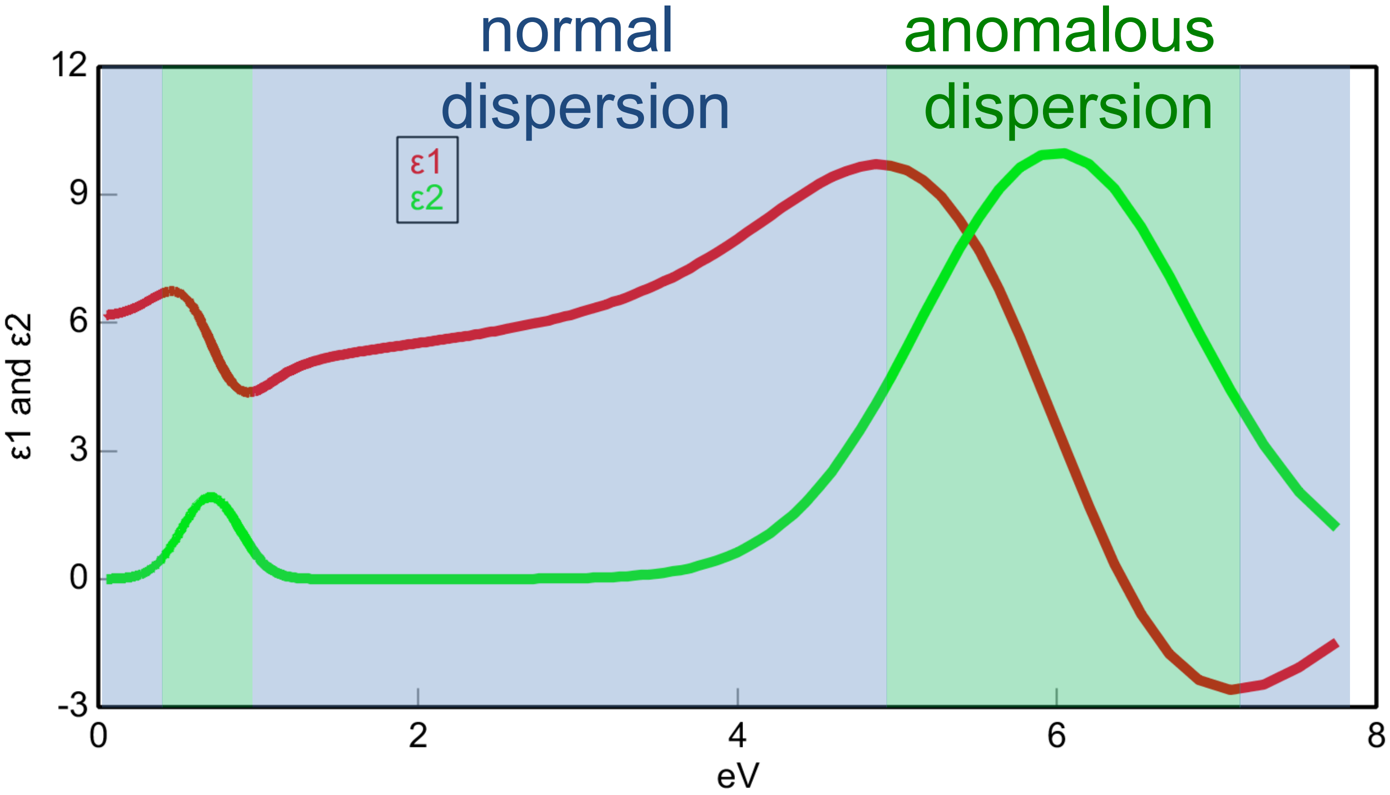


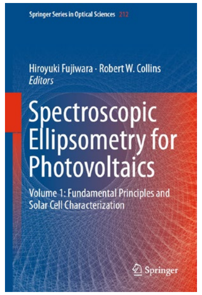


Optical Constants (dispersion)

- Dispersion refers to the variation in optical properties versus wavelength/frequency.





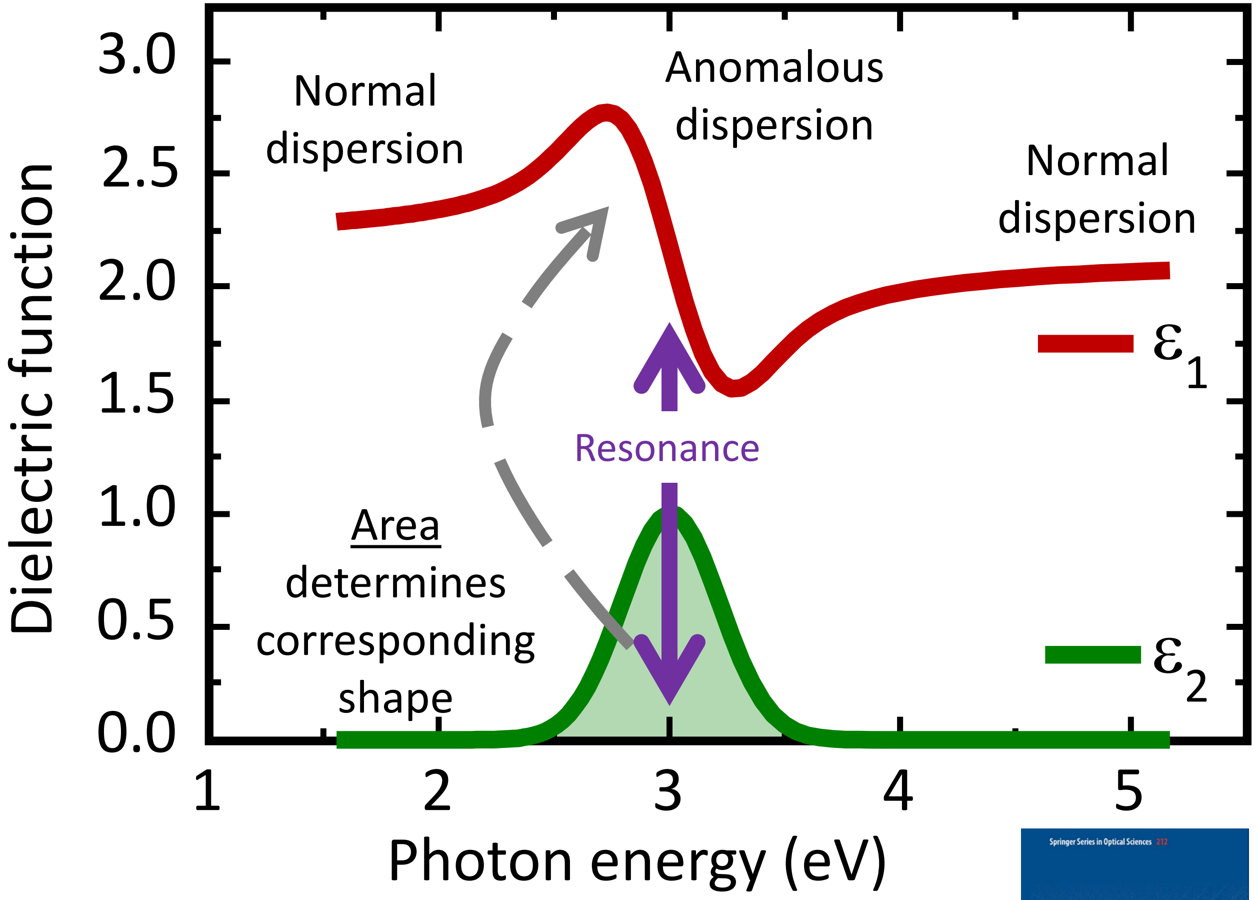


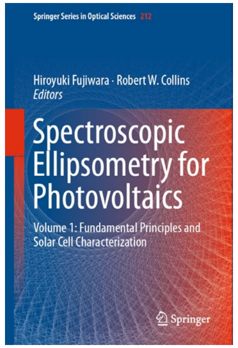
- Oscillating E-field causes dipole oscillations in the material

Kramers Kronig Consistency

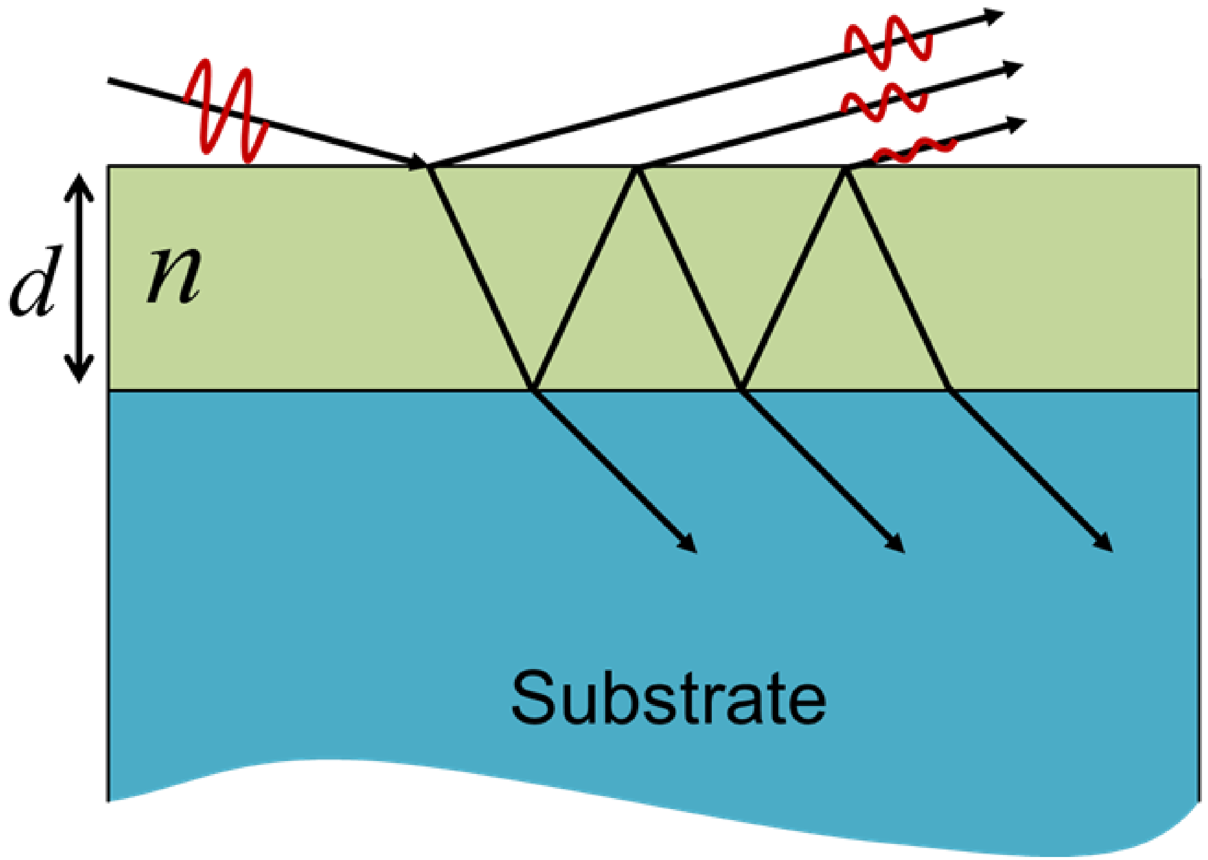
- The dipole response is like a mechanical oscillator
- Real and imaginary components are "connected" via Kramers-Kronig (KK) equations.

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





Light-Matter Interactions



$$\tilde{r}_p = \frac{E_{rp}}{E_{ip}} = \frac{n_t \cos\theta_i - n_i \cos\theta_t}{n_t \cos\theta_i + n_i \cos\theta_t}$$

$$\tilde{t}_p = \frac{E_{tp}}{E_{ip}} = \frac{2 n_i \cos\theta_i}{n_t \cos\theta_i + n_i \cos\theta_t}$$

$$\tilde{r}_s = \frac{E_{rs}}{E_{is}} = \frac{n_i \cos\theta_i - n_t \cos\theta_t}{n_i \cos\theta_i + n_t \cos\theta_t}$$

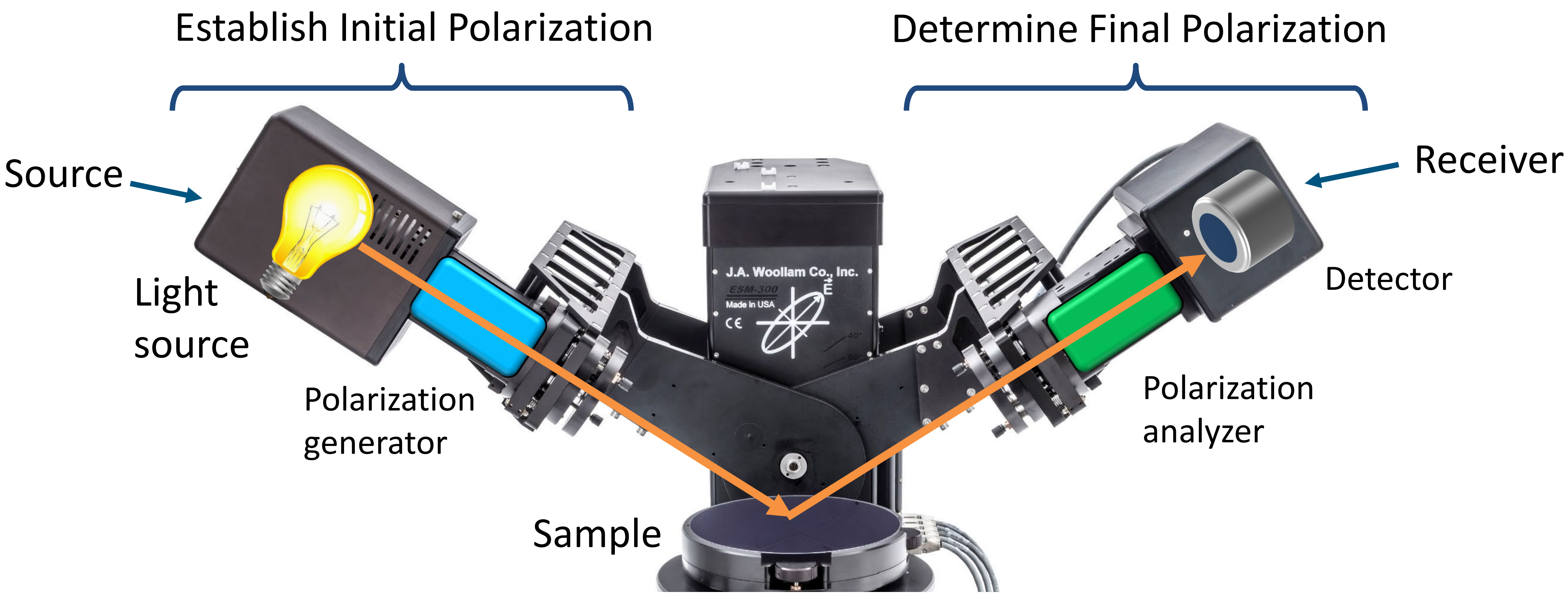
$$\tilde{t}_s = \frac{E_{ts}}{E_{is}} = \frac{2 n_i \cos\theta_i}{n_i \cos\theta_i + n_t \cos\theta_t}$$

Film “phase” thickness accounts for the travel “delay” for light within a layer

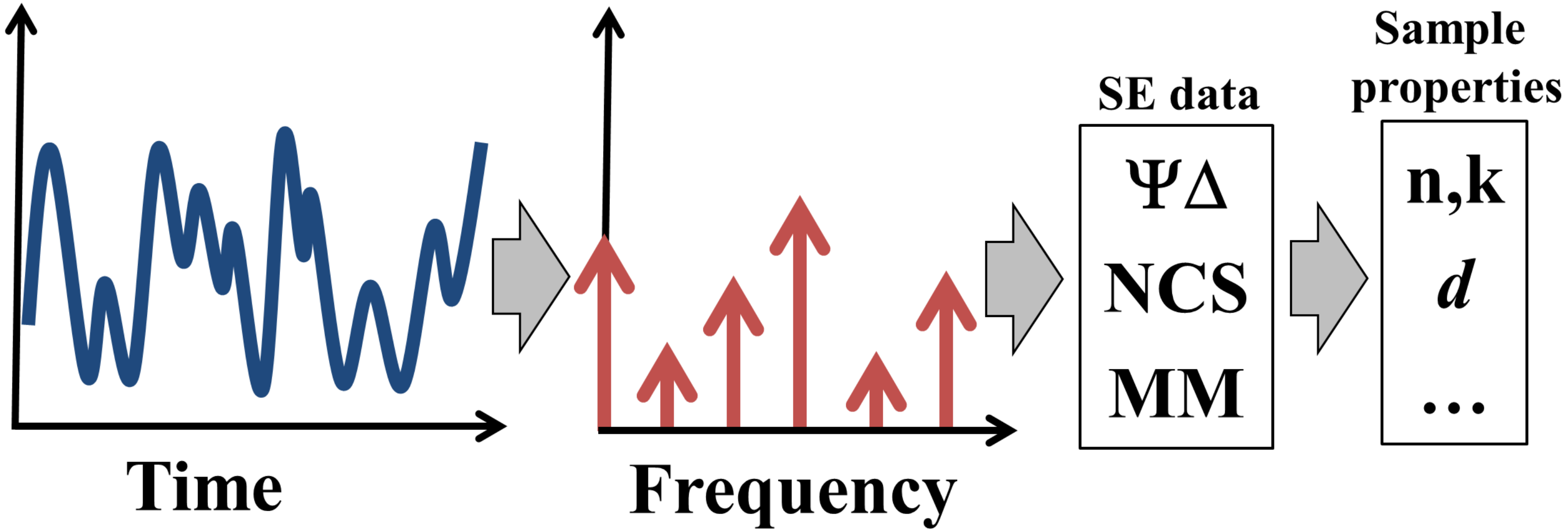
$$\beta = 2\pi \left(\frac{d}{\lambda} \right) n \cos\theta$$

Putting everything together

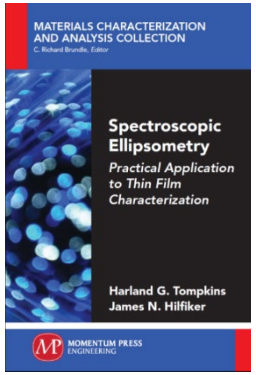
- Ellipsometry measures the <u>change in polarization</u> of light that reflects from or transmits through a sample.



Rotating Element Ellipsometers



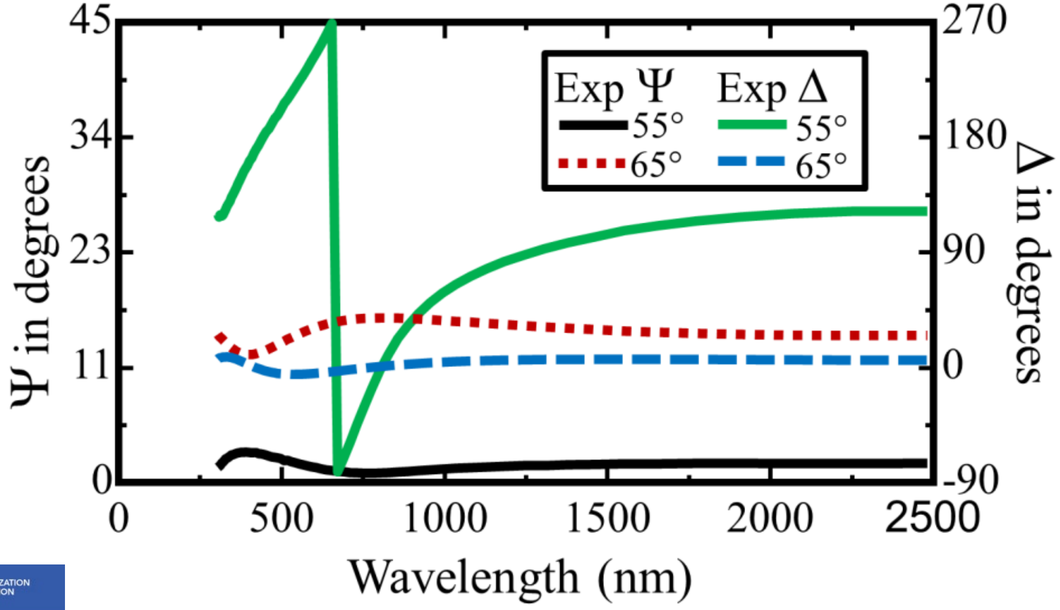
Ellipsometer Type	Frequency Content (normalized FC)
Rotating Analyzer/ Rotating Polarizer	2
Rotating Compensator	4
Dual Rotating Compensator	24



Converting Data to Results

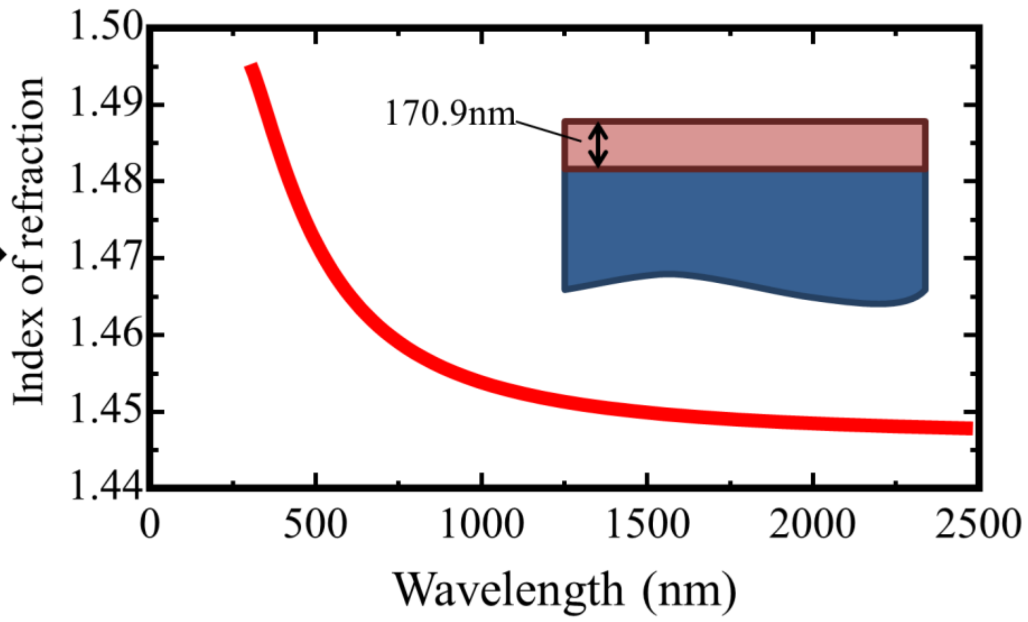
Experimental Data

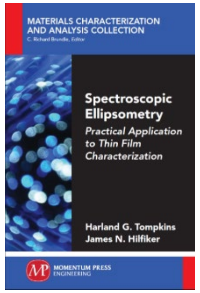
Psi, Delta



Sample properties

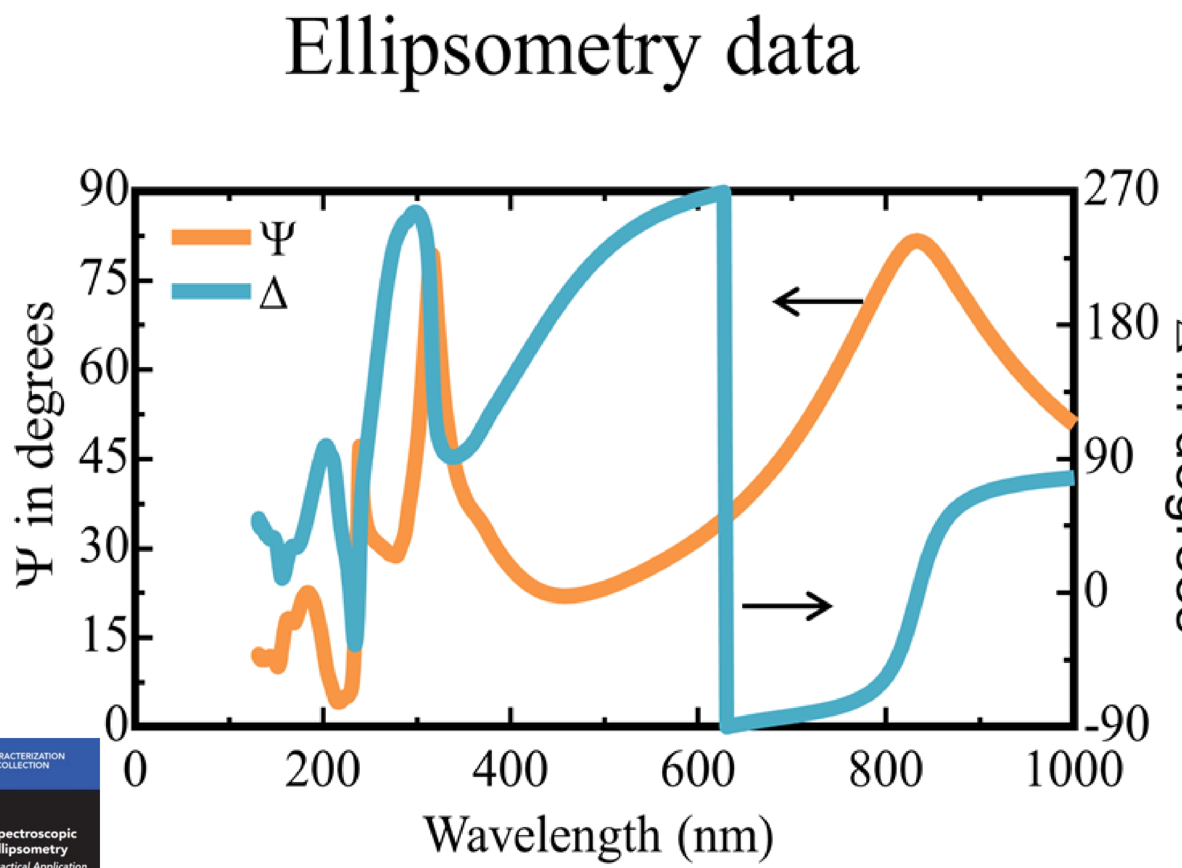
Film thickness, Optical constants
Surface roughness, Composition, Crystallinity…

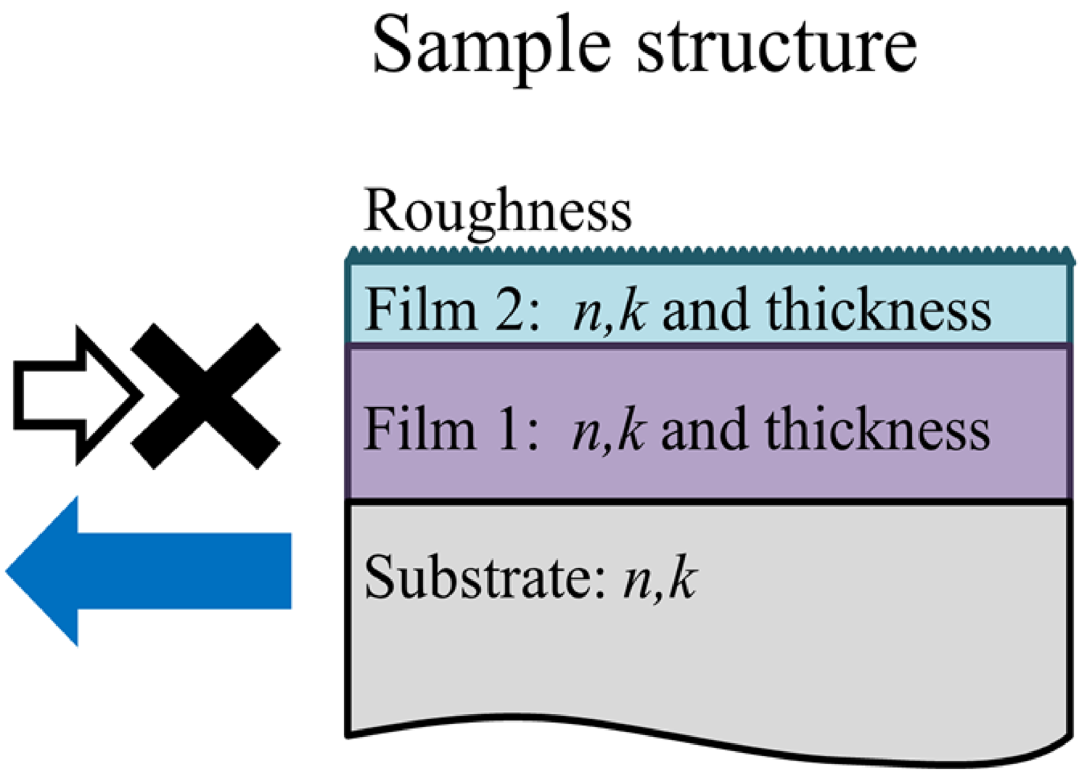


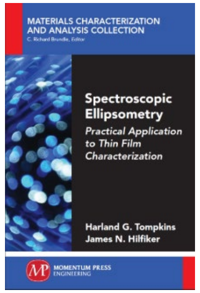


Inverse Problem

- Propose educated "guess" and check whether it matches experimental measurement.



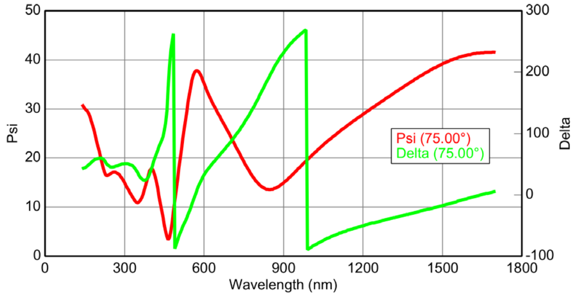




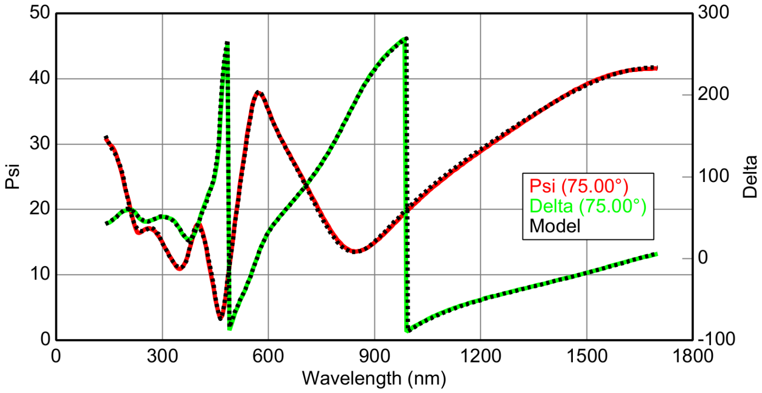
Basics Of Ellipsometry

Measurement

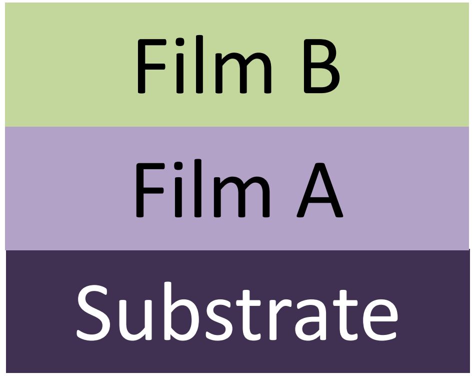
Variable Angle Spectroscopic Ellipsometric (VASE) Data

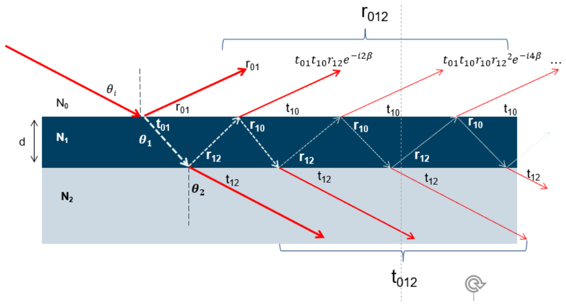


FIT

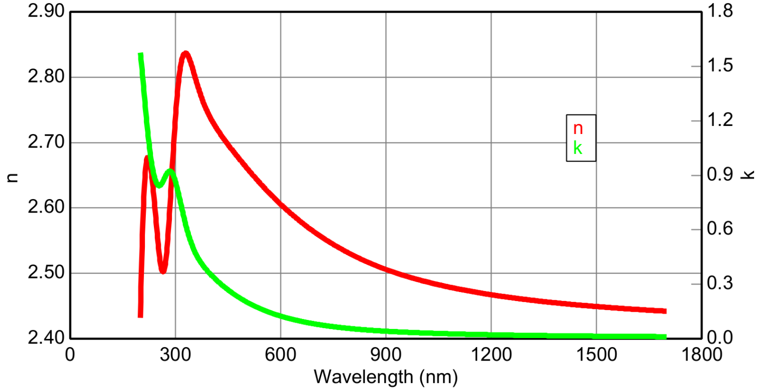


MODEL





RESULTS

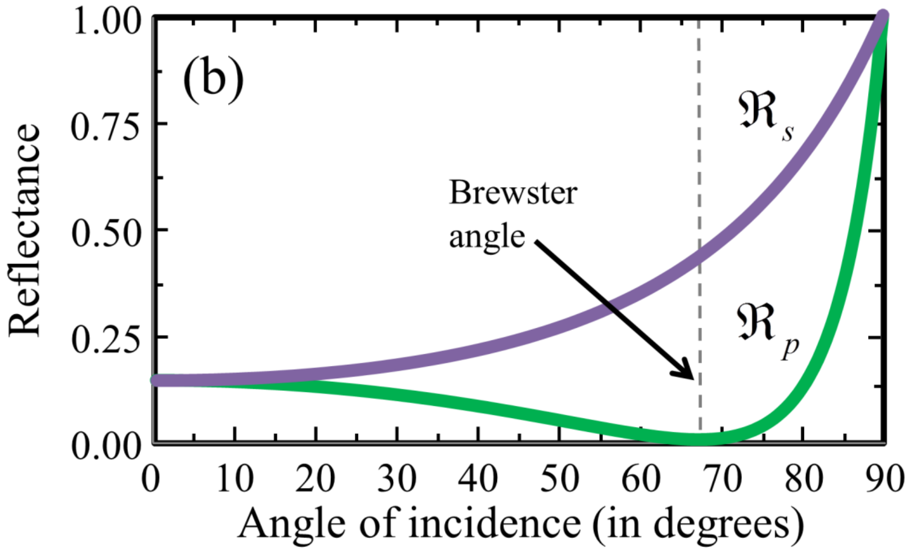


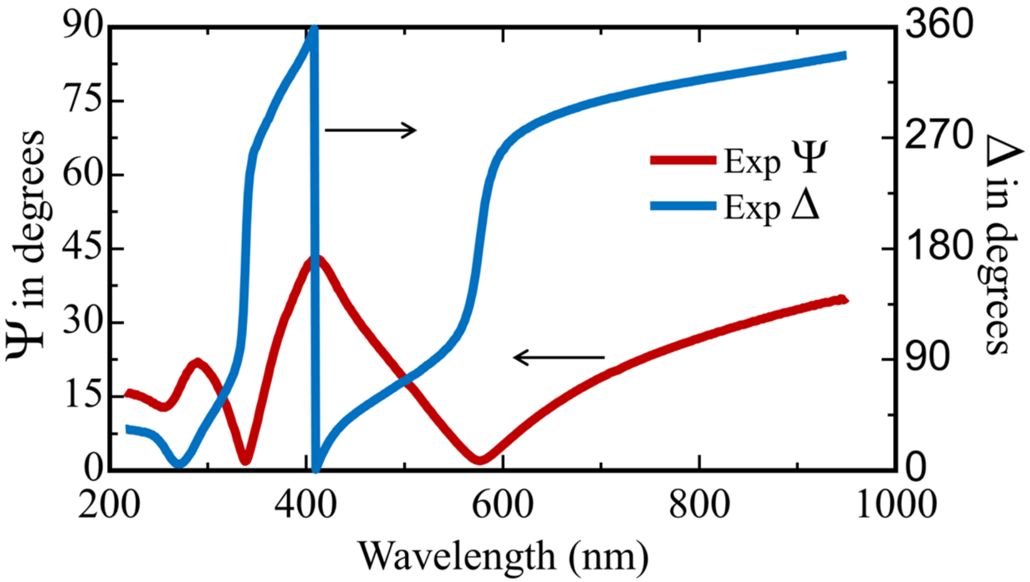
1… Measure Sample

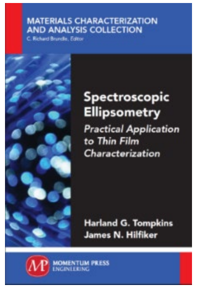
- Collect Ψ, Δ

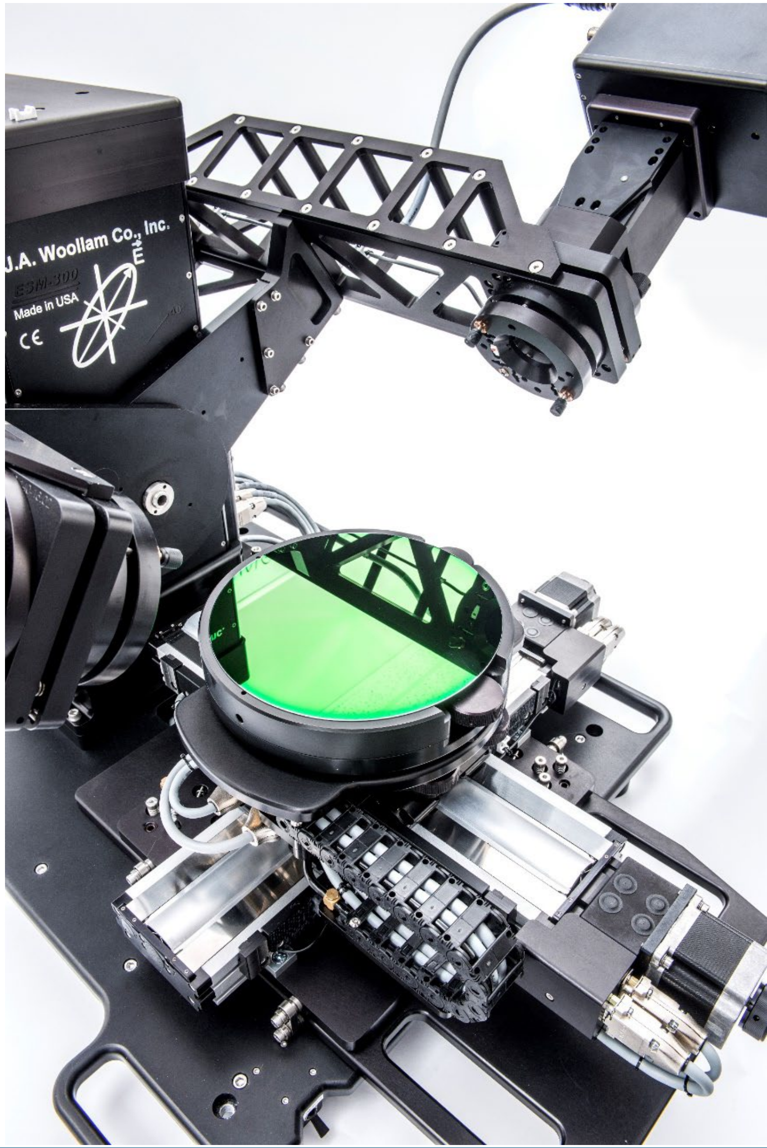
  -versus wavelength, angle

$$\tan(\Psi)e^{i\Delta} = \frac{|r_p|}{|r_s|}e^{i(\delta_p - \delta_s)}$$



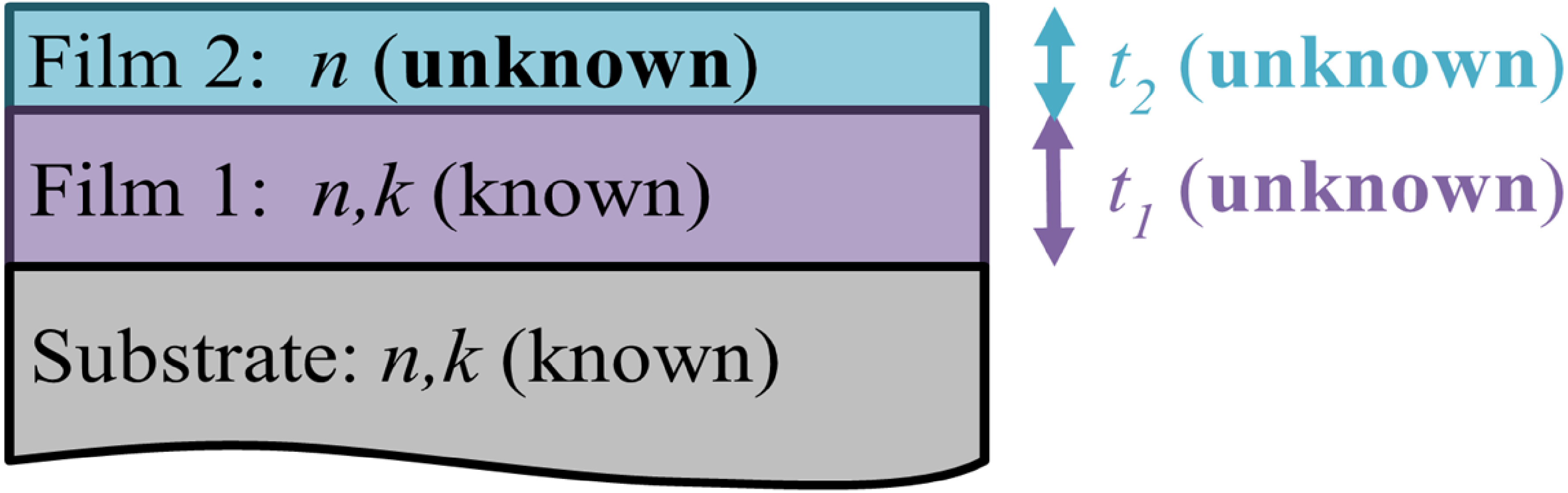


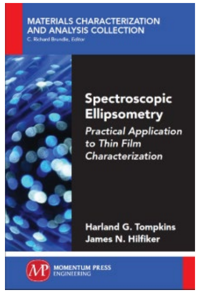




2…Build a Model

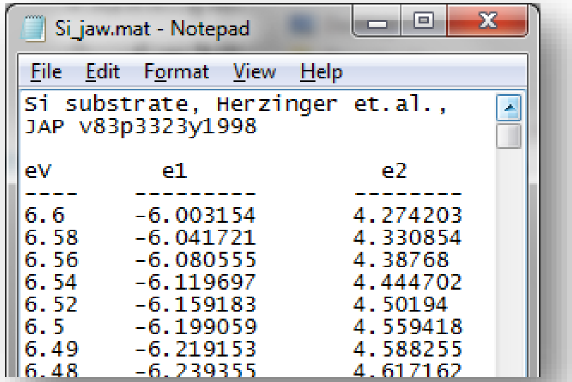
- Model is description of the sample
  - Each layer is described by a thickness & optical constants (*n* & *k*)
- Once we build a model, we can do theoretical calculations for Ψ & Δ



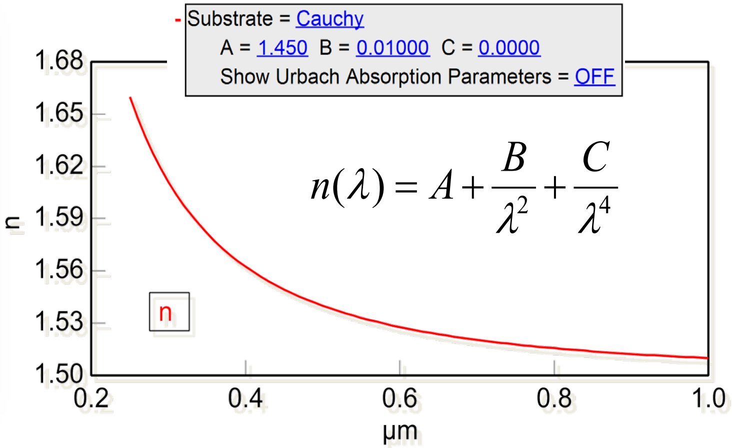


Where do we get optical constants?

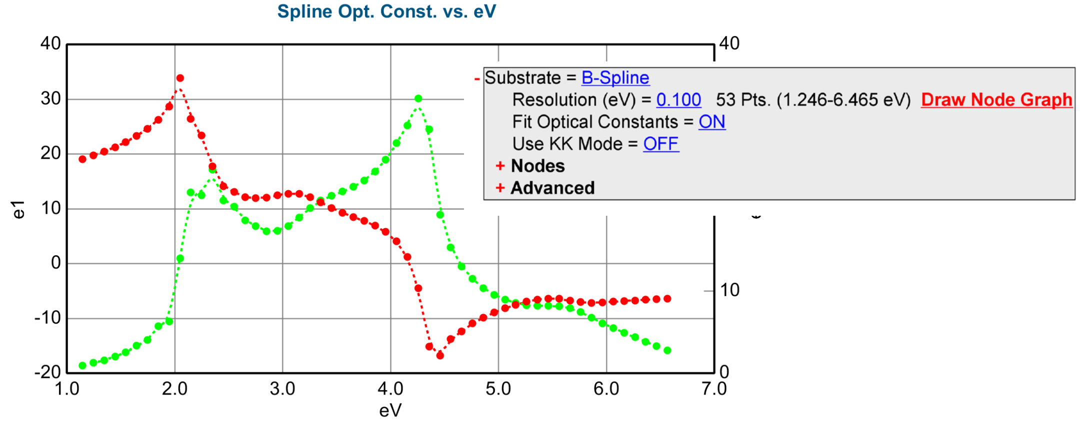
Tabulated Lists



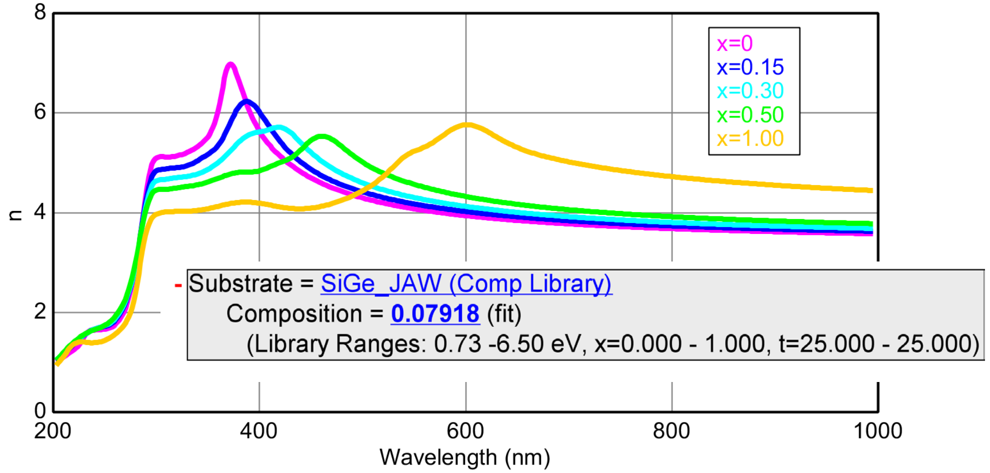
Cauchy



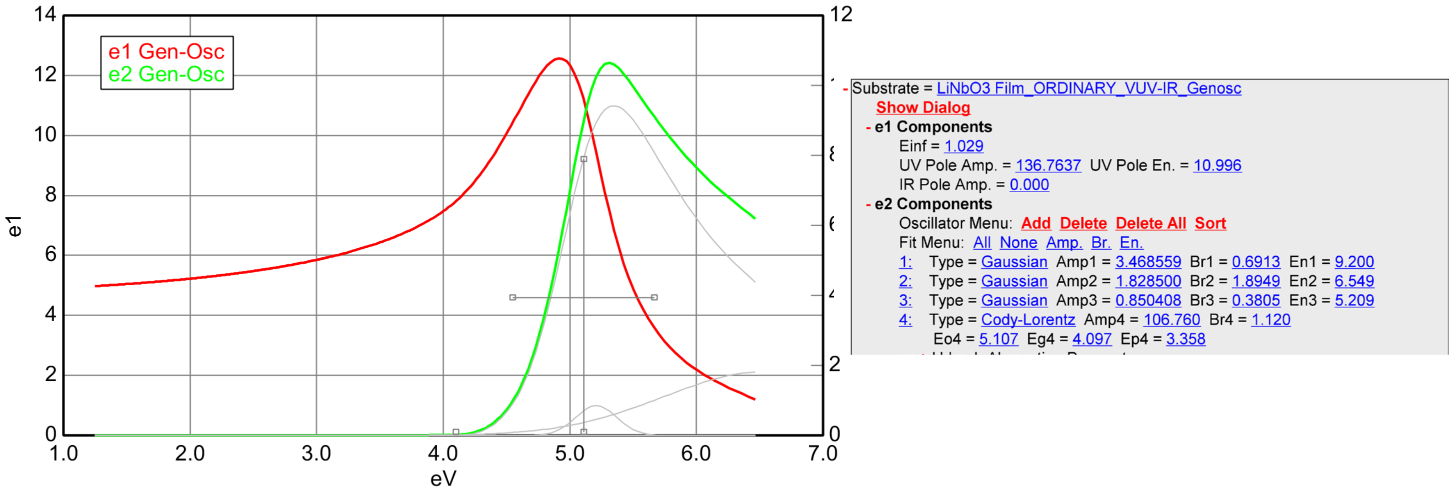
B-spline



Composition Libraries

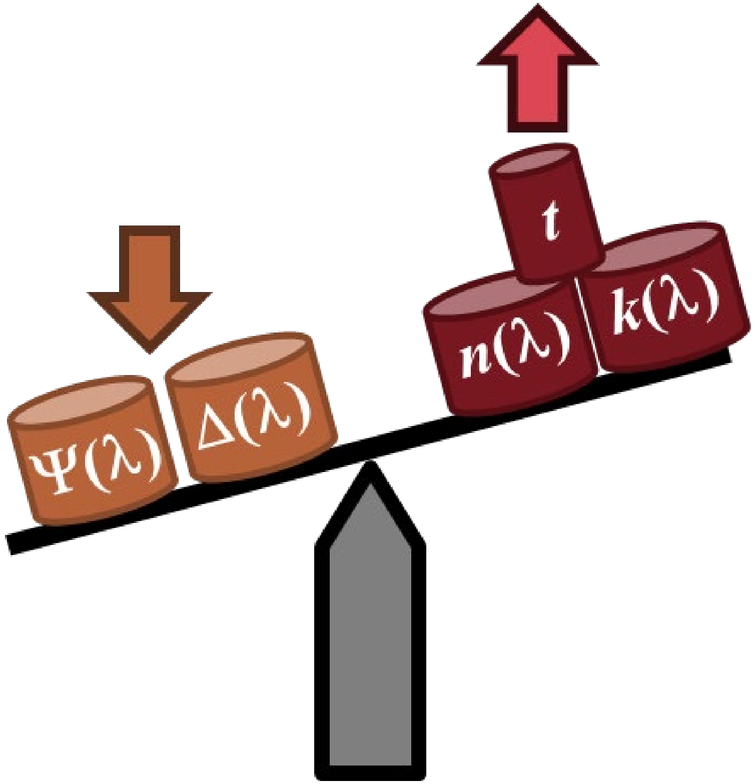


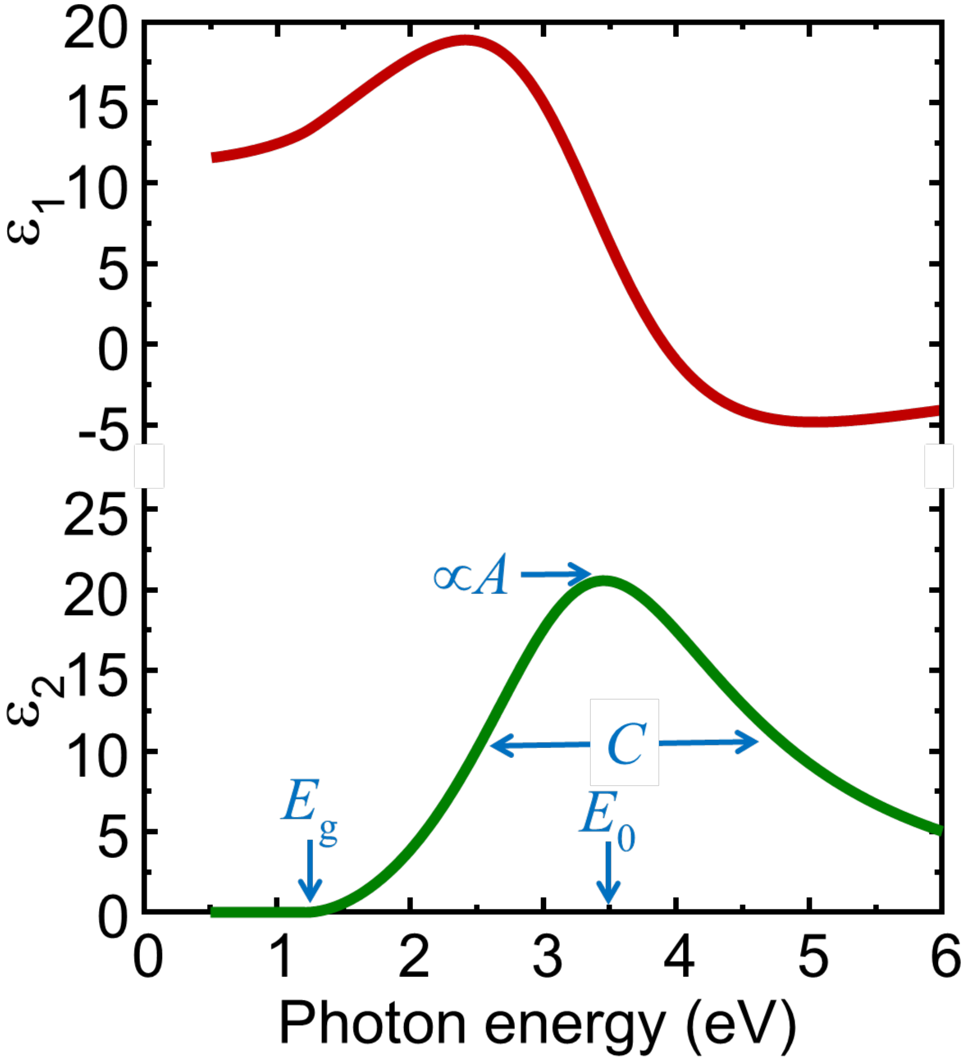
Gen-osc



Dispersion Equations

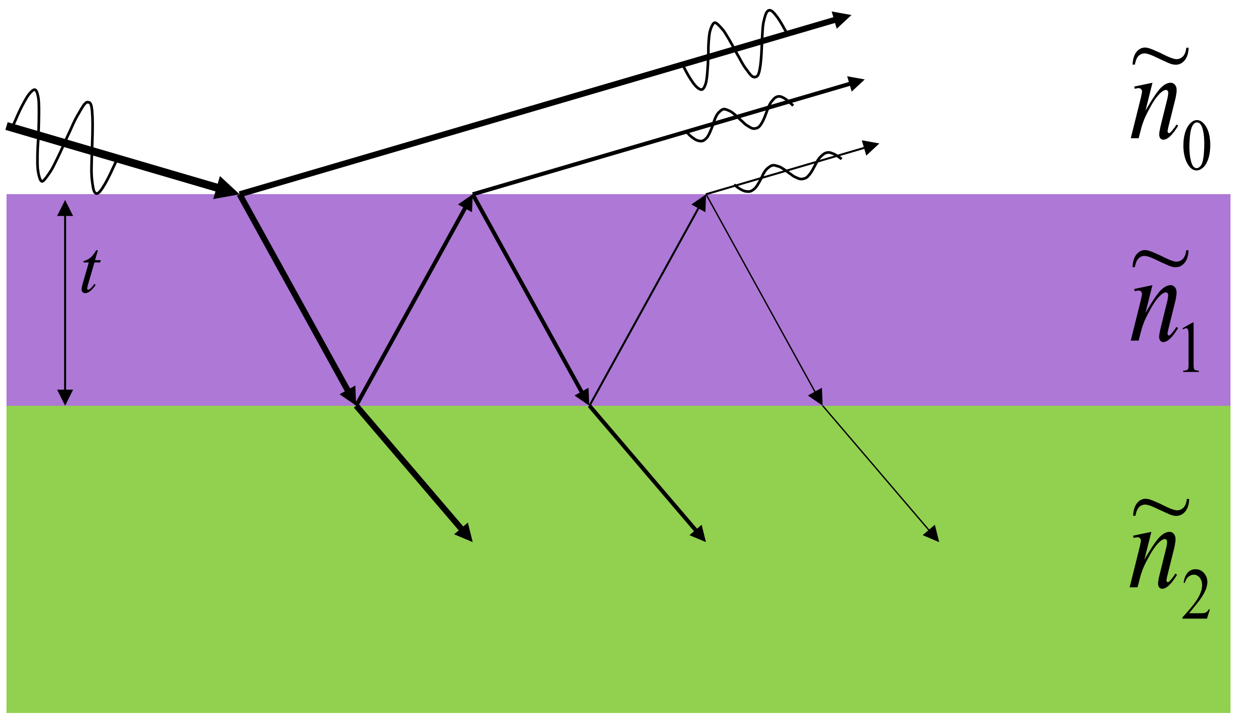
- Use equations to describe the shape of optical functions with a limited # of parameters.

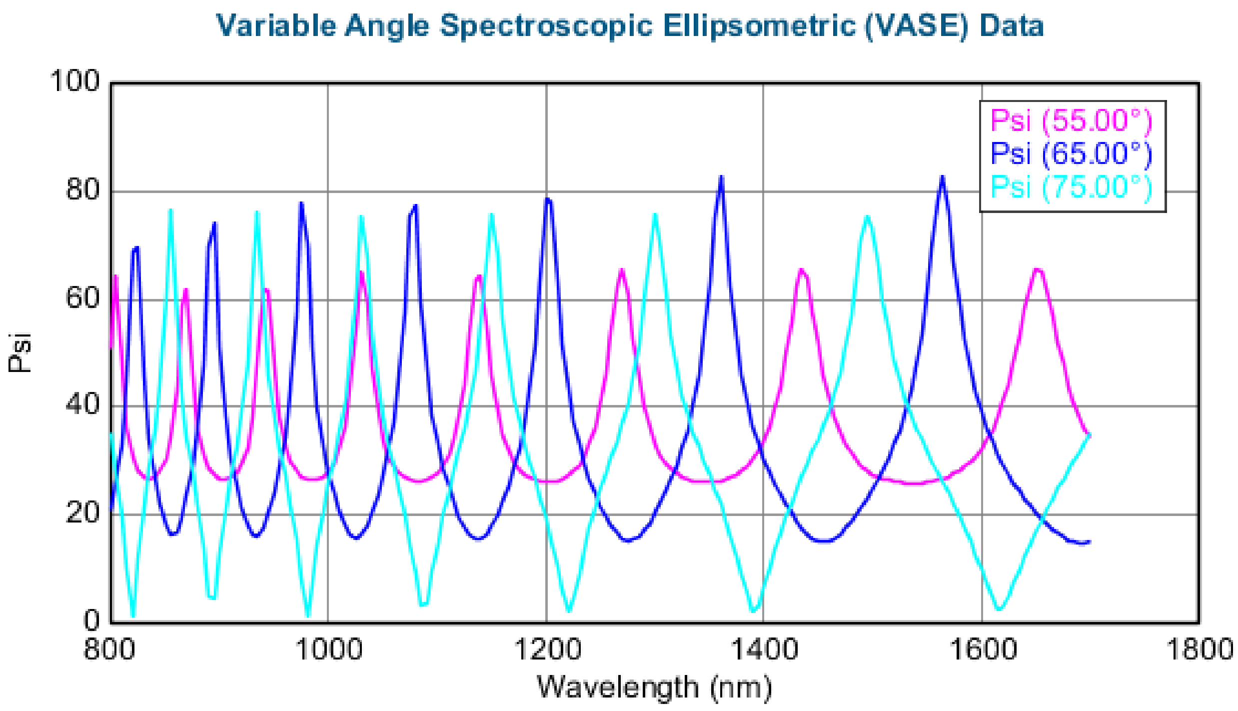




Importance of Wavelength

- Oscillation patterns in ellipsometry data are due to interference of surface-reflected light with beam that traveled through the film.

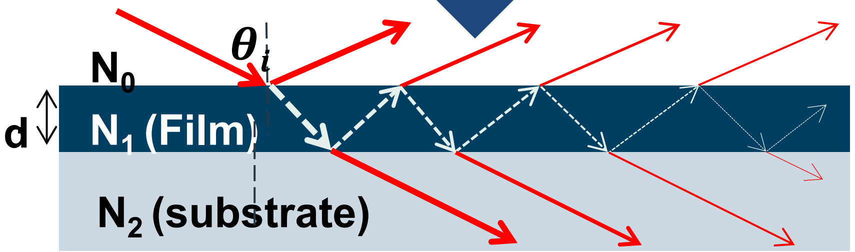




3. Generate data

- Calculate response from model and compare to Exp Data

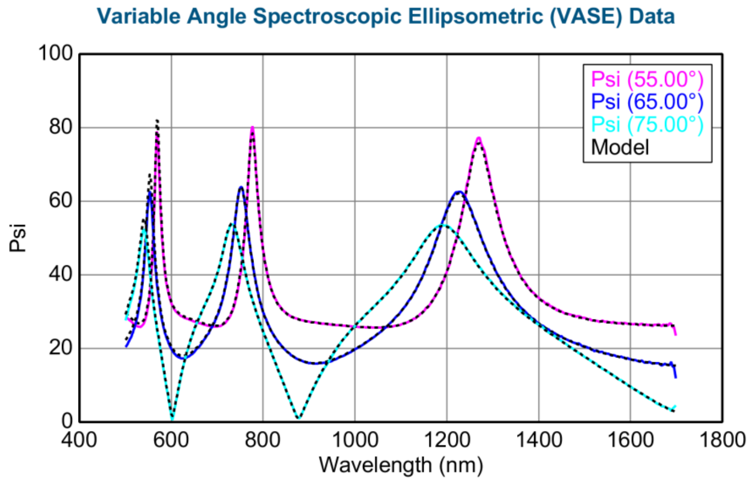
\- Layer # 1 = Biaxial Thickness # 1 = **640.77 nm** (fit)
Type = Uniaxial
Optical Constants: Difference Mode = OFF
\+ Ex = Cauchy Film
\+ Ez = Cauchy Film
Euler Angles: Phi = 0.00 Theta = 0.00
Substrate = SI_JAW

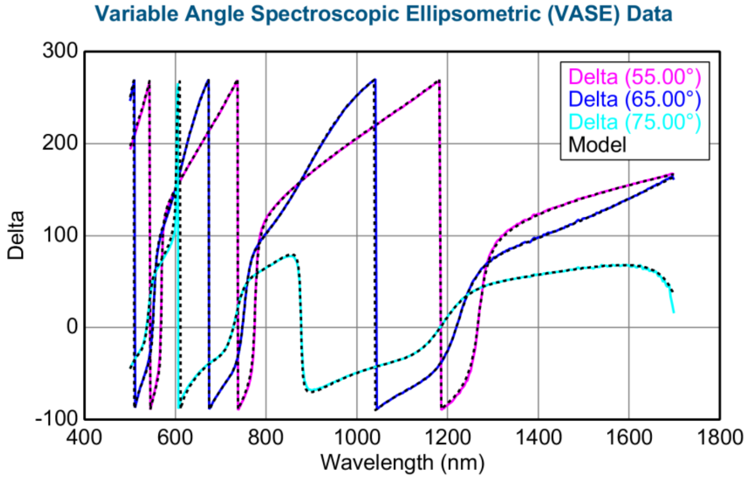


$$\tilde{r}_{p(total)} = \frac{\tilde{r}_{p01} + \tilde{r}_{p12}\, e^{-i2\beta}}{1 + \tilde{r}_{p01}\tilde{r}_{p12}\, e^{-i2\beta}}$$

$$\tilde{r}_{s(total)} = \frac{\tilde{r}_{s01} + \tilde{r}_{s12}\, e^{-i2\beta}}{1 + \tilde{r}_{s01}\tilde{r}_{s12}\, e^{-i2\beta}}$$

$$where\ \beta = 2\pi \left(\frac{d}{\lambda}\right) N_1 \cos\theta_1 = 2\pi \left(\frac{d}{\lambda}\right) \sqrt{N_1^2 - N_0^2 \sin^2\theta_0}$$

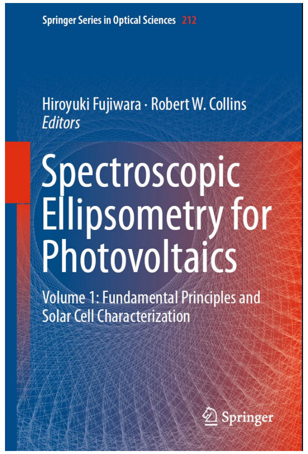


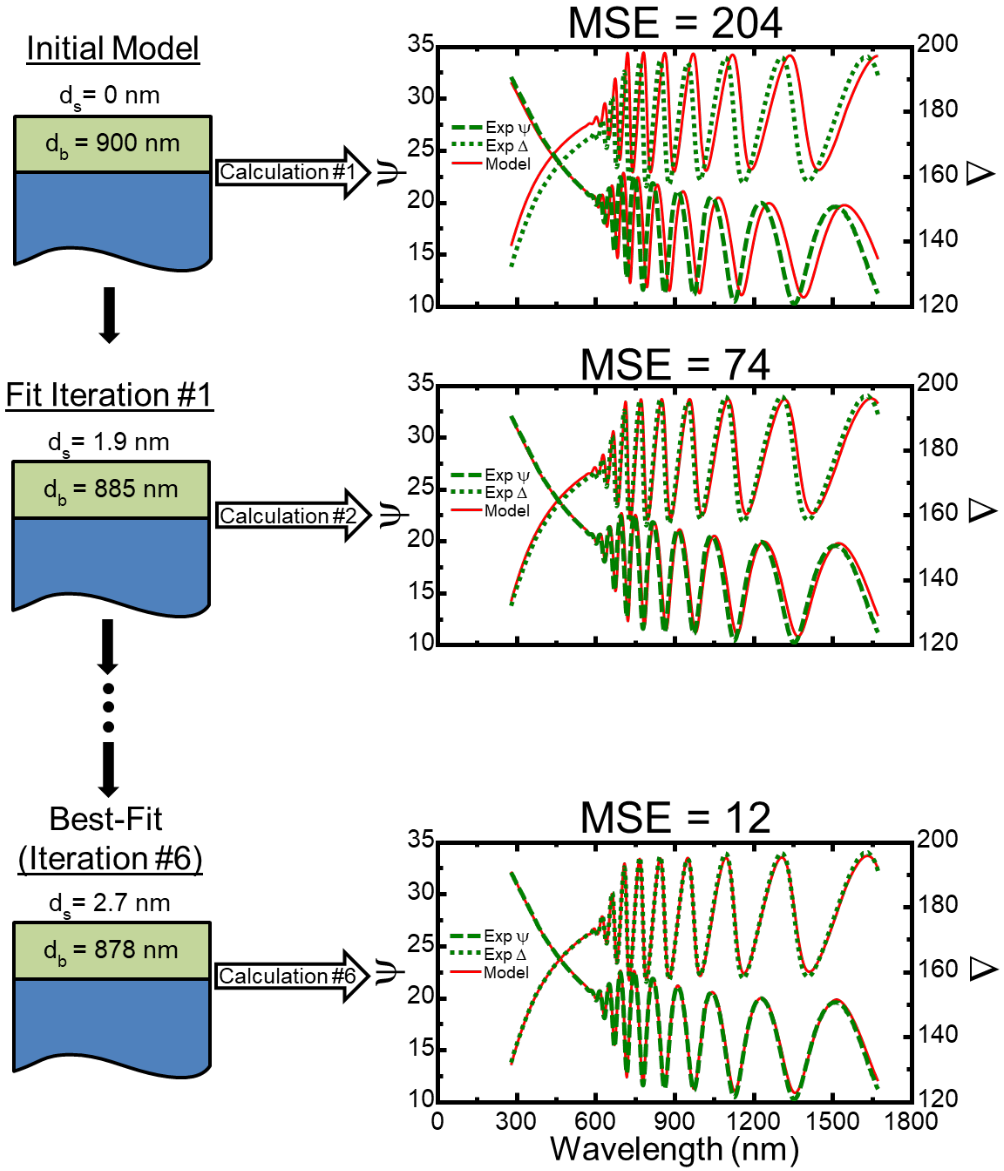


4. Data Fitting

- Unknown model parameters are varied to improve the match between "calculation" and "measurement"

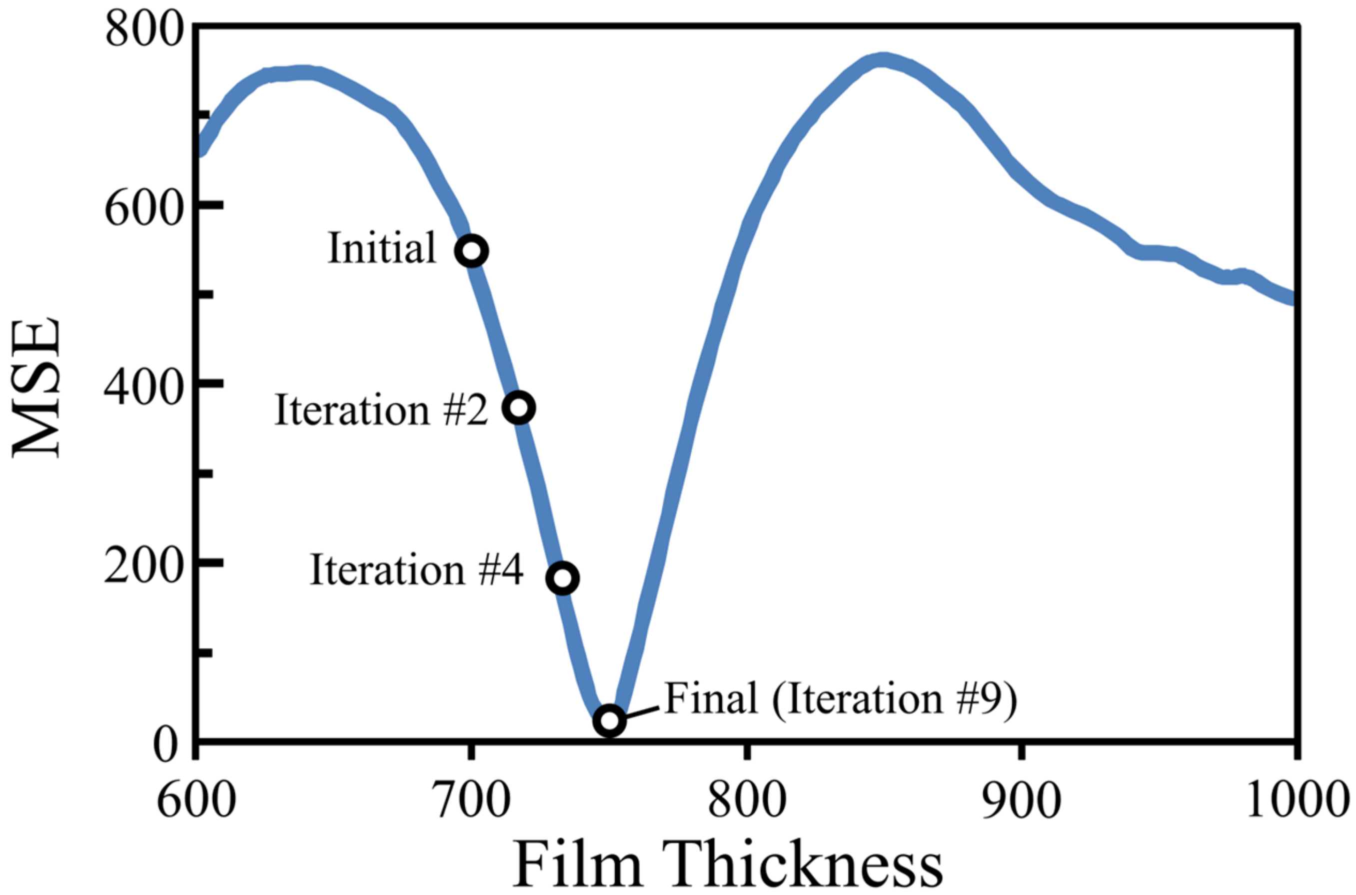
$$MSE \propto \sum \left(Mod - Exp\right)^2$$

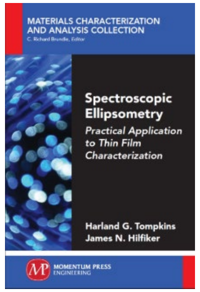




Levenberg-Marquardt Method

- Varies smoothly between the Inverse Hessian method (near the minimum) and the Steepest Descent method (far from the minimum).





Mean Squared Error

- Mean Squared Error (**MSE**) used to quantify the difference between experimental (E) and model-generated (G) data.
- CompleteEASE uses N, C, S as these values do not have discontinuities and are on the same scale (-1 to +1)

$$MSE_{NCS} = \sqrt{\frac{1}{3n-m}\sum_{i=1}^{n}\left[\left(\frac{N_{E_i}-N_{G_i}}{0.001}\right)^2+\left(\frac{C_{E_i}-C_{G_i}}{0.001}\right)^2+\left(\frac{S_{E_i}-S_{G_i}}{0.001}\right)^2\right]}$$

$$N = \cos(2\Psi)$$
$$C = \sin(2\Psi)\cos(\Delta)$$
$$S = \sin(2\Psi)\sin(\Delta)$$

*where n = total number of data points and m = number of variable "fit" parameters in the model

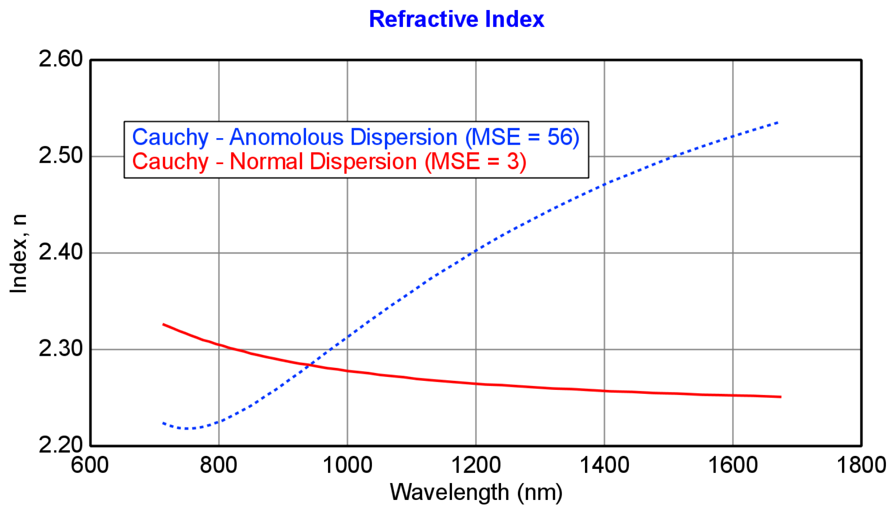
Theoretical "Best" MSE = 1
Fit to data is at same level as the estimated error of experimental measurements

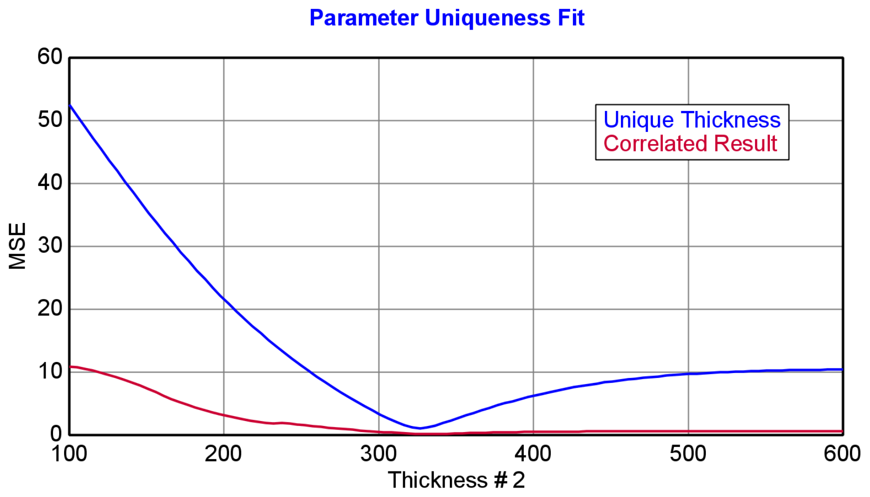
5. Evaluate Results

- How well does experimental and generated data match? How low is MSE? Can it be reduced further by increasing model complexity?

- Are fit parameters physical?
  - Normal dispersion, K-K consistency

- Check other mathematical “goodness of fit” indicators
  - Correlation matrix
  - Uniqueness Test
  - Error bars

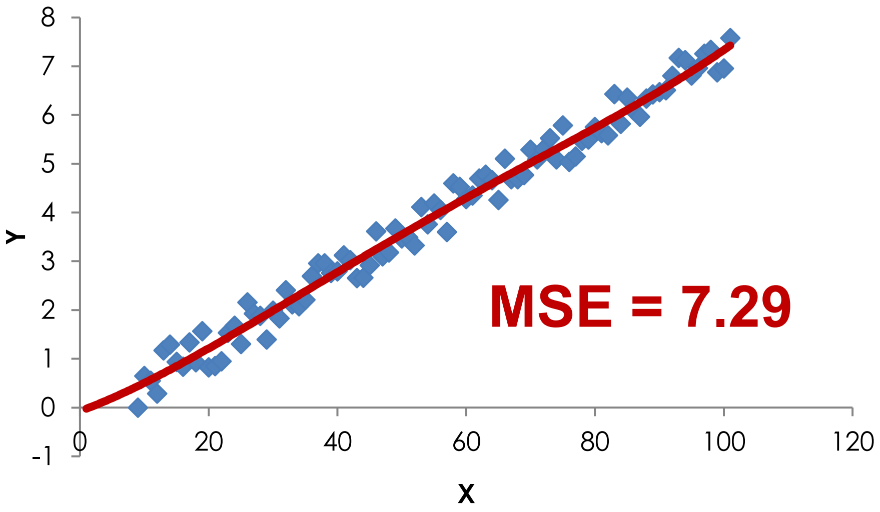




Evaluating Results: General Rules

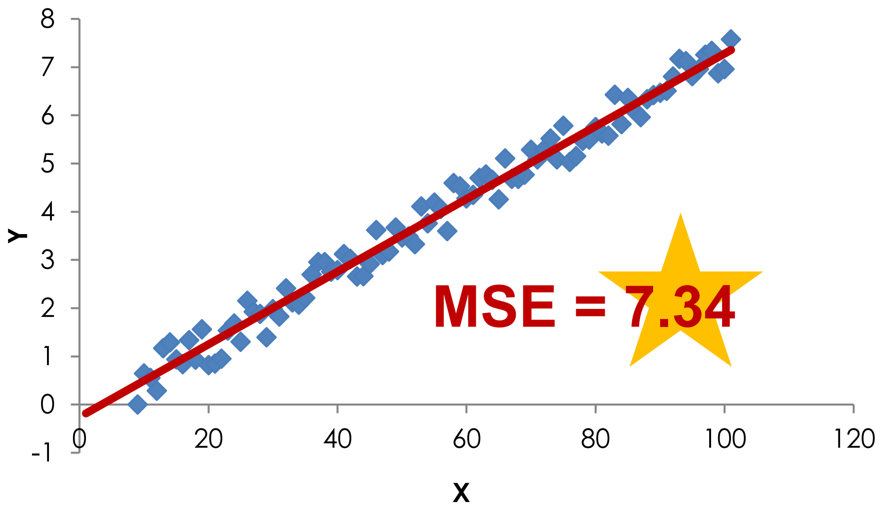
- Find the **simplest optical model** that fits Experimental Data
- **Verify uniqueness** of the model
  - Find minimum # of fit parameters which give the same goodness-of-fit

$Model\text{:}\ \ Y = A \cdot X^4 + B \cdot X^4 + C \cdot X^2 + D \cdot X + \mathrm{E}$



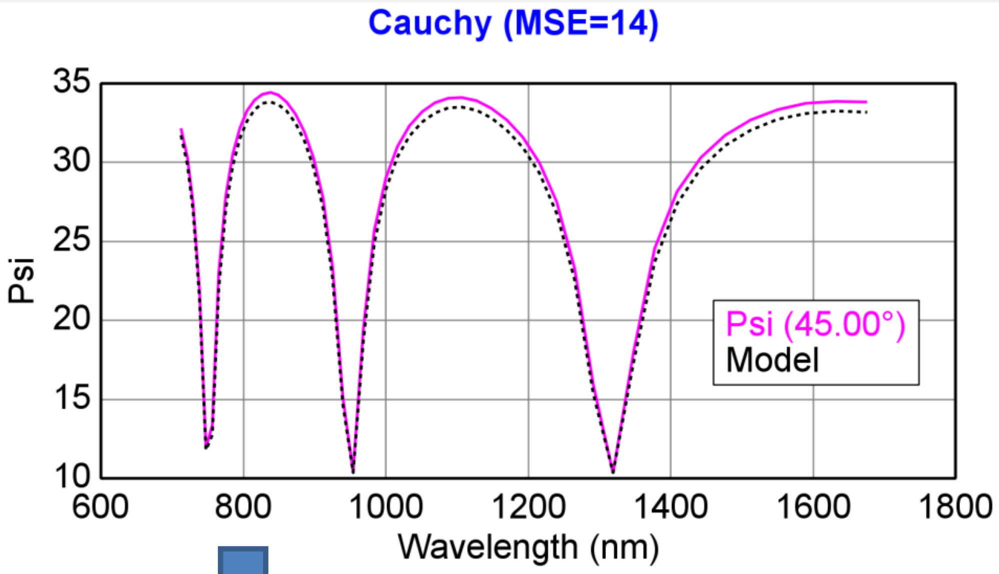
	Model Values	
	Polynomial	Linear
A	.0898	3.00
B	-.4095	.539
C	.566	
D	2.77	
E	.552	

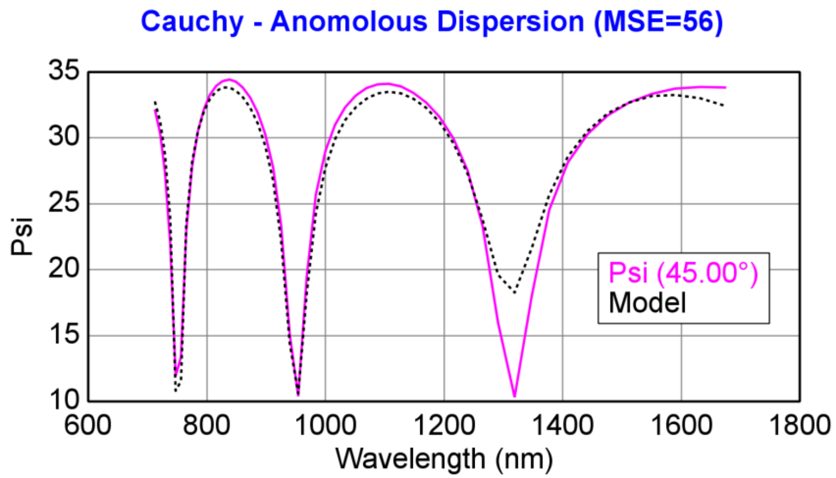
$Model\text{:}\ \ Y = A \cdot X + B$

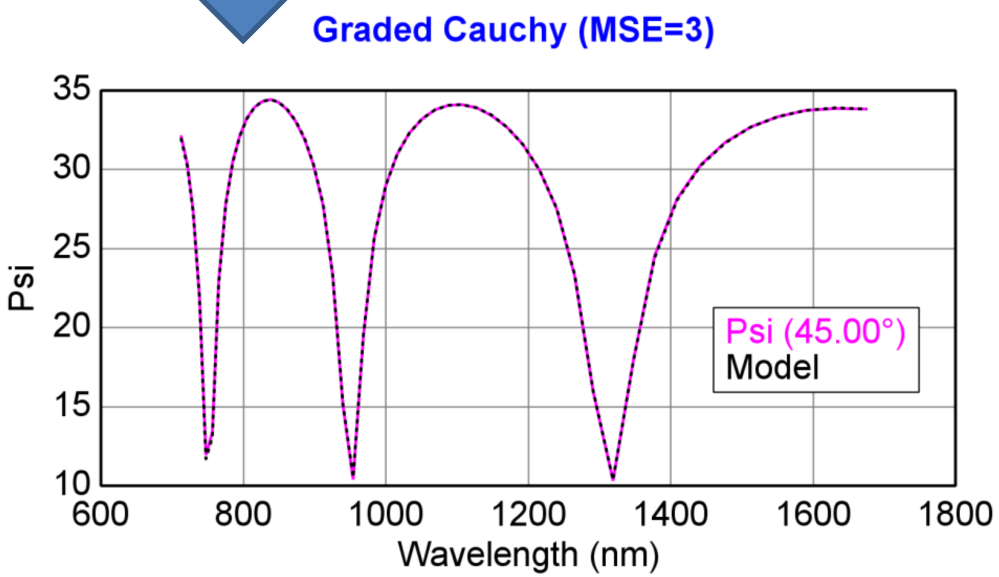


Comparison - MSE

- Model should match Exp. curves "by eye".
- MSE quantifies the match
- Additional Model Complexity is justified <u>if</u> the MSE improves "significantly".



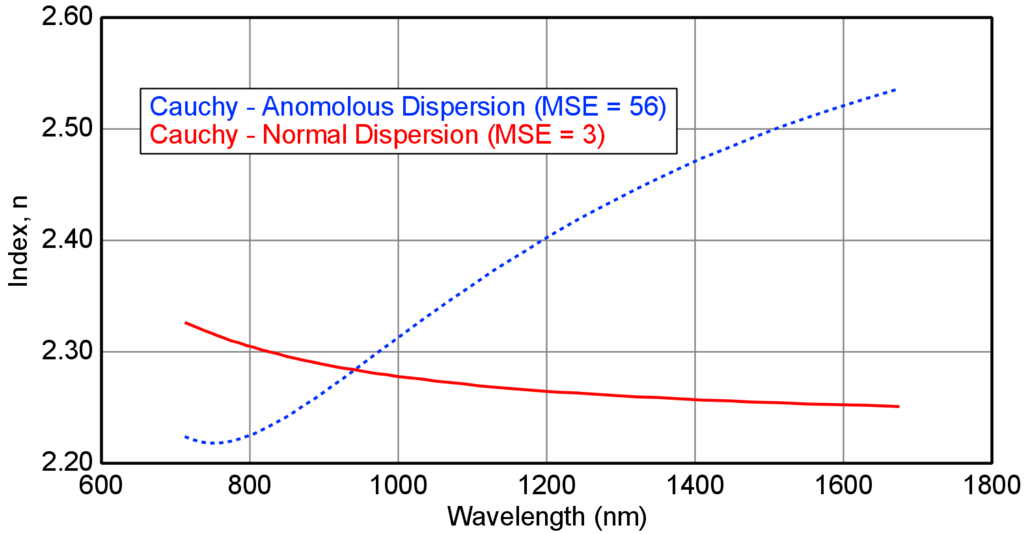




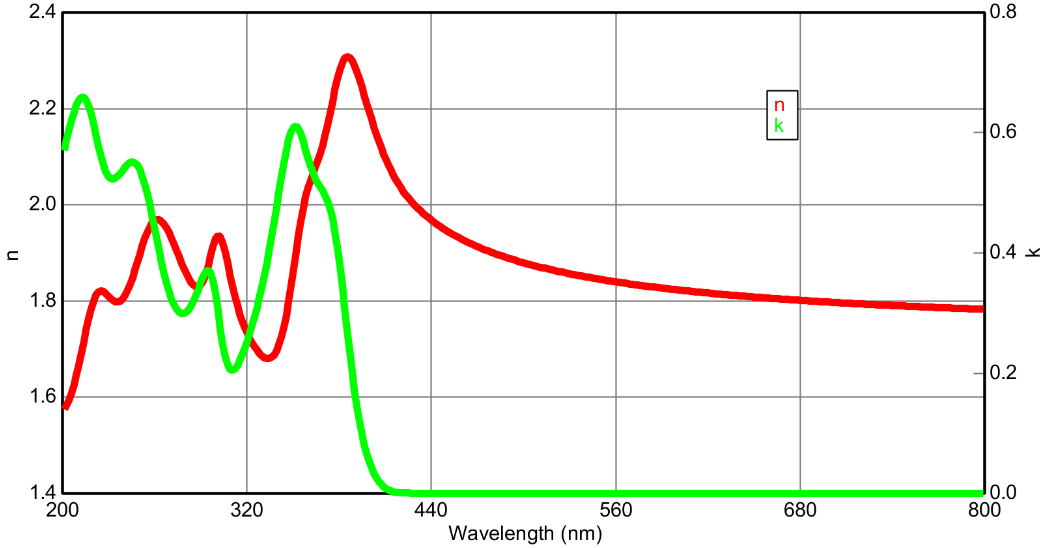
When poor fit, results are meaningless!

“Physical” Fit Parameters

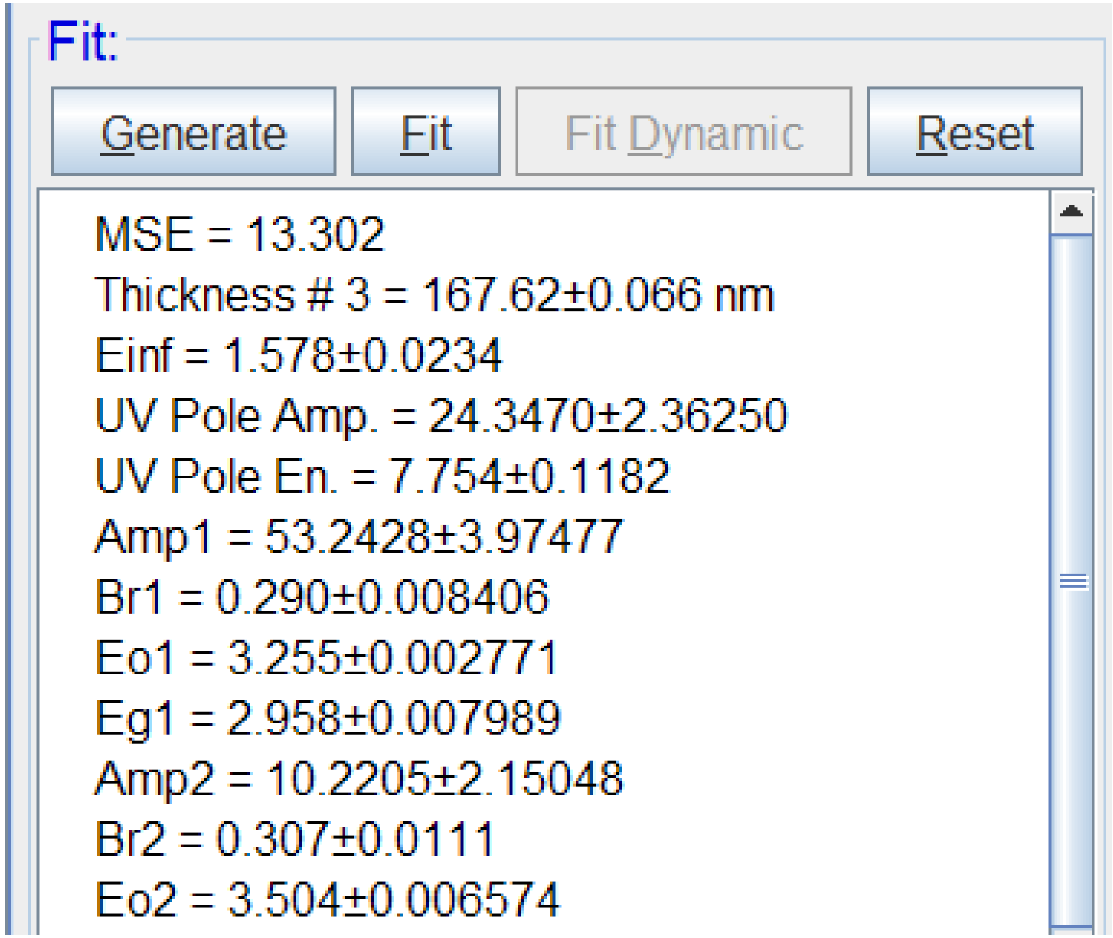
- Normal – Anomalous Dispersion
  - When transparent, index increases toward shorter wavelengths.



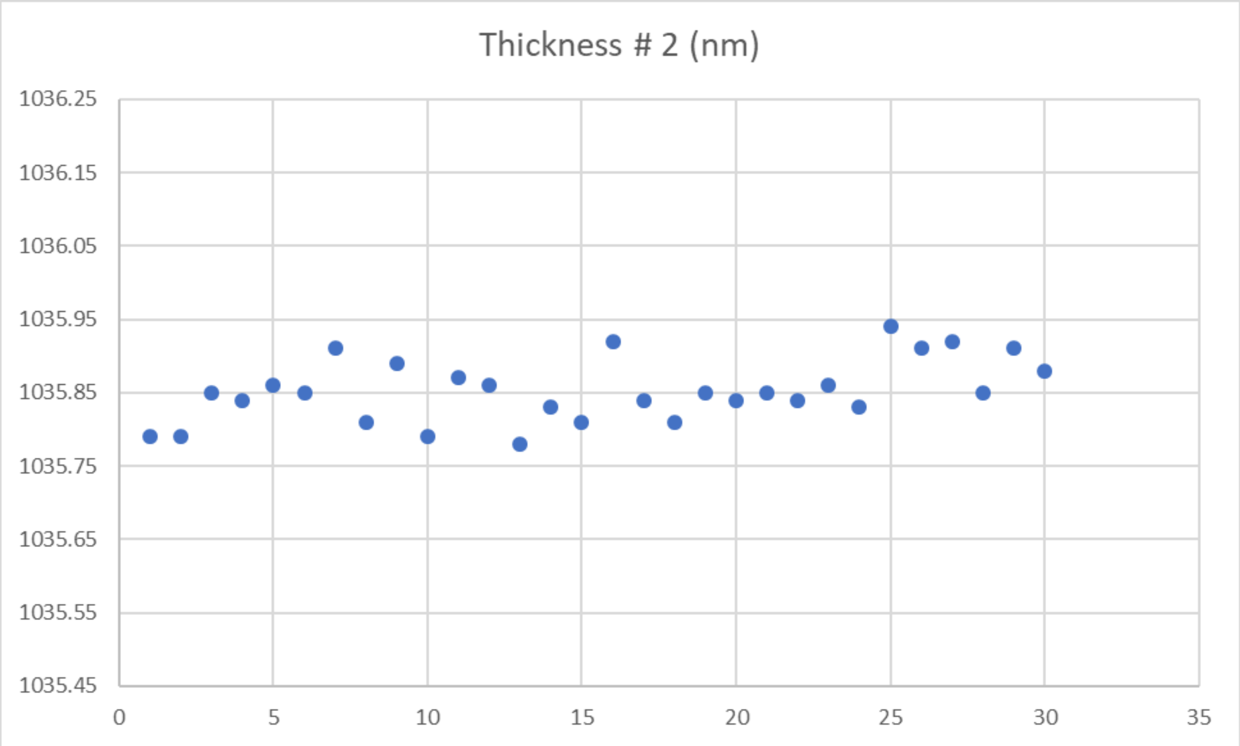
  - When absorbing, the index “rolls-over” to follow Kramers-Kronig consistency.



90% Confidence Limits



Confidence Limits only account for random error, not systematic error!



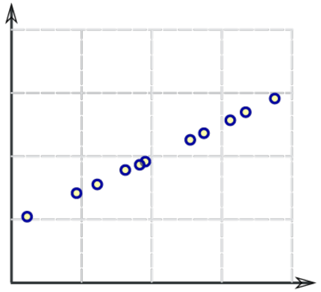
Correlation Matrix

Correlation defines relationship between 2 parameters

Correlation Matrix

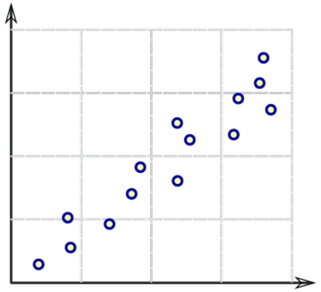
	Roughness	Thickness # 2	Einf	UV Pole Amp.	UV Pole En.	Amp1	Br1
Roughness	1.000	0.067	0.057	-0.056	-0.181	-0.024	0.027
Thickness # 2	0.067	1.000	0.113	0.020	-0.078	-0.095	-0.051
Einf	0.057	0.113	1.000	0.799	-0.474	-0.969	-0.938
UV Pole Amp.	-0.056	0.020	0.799	1.000	0.110	-0.918	-0.873
UV Pole En.	-0.181	-0.078	-0.474	0.110	1.000	0.247	0.342
Amp1	-0.024	-0.095	-0.969	-0.918	0.247	1.000	0.942
Br1	0.027	-0.051	-0.938	-0.873	0.342	0.942	1.000
Eo1	0.054	0.142	0.518	0.663	0.314	-0.645	-0.402
Eg1	0.062	0.192	0.596	0.642	0.122	-0.682	-0.428
Ep1	-0.025	-0.097	-0.967	-0.919	0.239	1.000	0.938
Thickness # 1	0.027	0.133	0.368	0.288	-0.109	-0.366	-0.293
# Back Reflections	0.029	-0.755	-0.052	-0.027	0.009	0.053	0.034

Perfect Positive Correlation



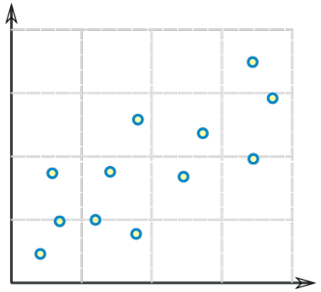
1

High Positive Correlation



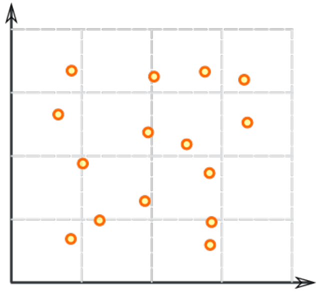
0.9

Low Positive Correlation



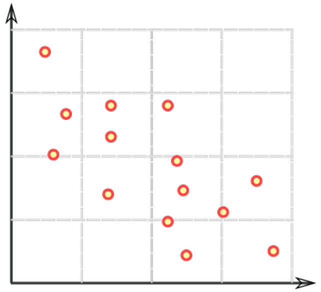
0.5

No Correlation



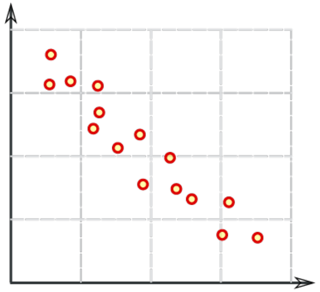
0

Low Negative Correlation



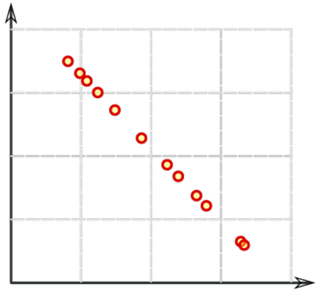
-0.5

High Negative Correlation



-0.9

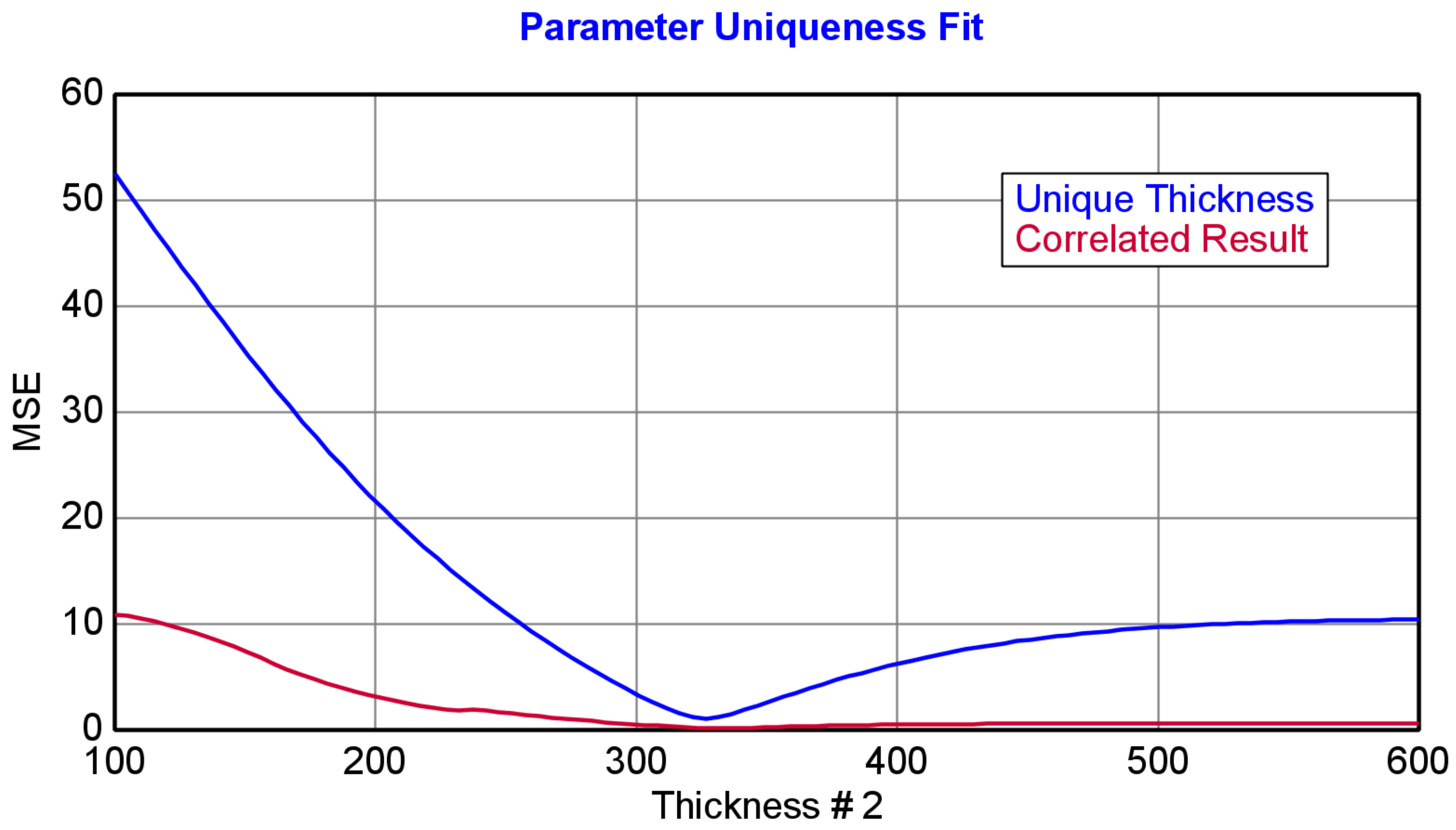
Perfect Negative Correlation



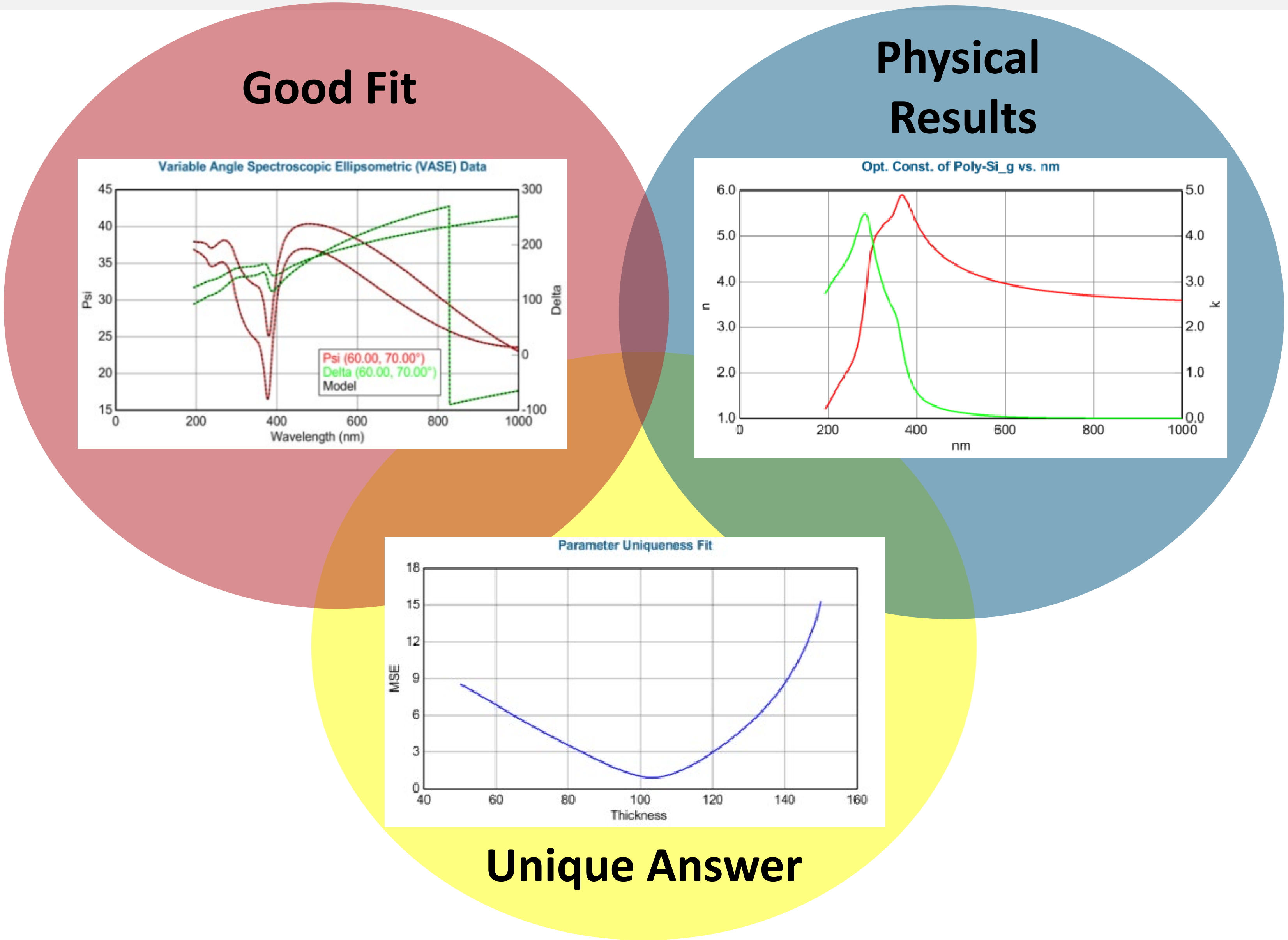
-1

Parameter Uniqueness

- Test for True Correlation (Parameter Uniqueness):
  - Can same MSE be achieved with one parameter fixed at a perturbed value?

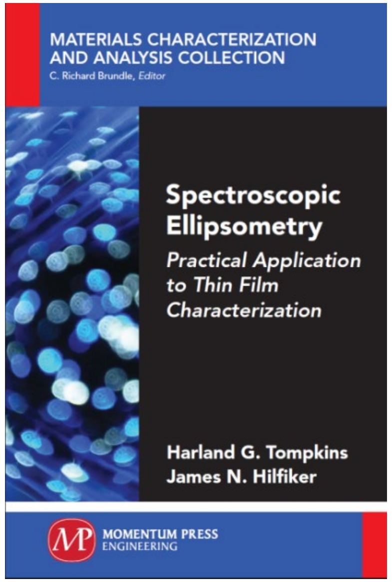


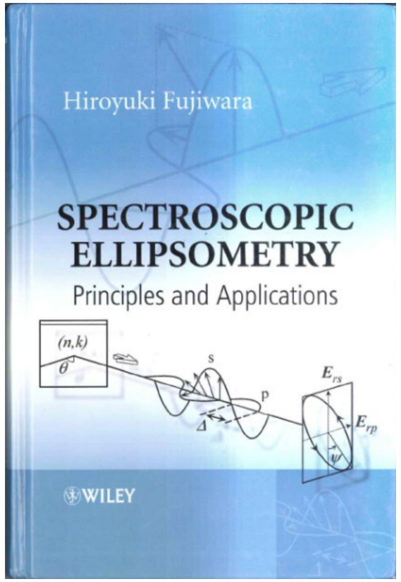
Correct Results



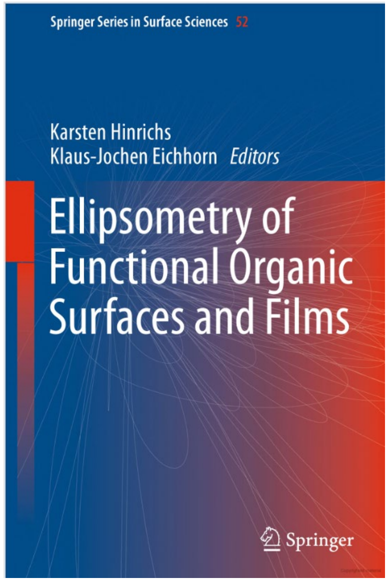
Spectroscopic Ellipsometry References

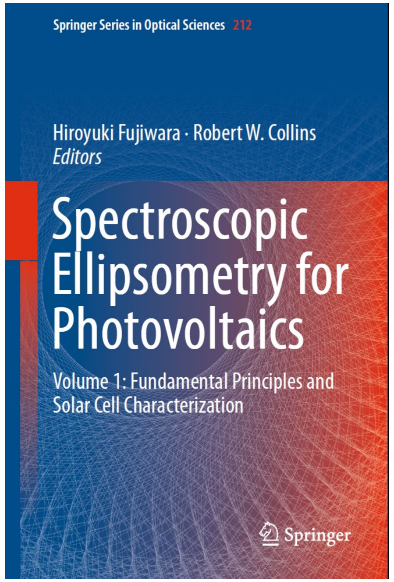
Beginner & Intermediate

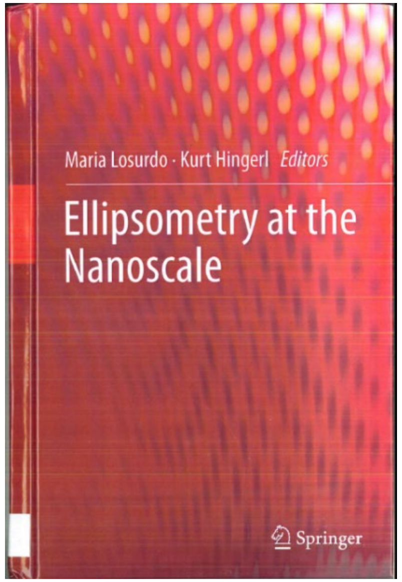




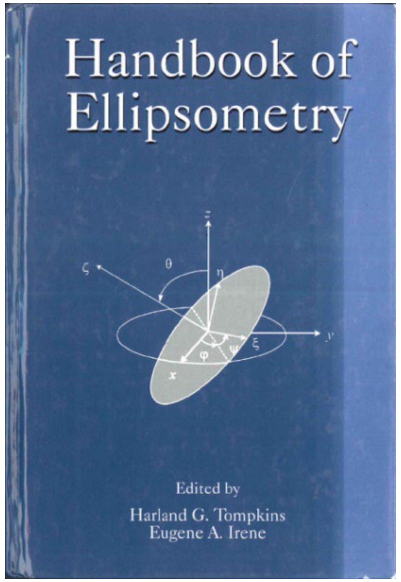
Applications

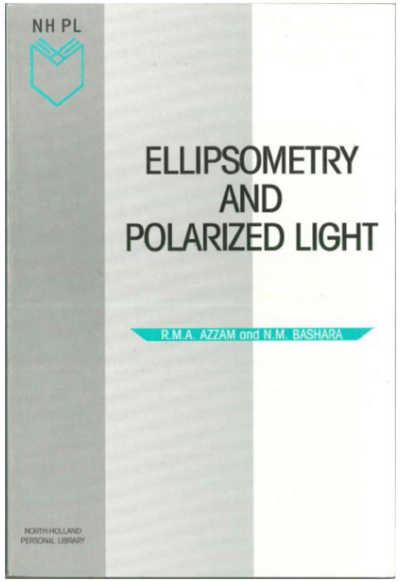






Advanced





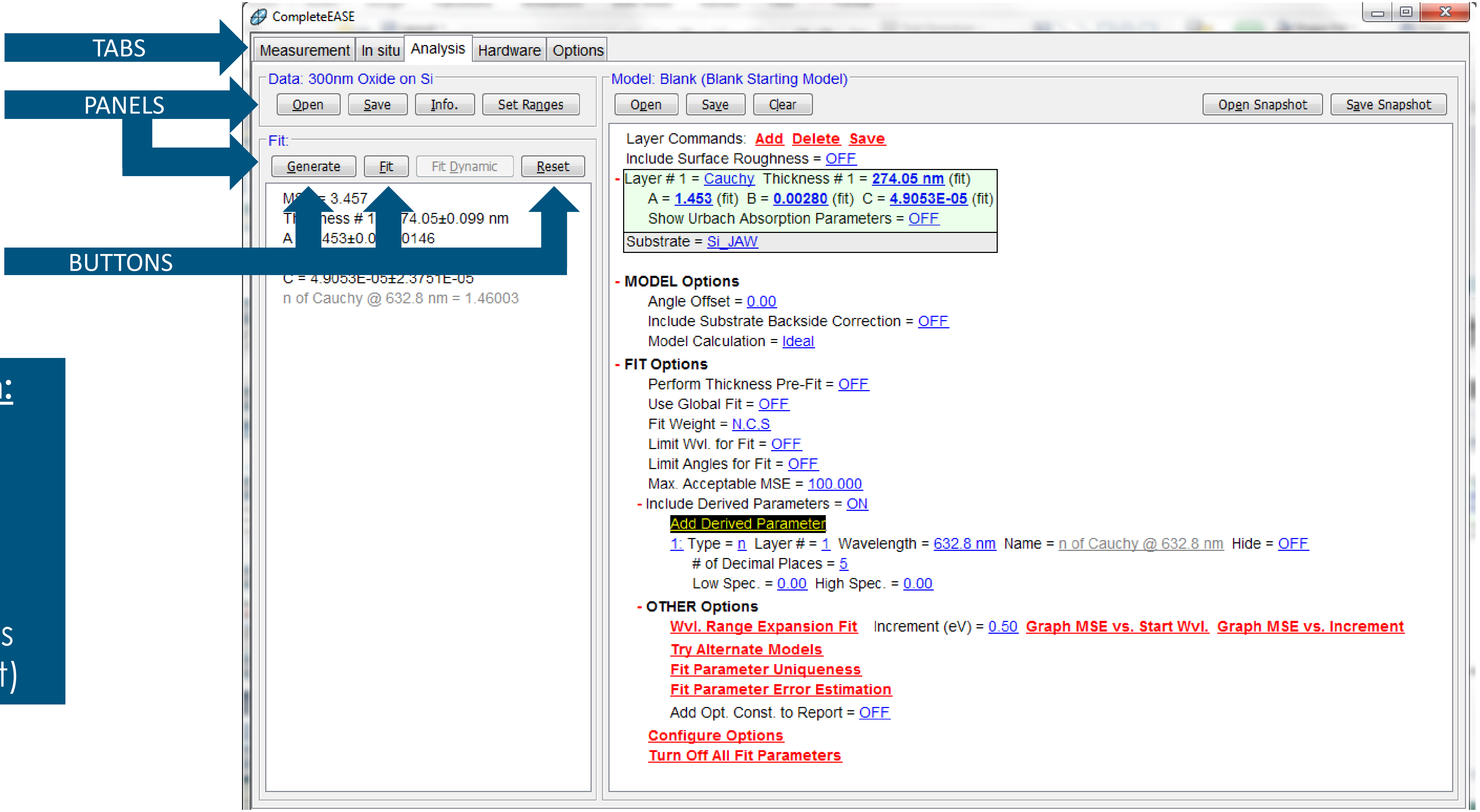
Break!

J.A. Woollam

Ellipsometry Solutions

CompleteEASE Navigation

Terminology in CompleteEASE



Navigate With:

Tabs

Panels

Buttons

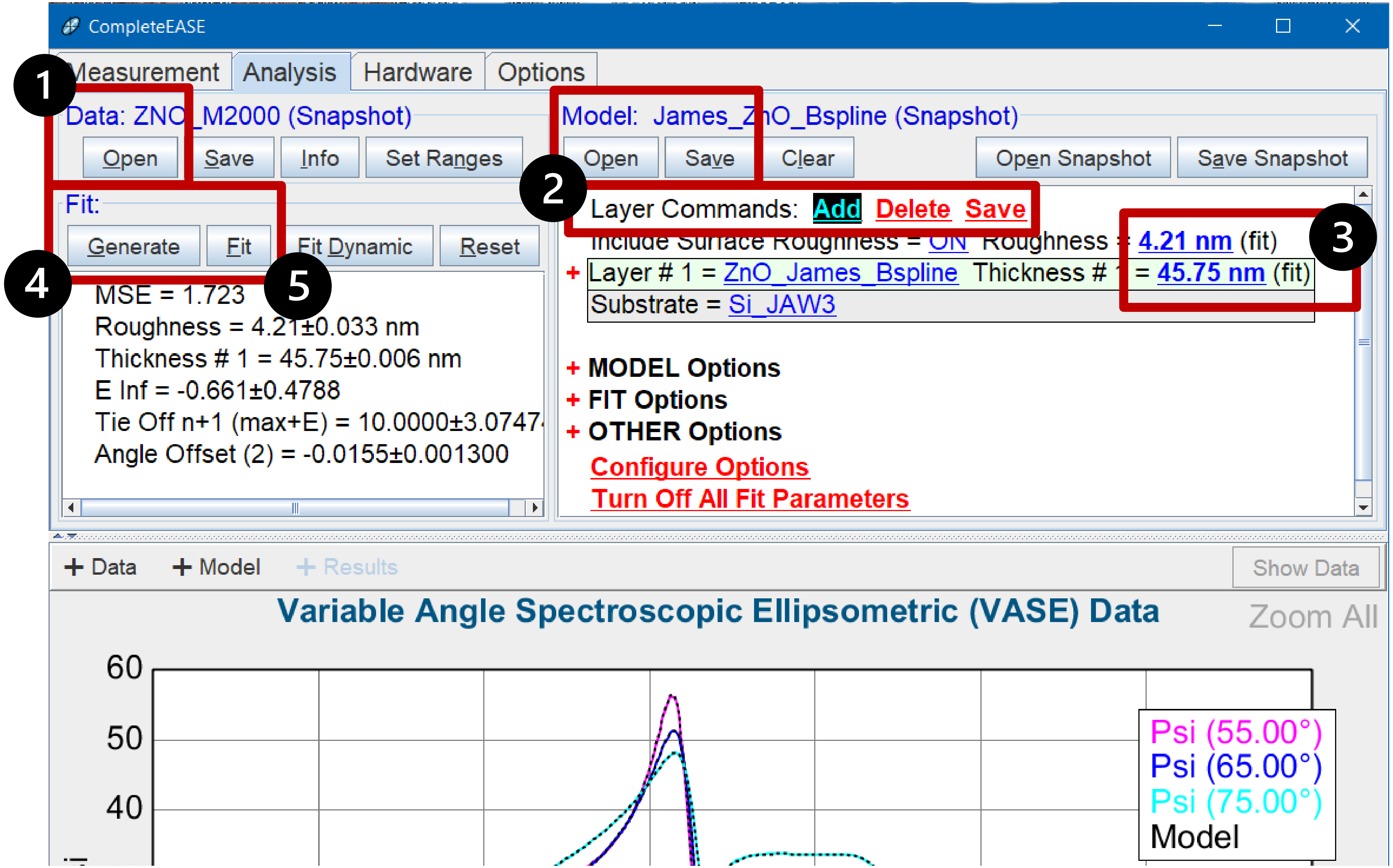
Mouse buttons (Left and Right)

Fitting Data - Analysis Tab

1. Open Data
2. Build Model
   - Open Model

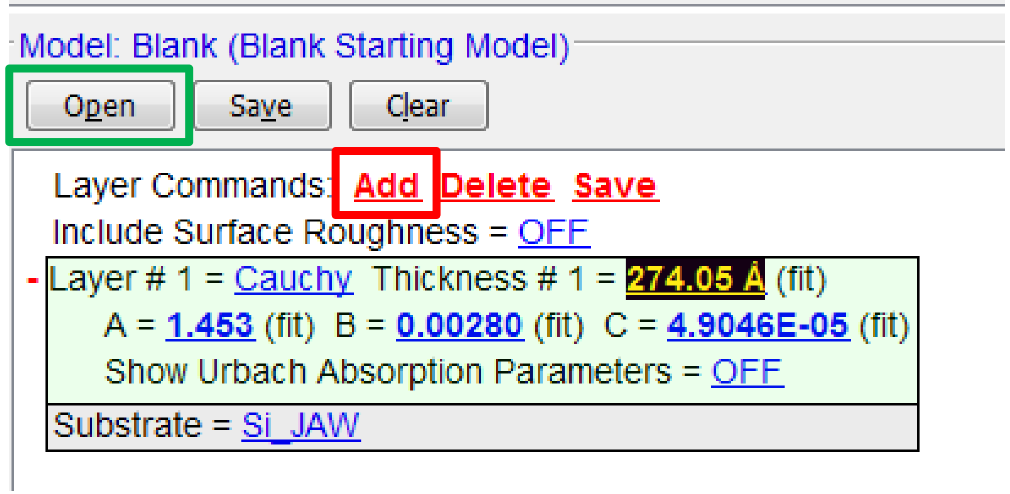
   Or

   - Add Layers
3. Designate Fit parameters
4. Generate
5. Fit

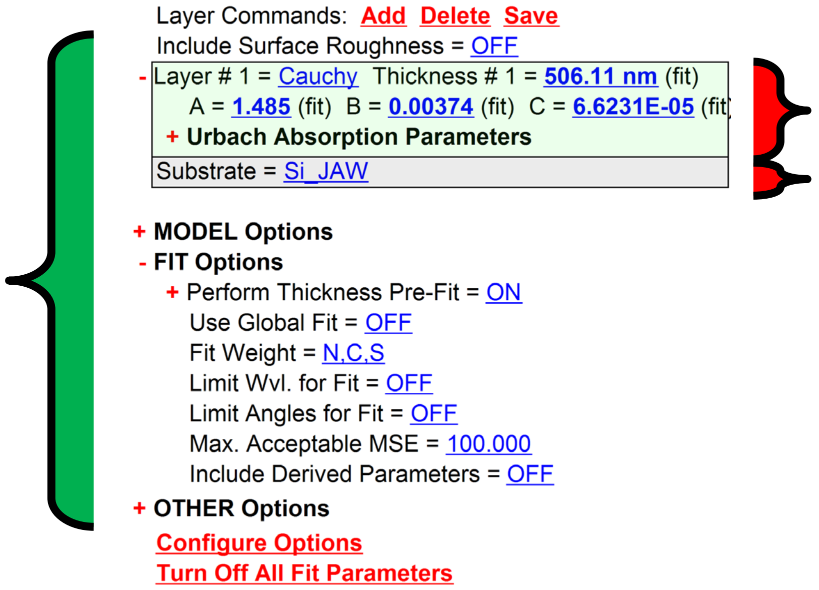


Mat vs. Mod Files

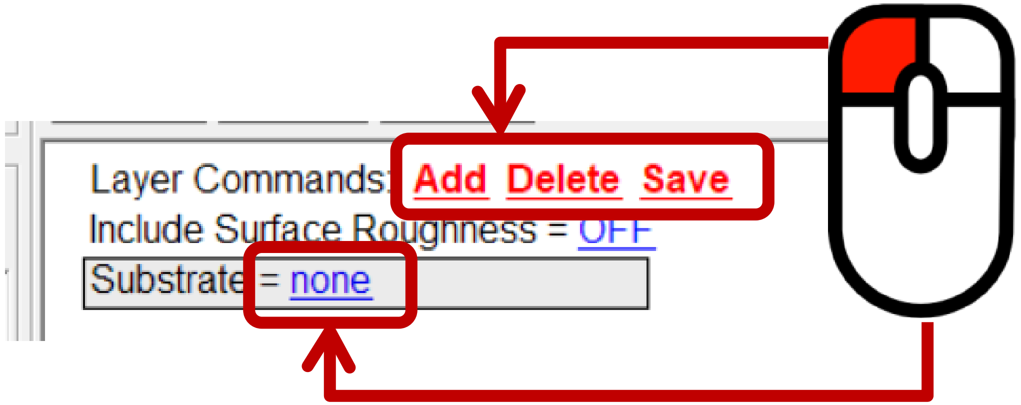
- Material File (.mat)
  Optical constants or parameters for a layer.
- Model (.mod)
  Layered structure with fit parameters and options to be considered during fitting.



Model



Materials (Layers)



Ctrl + Add to add as Top layer in a model

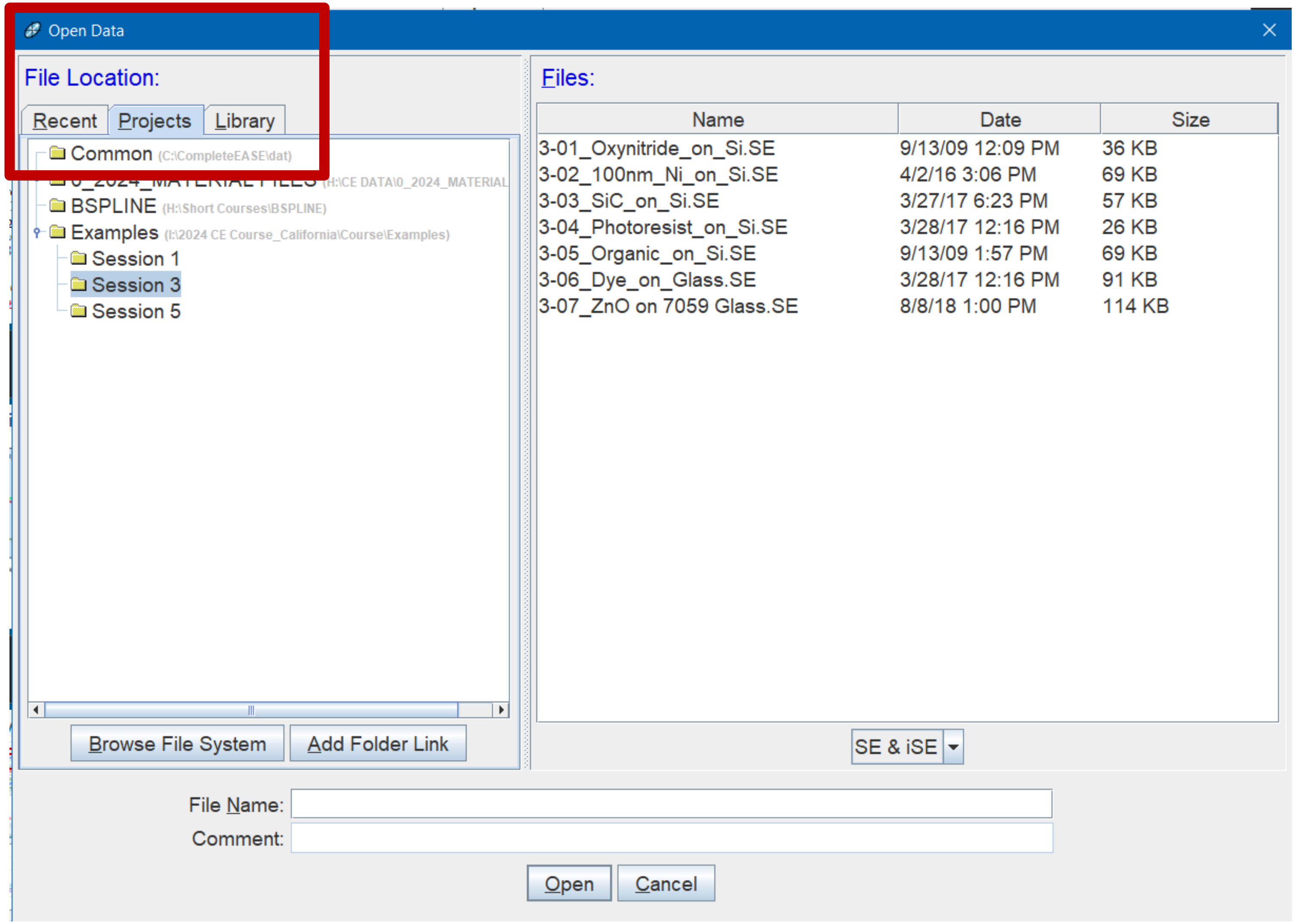
CompleteEASE File Dialog

Recent: Opened files and locations.

Projects: Folder links added by user.

Library: Special read-only folders located in the Common directory

COMMON Folder Locations
C:\CompleteEASE\MAT\
C:\CompleteEASE\MOD\
C:\CompleteEASE\DAT\

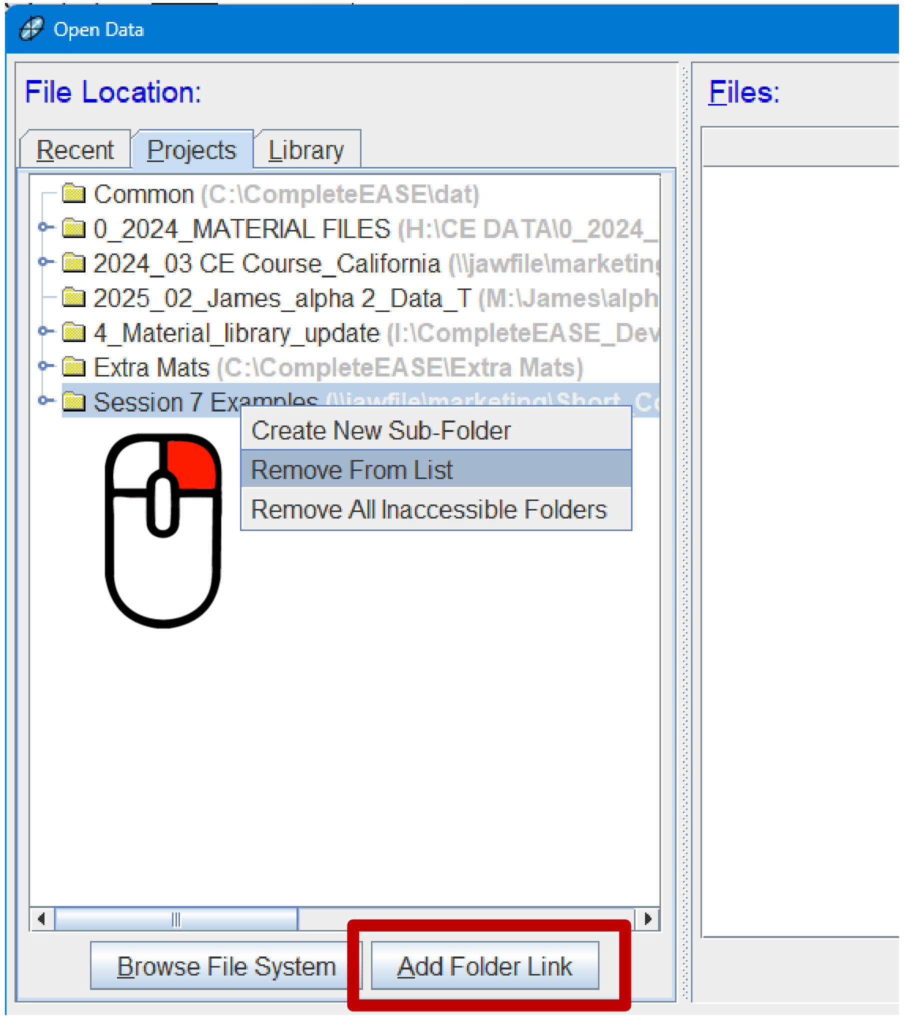


Folder Operations

- Folders in CE are "links"

Right-Click mouse options:

- **Add Folder Links** to Projects
- **Remove From List** breaks the "link" but does not delete the folder
- **Create New Sub-Folder**
- Subfolder levels are adjustable under Options\Edit Configuration



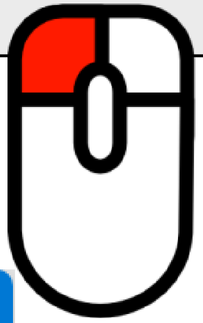
Use drag-and-drop to add folders from Windows Explorer to add to Projects list

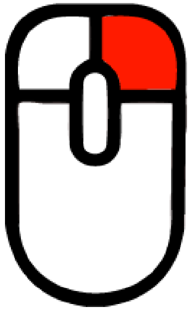
Turning on/off fit parameters

Roughness = **3.12 nm** (fit)

+ Layer # 1 = Cr2O3_James_VUV Thickness # 1 = **150.42 nm** (fit)

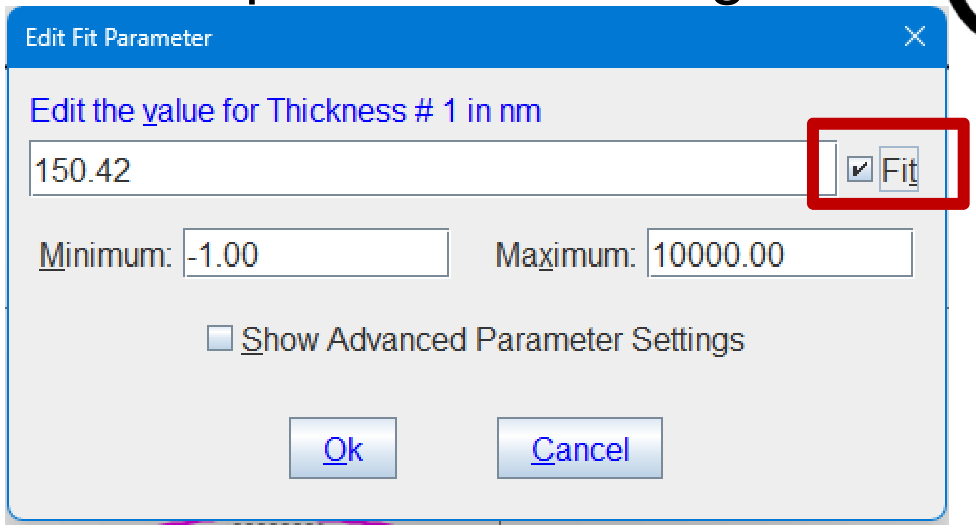
Substrate = Si_JAW3





Right-mouse button toggles fit on/off

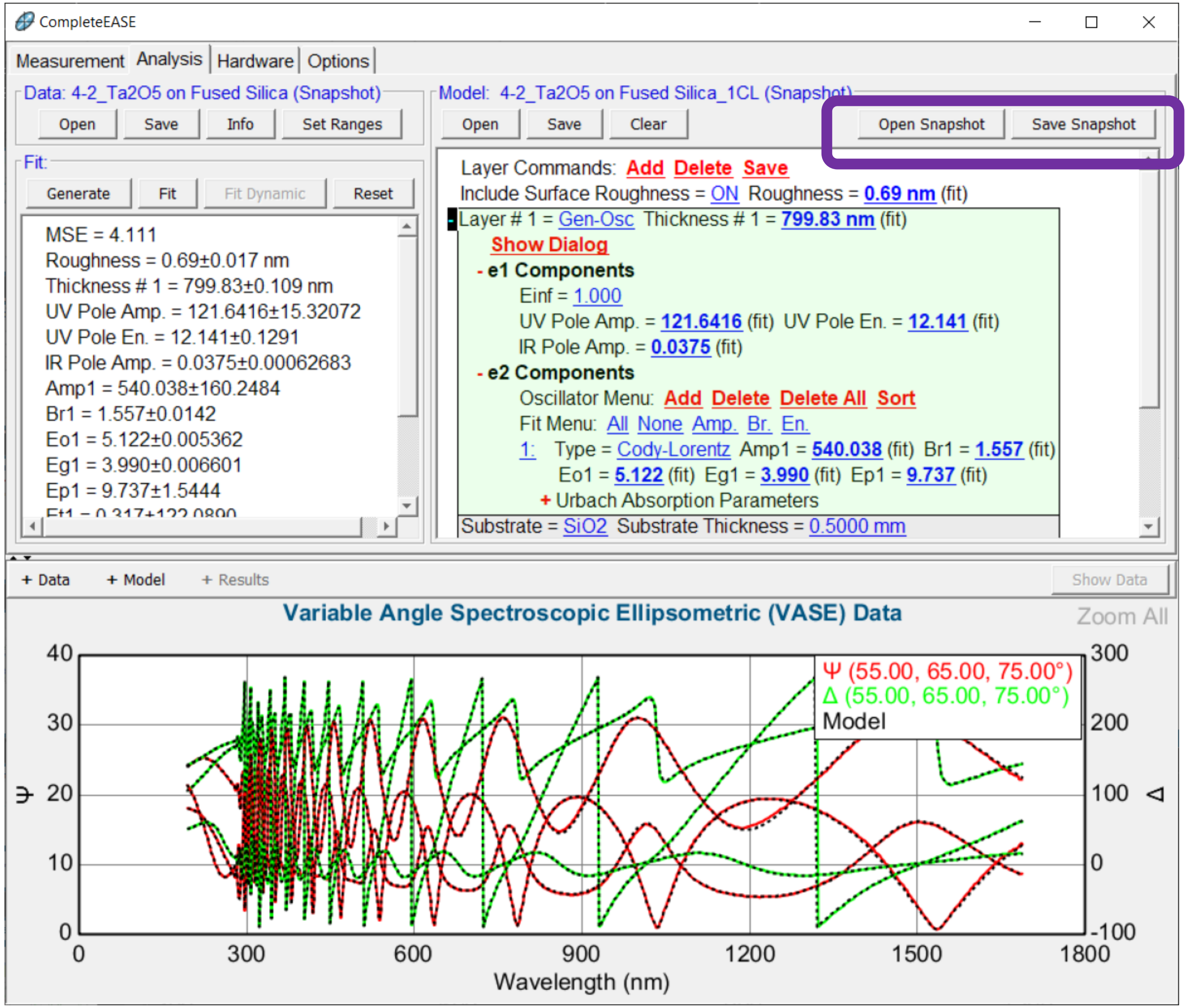
Left-mouse button opens “edit fit parameter” dialog



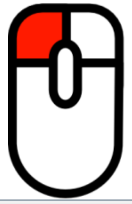
Snapshot Files (.SEsnap)

- Great way to share your results in a single file.
- NOT an image.
- Compresses the data, model & fit results together

.SEsnap file extension

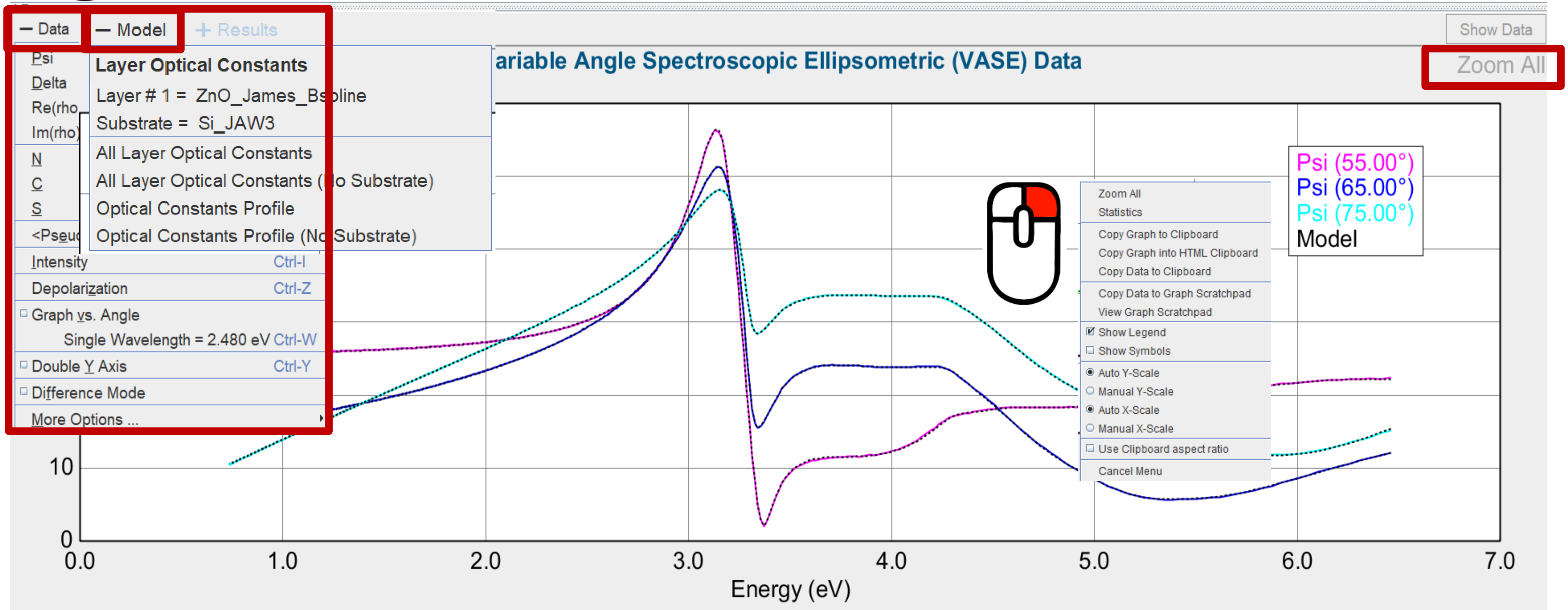


Graph Options

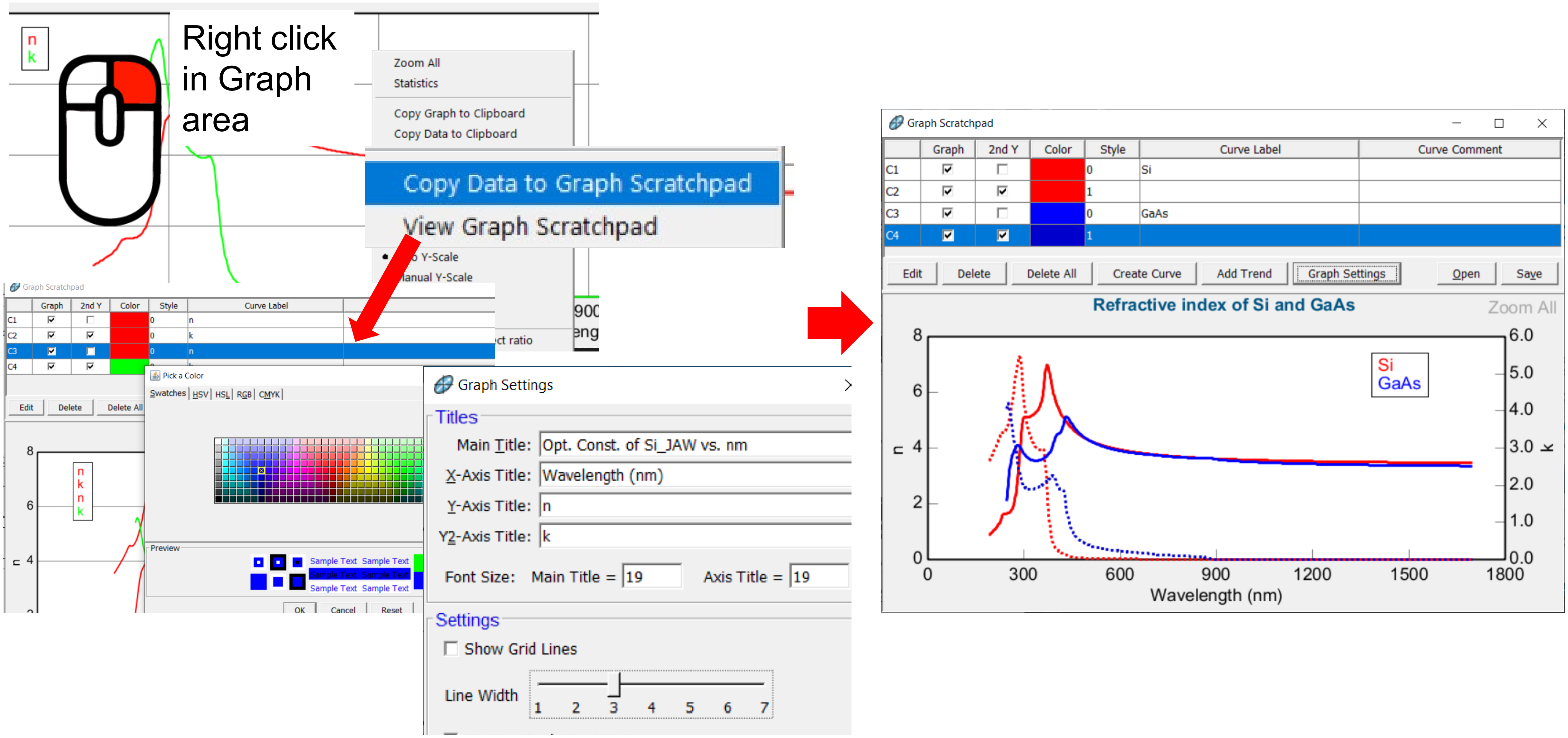


Left-click & drag the mouse to range-select wavelengths.

"Zoom All" (or double-click on graph) expands to full range.



Scratch Pad



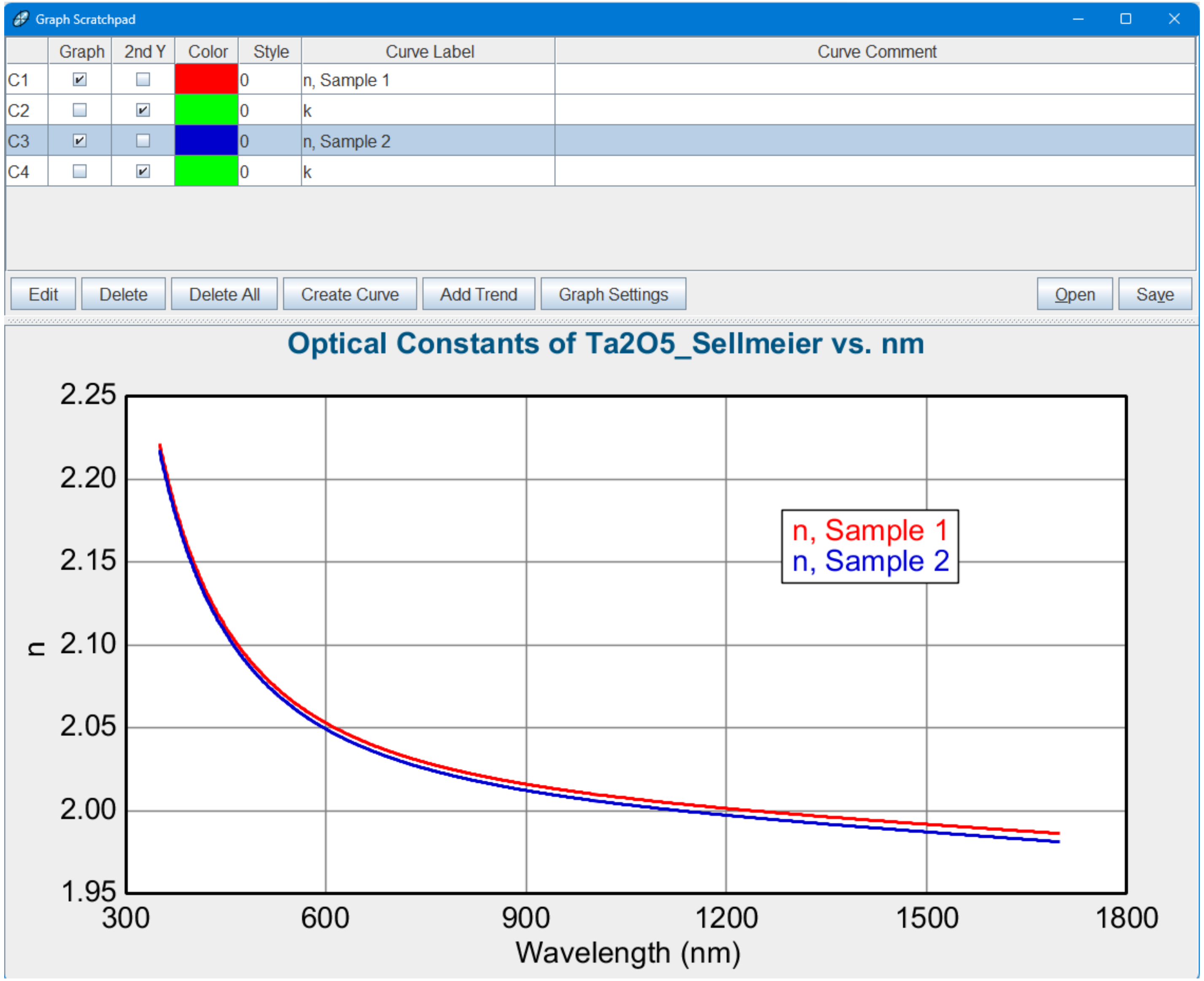
Right click in Graph area
Zoom All
Statistics
Copy Graph to Clipboard
Copy Data to Clipboard
Copy Data to Graph Scratchpad
View Graph Scratchpad
Graph Scratchpad
Graph
2nd Y
Color
Style
Curve Label
Curve Comment
C1
C2
C3
C4
Si
GaAs
Edit
Delete
Delete All
Create Curve
Add Trend
Graph Settings
Open
Save
Refractive index of Si and GaAs
Zoom All
Wavelength (nm)
n
k
Pick a Color
Swatches
HSV
HSL
RGB
CMYK
Preview
Sample Text
OK
Cancel
Reset
Graph Settings
Titles
Main Title: Opt. Const. of Si_JAW vs. nm
X-Axis Title: Wavelength (nm)
Y-Axis Title: n
Y2-Axis Title: k
Font Size: Main Title = 19 Axis Title = 19
Settings
Show Grid Lines
Line Width

1-1: File Navigation

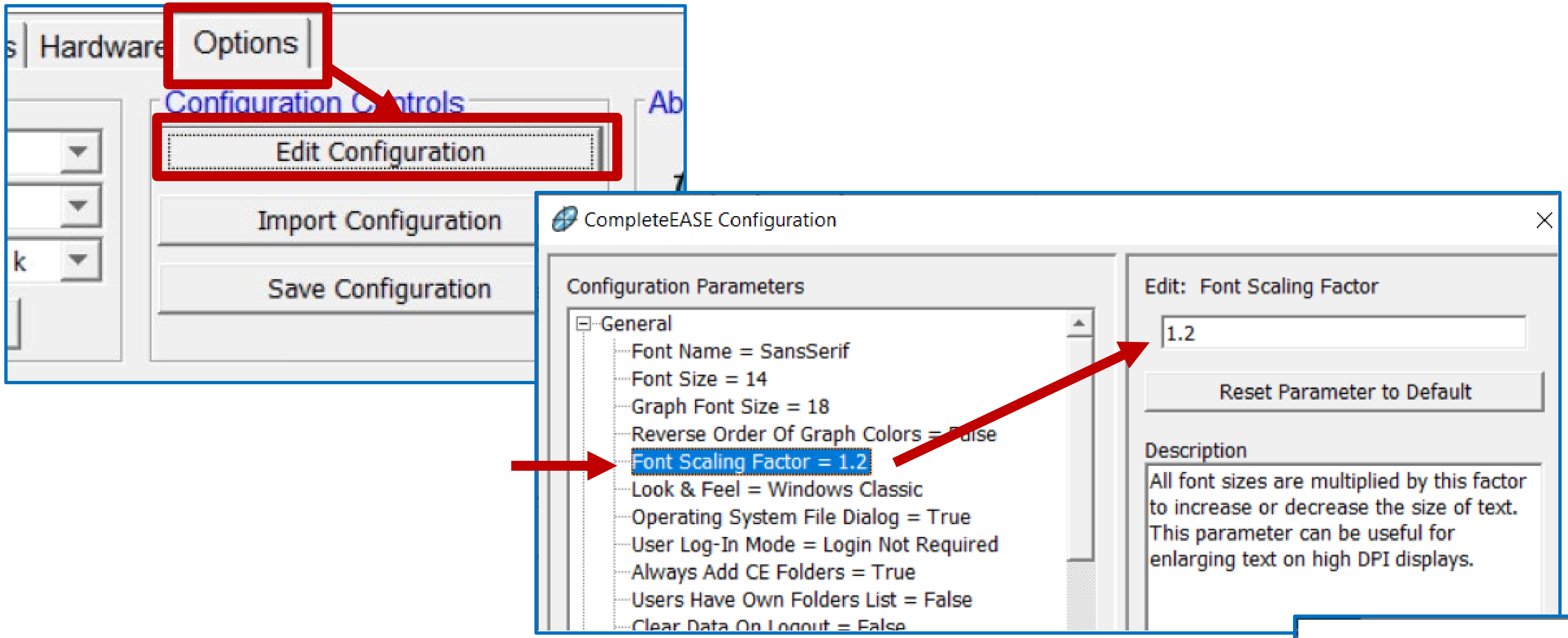
- Working with Data, Models, Materials, and Snapshots
  (FROM THE ANALYSIS TAB)

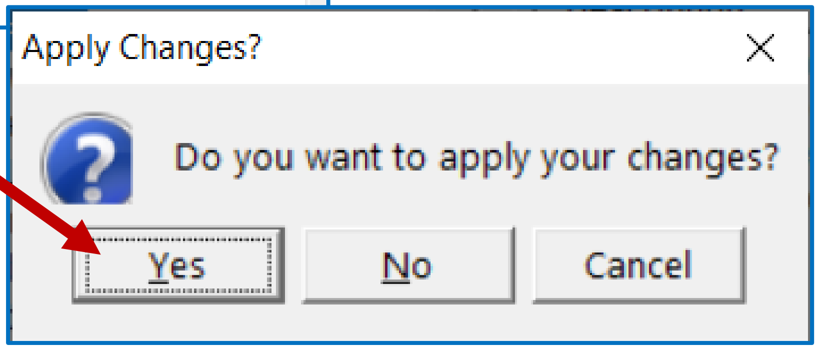
1. Add **Examples** and **Session 1** Folders to CompleteEASE “Projects”
   Open Data File: **1-01_Ta2O5_Sample1.SE**
2. Open Model: **Ta2O5 on FS.mod**
3. **Generate** and **Fit**
4. Save Snapshot: **Sample1.SESnap**
   - Copy optical constants to the Graph Scratchpad
5. Open Snapshot: **1-01_Ta2O5 on FS_Sample2.Sesnap**
   - Copy optical constants to the Graph Scratchpad (Compare results)

1-1: Ta2O5 on FS - RESULTS



Change Display on High-Res Monitors





- Restart CompleteEASE to make the changes

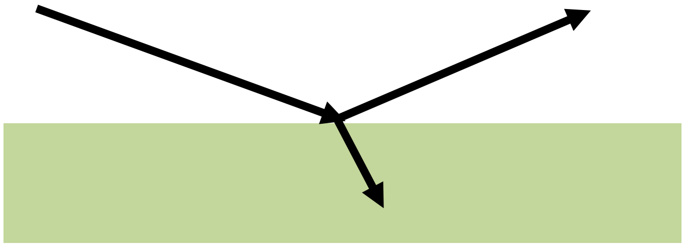
J.A. Woollam

Ellipsometry Solutions

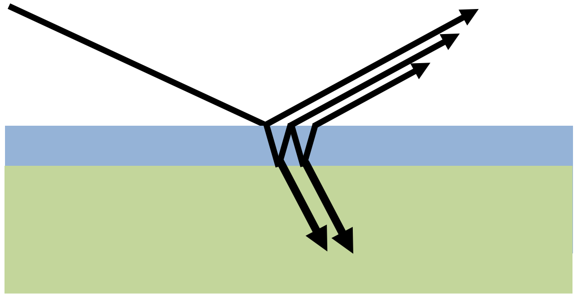
Crystalline Semiconductors

What are we measuring?

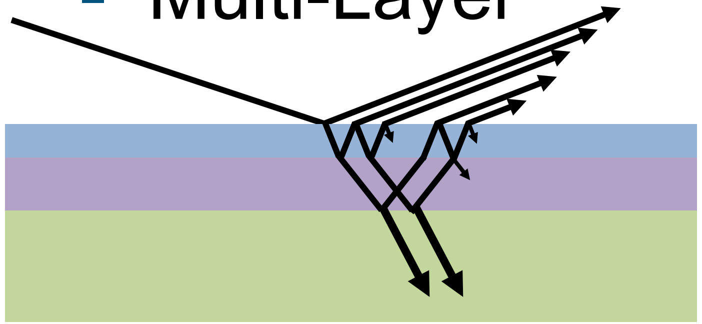
- Substrate



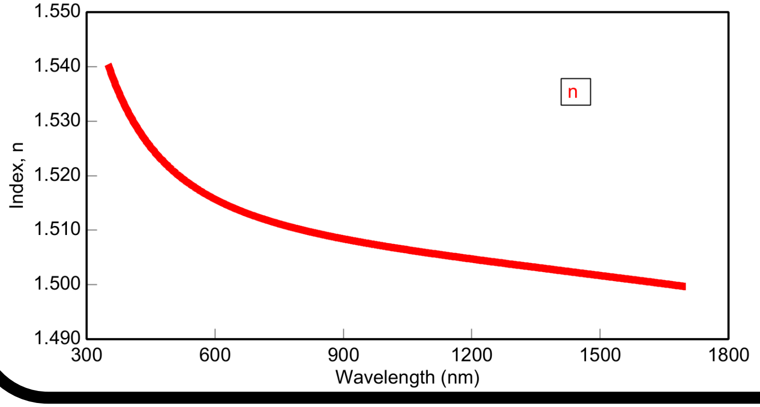
- Single-Layer



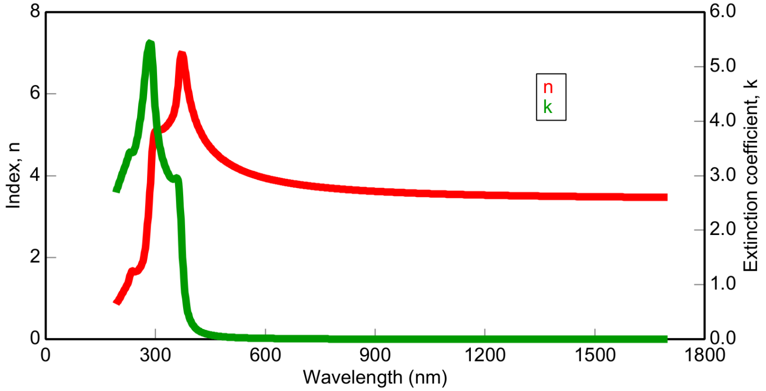
- Multi-Layer



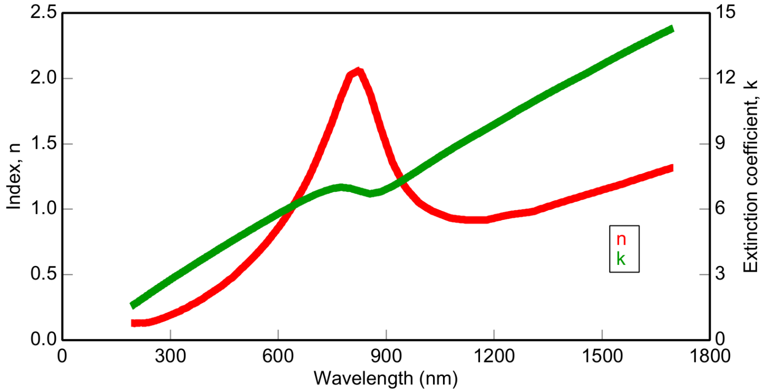
Dielectrics:
Glass, plastic, sapphire, SiC …



Semiconductors:
Si, GaAs, InP, Ge…



Metals:
Al, Au, Cu, Ni, Pt,…



Semiconductor Substrates

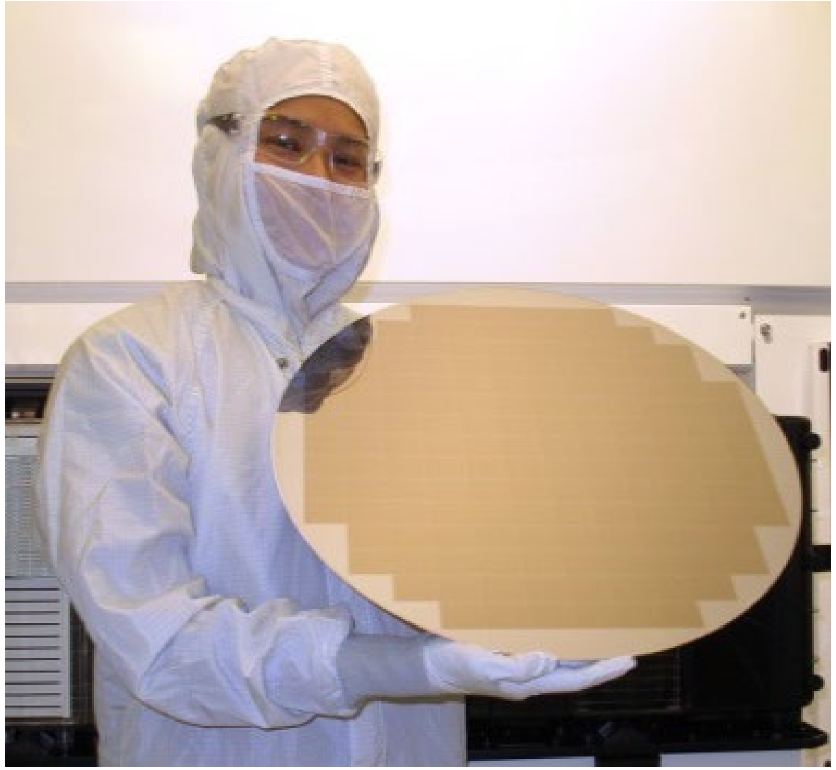
- Use library optical constants – no fitting needed
- The only fit parameter is the native oxide thickness

Include Surface Roughness = OFF

Layer # 1 = NTVE_JAW	Thickness # 1 = **10.00 Å** (fit)
Substrate = Si_JAW	

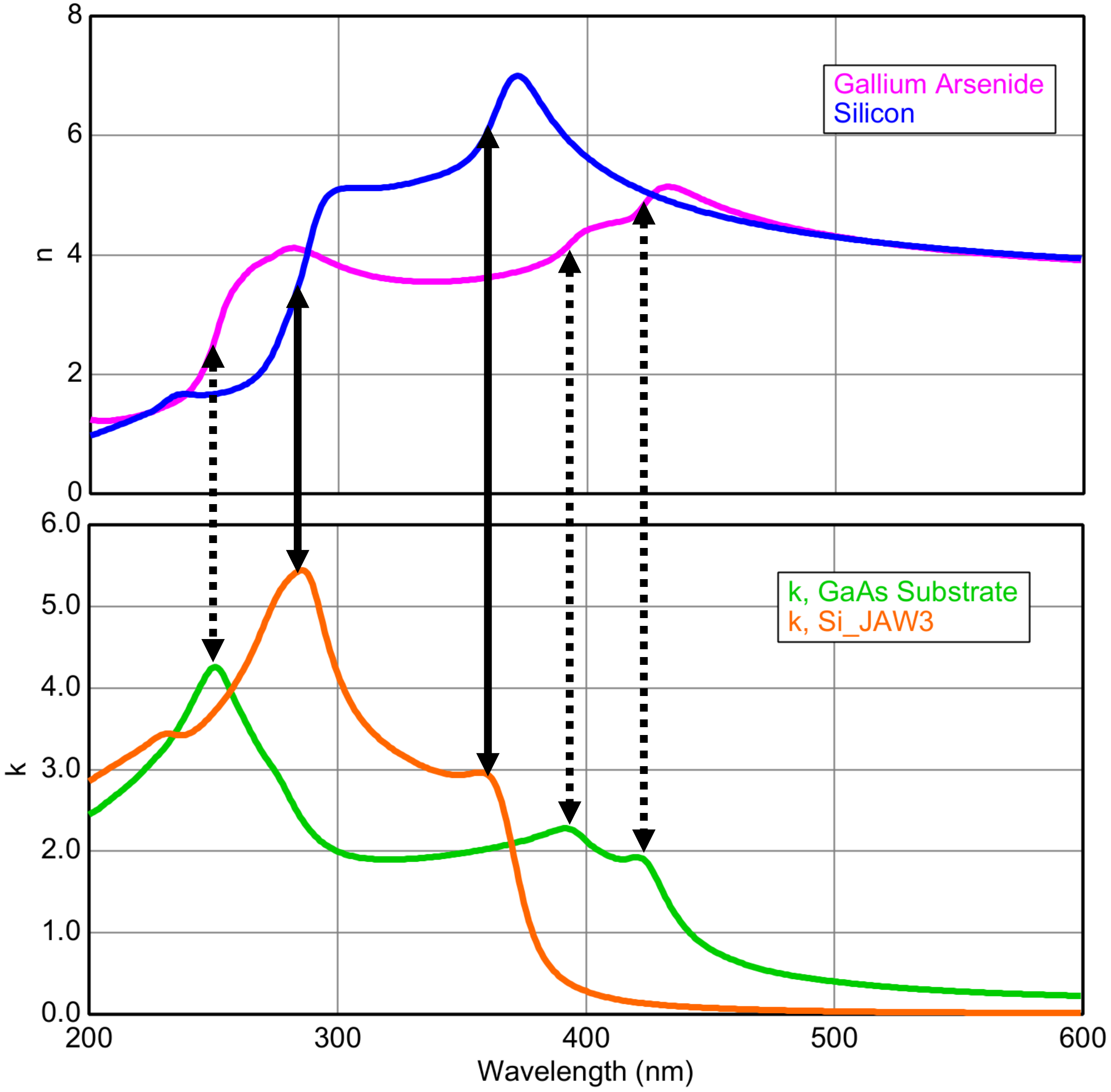
Semiconductor Substrates

- Substrates are crystalline – they have well-known optical constants.
- Consistent from wafer-to-wafer in UV-NIR region
- Doping must be extreme to affect UV-NIR optical constants
- Thin oxide forms quickly but stabilizes at thickness from 1 to 3 nm (typical)

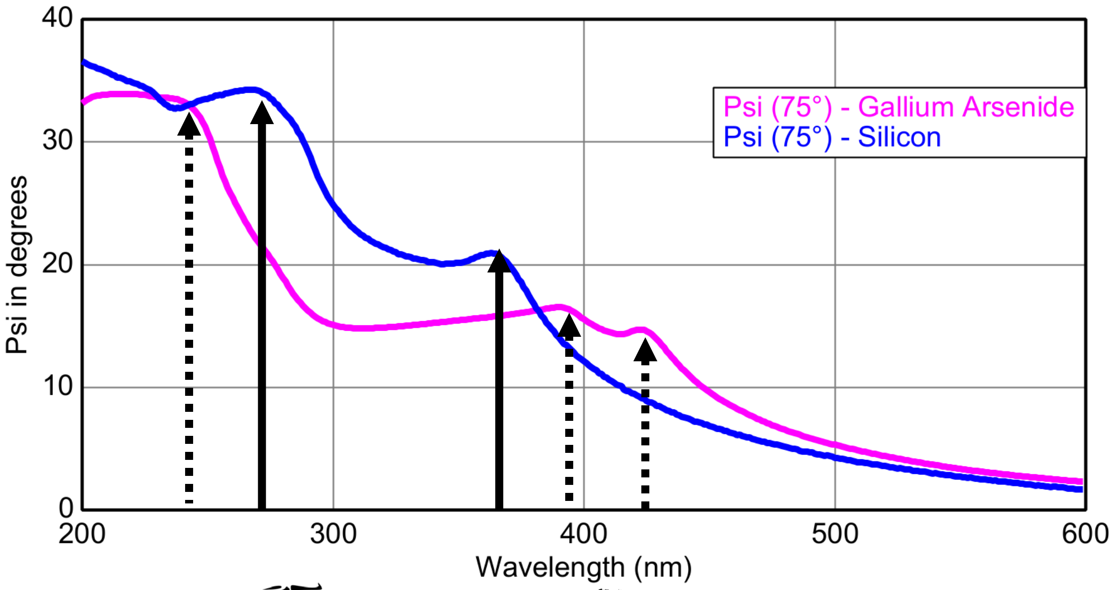


WATCH OUT!
Double-side polished wafers will have "strange" behavior in the near infrared (E below bandgap)

Optical Constant Features – Crystalline Semiconductors

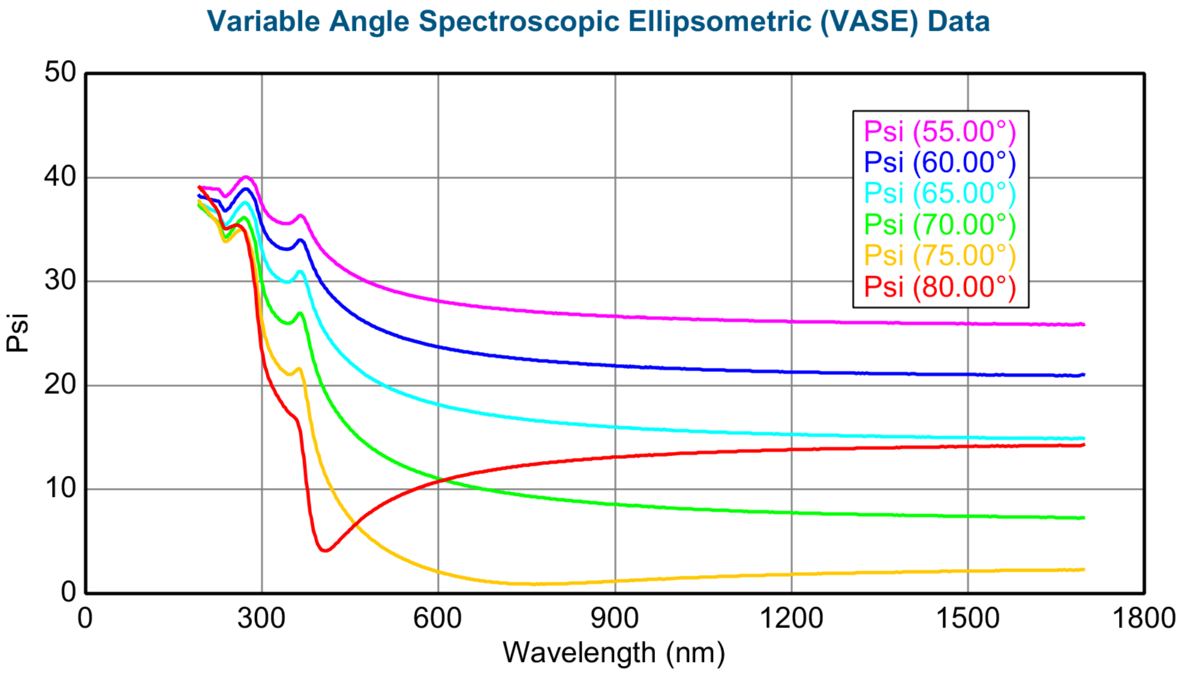


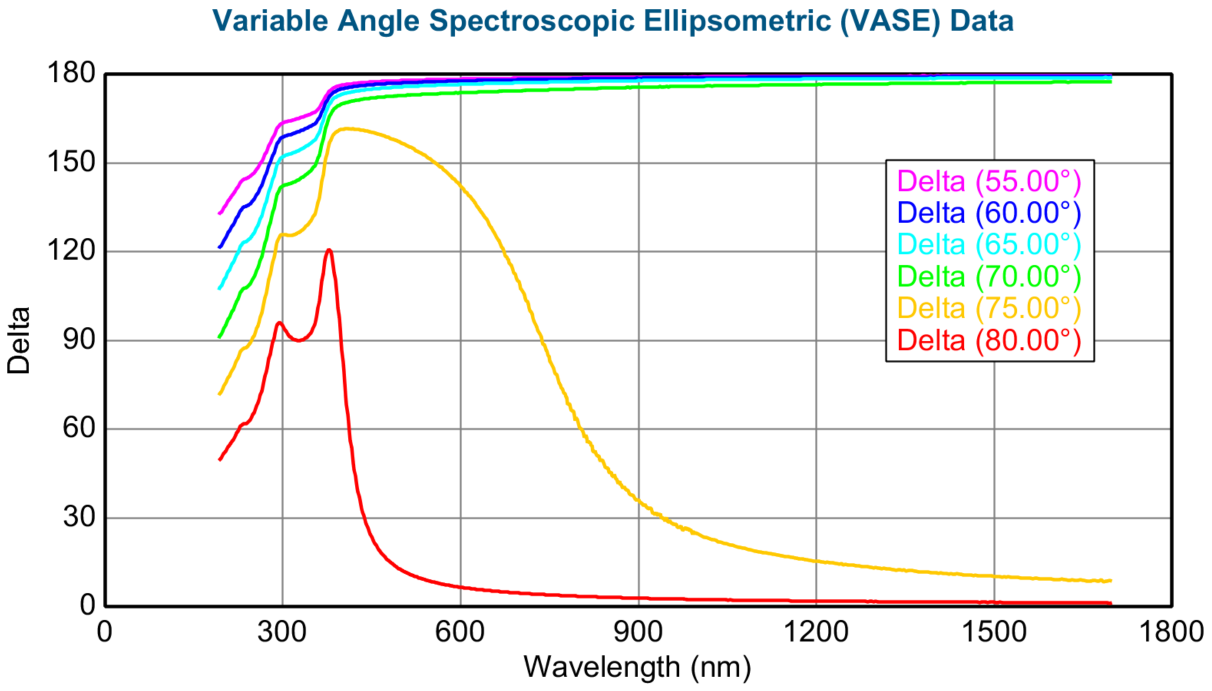
Data features appear at “critical points” where the semiconductor absorbs light (very specific energies)



Semiconductor Substrates – Data Features

- Ψ mimics optical constants, data features (bumps) form a "fingerprint" for semiconductor (related to electronic transitions)
- Δ near 0° or 180° except when absorbing or surface layer.





Semiconductor Substrates – Strategy

1. Build Model with Semiconductor Optical Constants from Library*.
2. Add native oxide from Library*.
3. Fit the Oxide Thickness.

*Semiconductor Folder holds optical constants for both semiconductors and native oxides.

Layer Commands: **Add** **Delete** **Save**

Include Surface Roughness = OFF

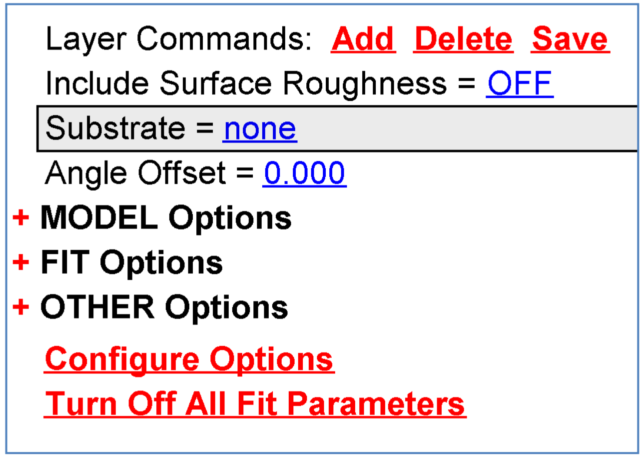
Layer # 1 = NTVE_JAW	Thickness # 1 = **10.00 Å** (fit)
Substrate = Si_JAW	

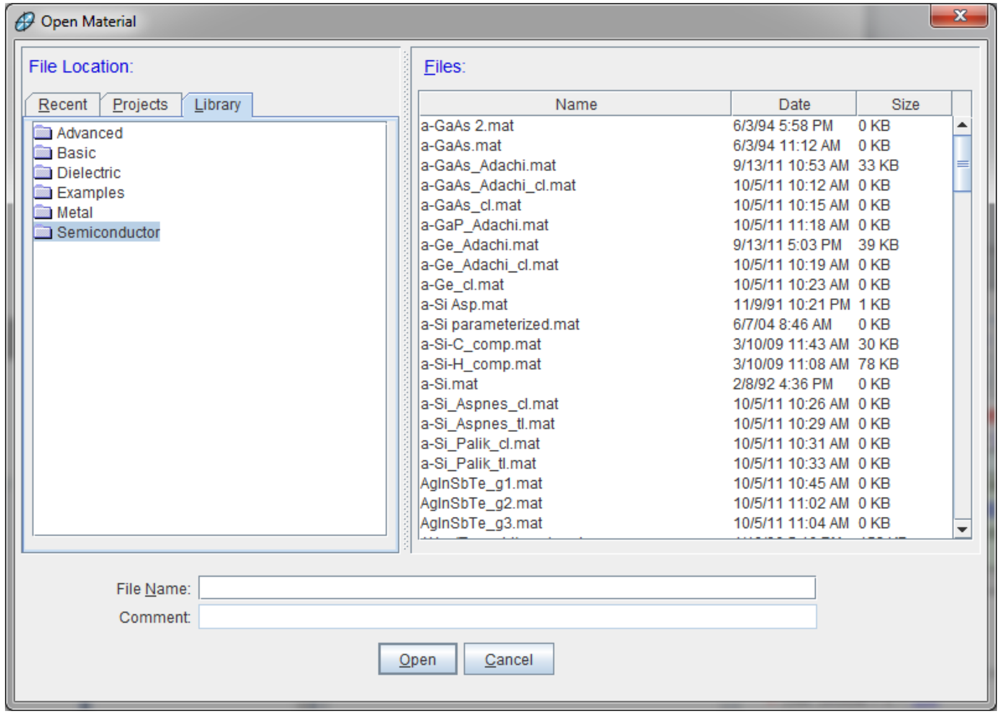
WARNING

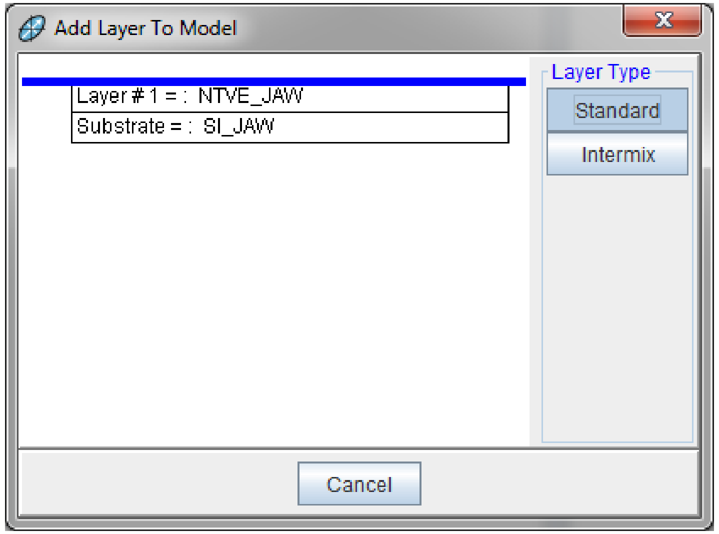
Don't fit surface roughness:
native oxide should take care of small roughness

Building a Model

1. Start from “BLANK” Model (Clear Model Button)
2. Click on Layer Name to replace Material File.
3. Press Add to add a layer to Model*.



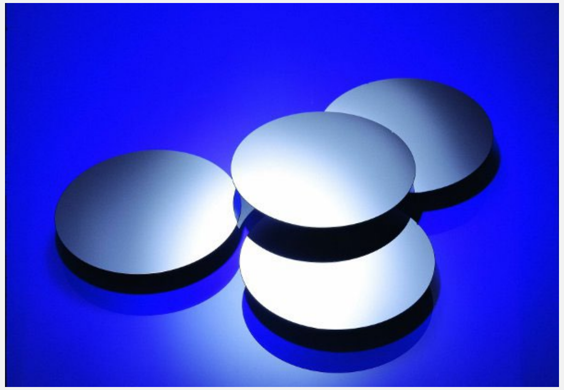




* short cut: CTRL+ Add adds layer on top of current stack without showing dialog

1-2: Bare Si Wafer

- Si wafers are the most common substrate used for ellipsometry data. Fortunately, they are also the easiest to work with!

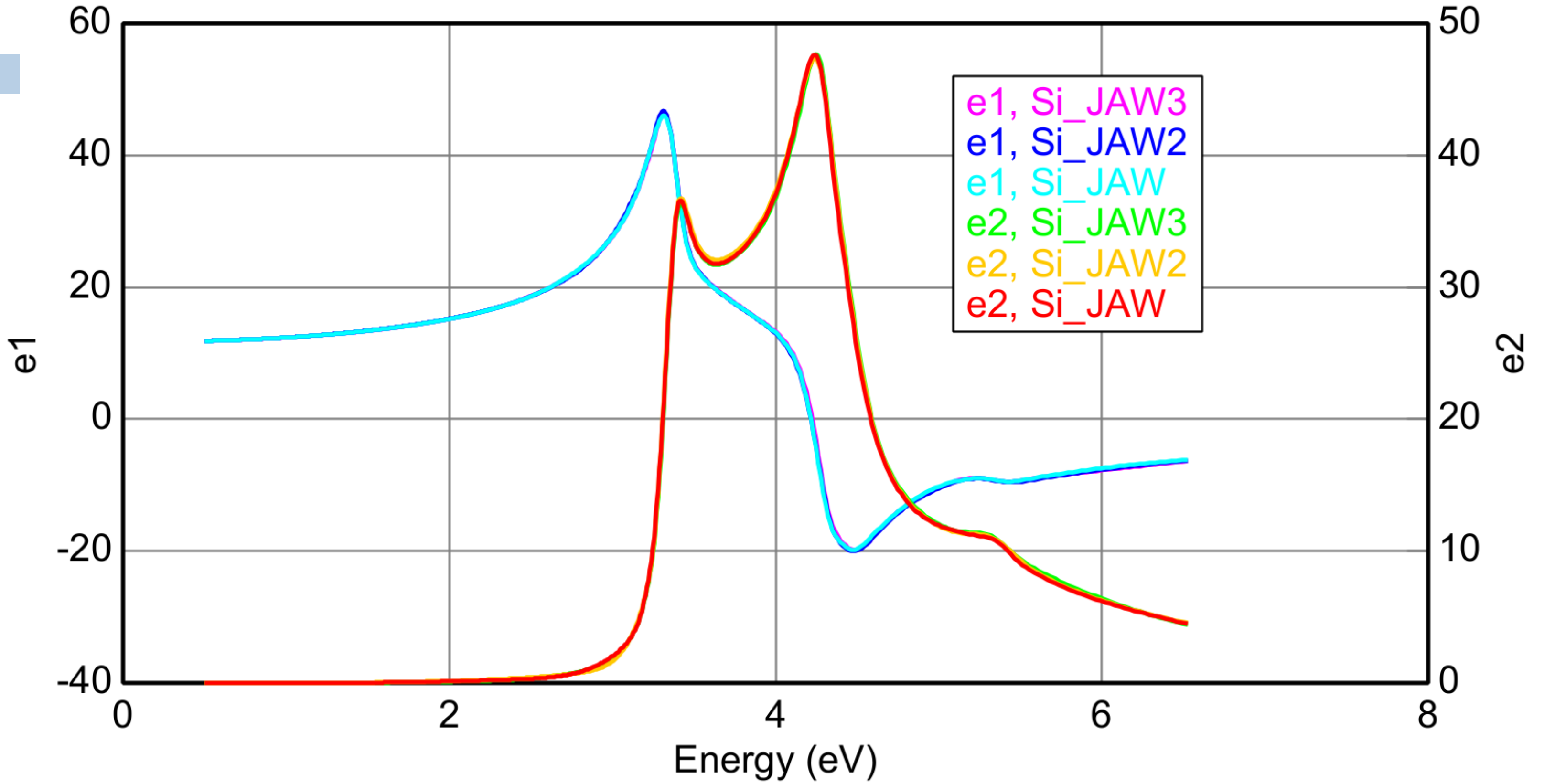


- Open Data: "1-2 Bare Si Wafer.SE"
- Start from "Blank" Model.
  - Add **Si_JAW.mat** for the substrate
  - Add **Ntve_JAW.mat** for the surface oxide.
- Enter a guess for oxide thickness.
- Right-Click on thickness to turn ON "fitting" for this parameter.
- Generate, then Fit.

Why so many Silicon Material files?

– Si_JAW.mat – great from 190 nm to 1700 nm, but "old" (created in 1998)
– Si_JAW2.mat – extended to VUV wavelengths
– Si_JAW3.mat – extended to both VUV and mid-IR wavelengths

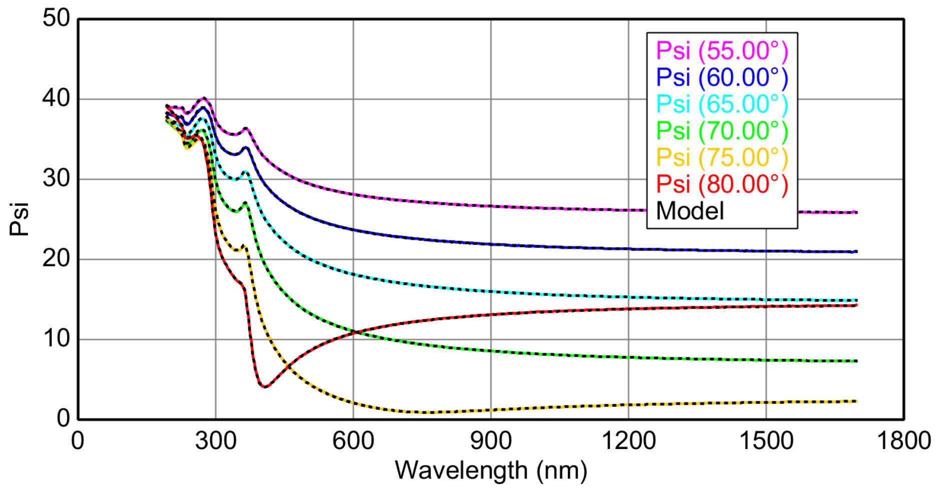
Si_JAW.mat	3/31/98 2:29 PM
Si_JAW2.mat	4/2/10 9:46 AM
Si_JAW3.mat	2/14/18 10:44 PM
Si_Temp_JAW(-25_500C).mat	2/19/18 12:21 PM
Si.mat	10/19/94 7:05 PM



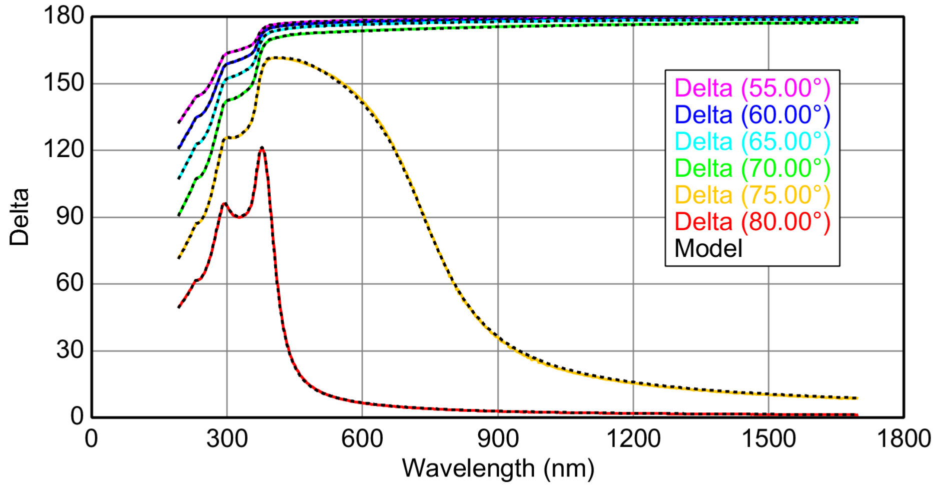
1-2: Bare Si Wafer - RESULTS

Experimental Data Fits

Variable Angle Spectroscopic Ellipsometric (VASE) Data



Variable Angle Spectroscopic Ellipsometric (VASE) Data



Resulting Thickness

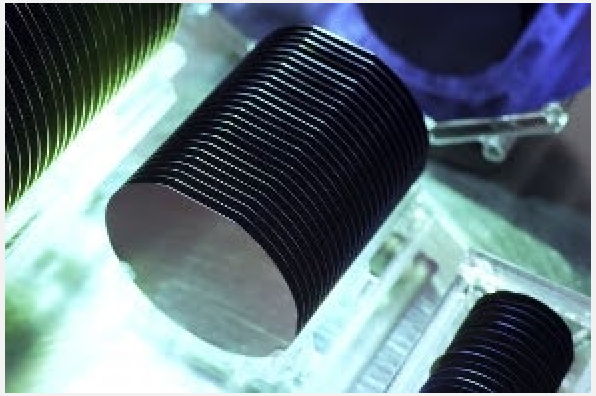
MSE = 1.297

Thickness # 1 = 16.71 ± 0.012 Å

Layer # 1 = NTVE_JAW	Thickness # 1 = **16.71 Å** (fi
Substrate = Si_JAW	

1-3, 1-4: Bare Semiconductor Wafers

- Build Model for each wafer.
- Determine native oxide thickness.

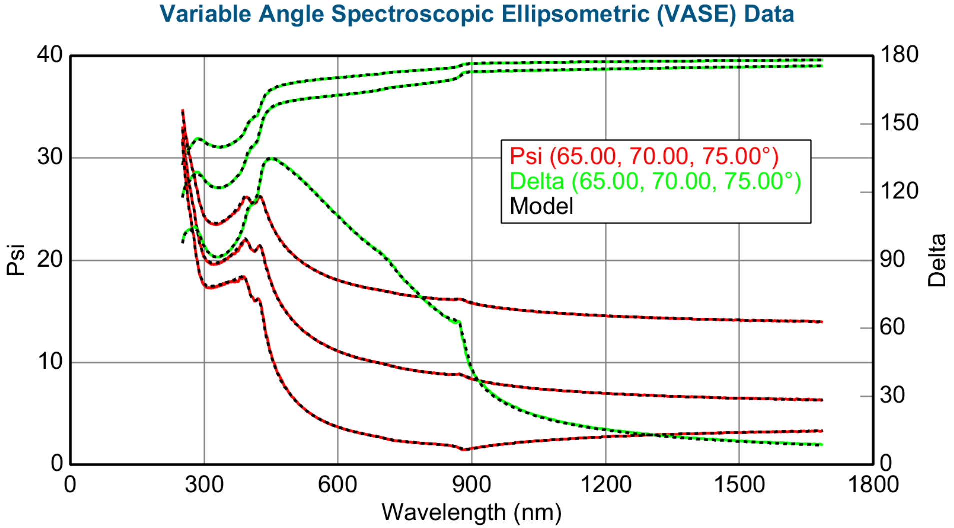


- "1-3 GaAs wafer.SE"
  - GaAs.mat, GaAs oxide.mat

- "1-4 InP wafer.SE"
  - InP.mat, InP oxide.mat

1-3, 1-4: Semiconductor wafers - RESULTS

GaAs:



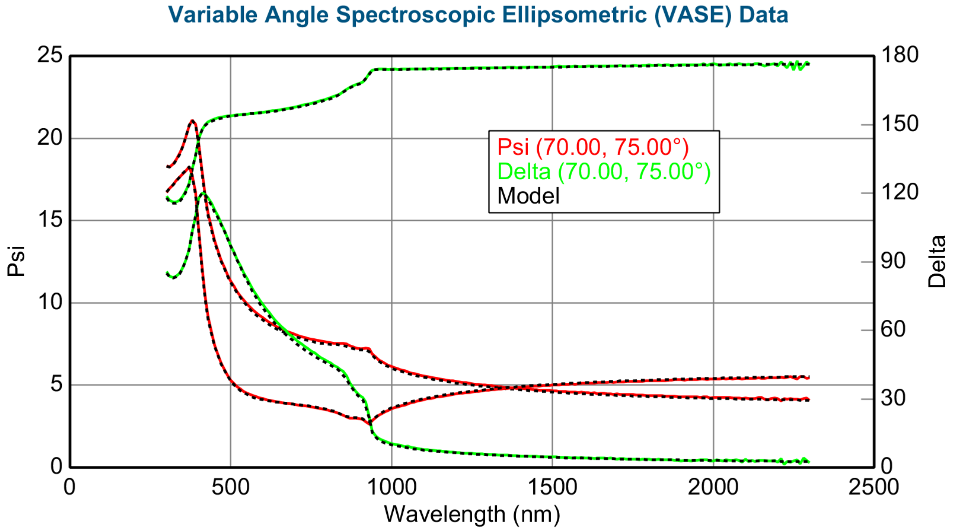
Thickness Results

MSE = 1.861

Thickness # 1 = 24.46 ± 0.025 Å

Layer # 1 = GaAs Oxide Thickness # 1 = **24.46 Å** (fit)
Substrate = GaAs

InP:



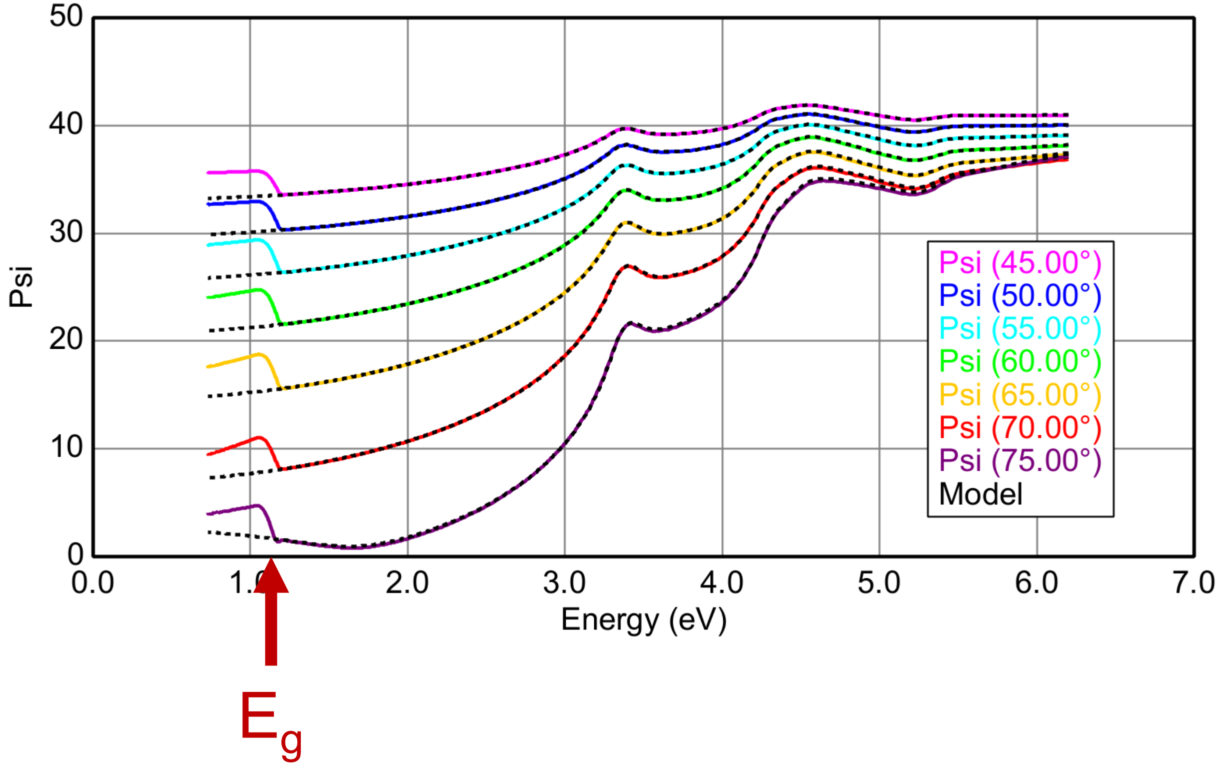
MSE = 1.844

Thickness # 1 = 20.78 ± 0.107 Å

Layer # 1 = InP Oxide Thickness # 1 = **20.78 Å** (fit)
Substrate = InP

Double-Side Polished Wafers

- Identifying data from double-side polished wafer:
  Data will show a "step" at the semiconductor bandgap.
- How to handle:
  - Exclude NIR when fitting
  - Roughen backside of substrate
  - Model "backside reflections"

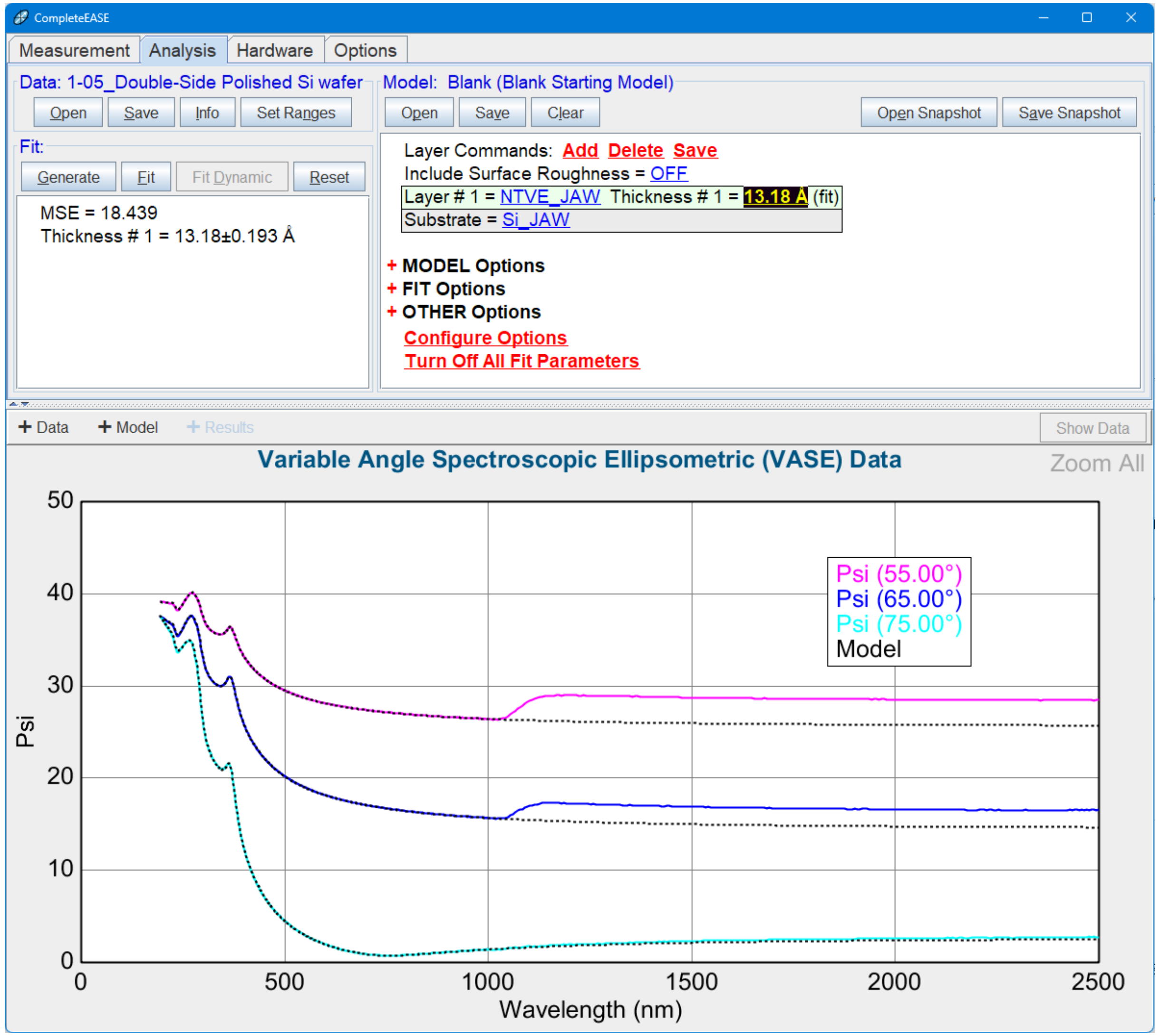


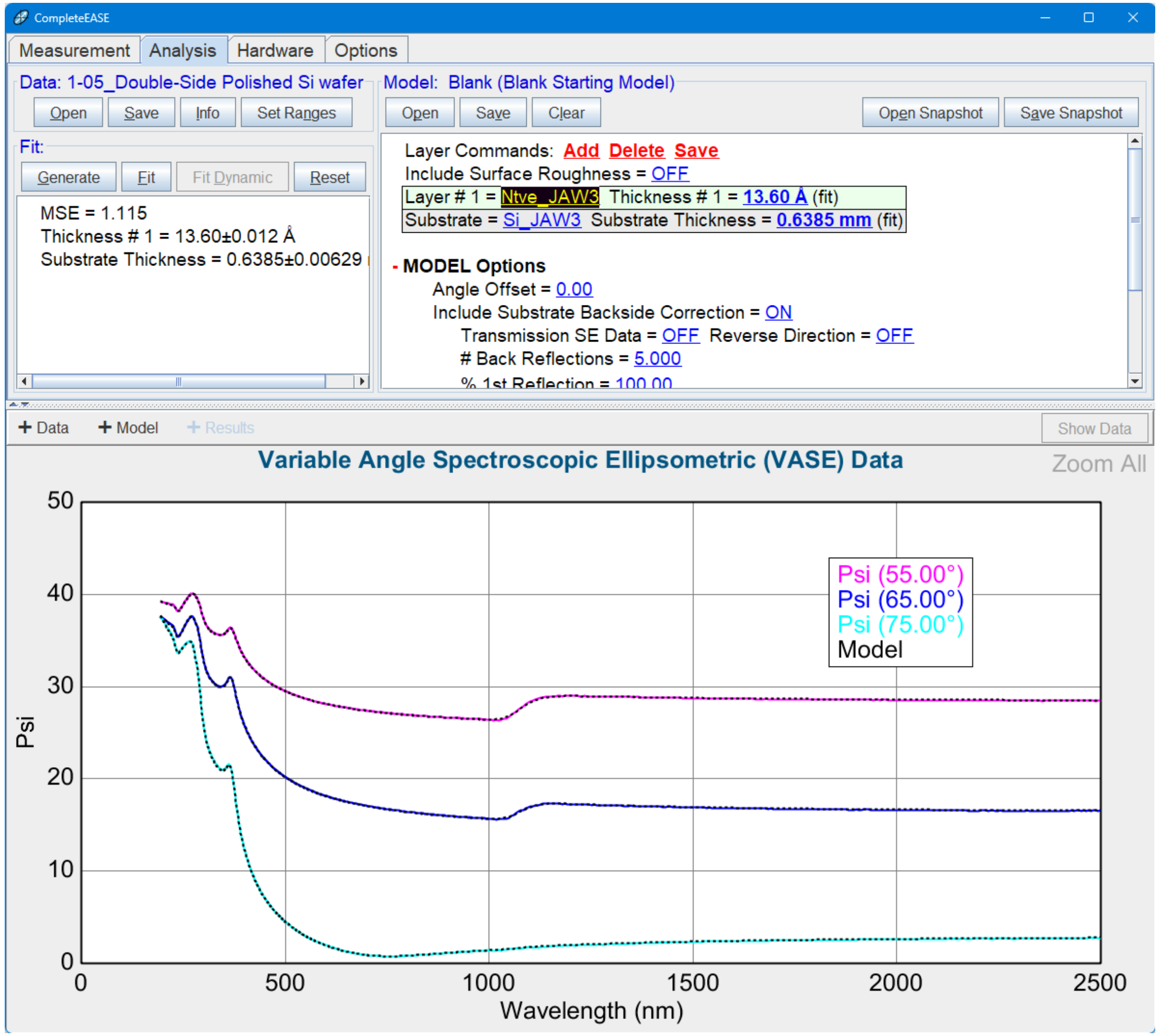
WARNING
What if there are films on the "back" side?

1-5: Double-side polished silicon (Extra credit)

- Demonstrate how to fit data from a double-side polished silicon wafer

1-5: dsp silicon - RESULTS





J.A. Woollam
Ellipsometry Solutions

Transparent Glass Substrates

Transparent (Glass) Substrates

- Measure “your” bare glass.
- Describe the index with **Cauchy** or **Sellmeier** – this should match the Ψ data.
- Add surface roughness to fit Δ

Roughness = **1.34 nm** (fit)

\- Substrate = Cauchy

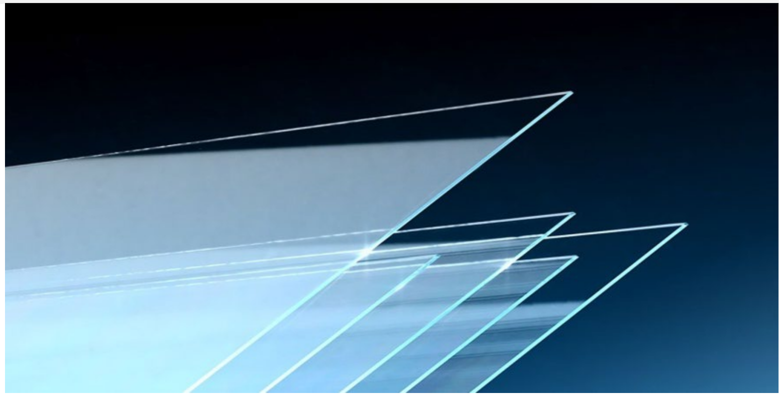
A = **1.504** (fit) B = **0.00496** (fit) C = **4.1073E-06** (fit)

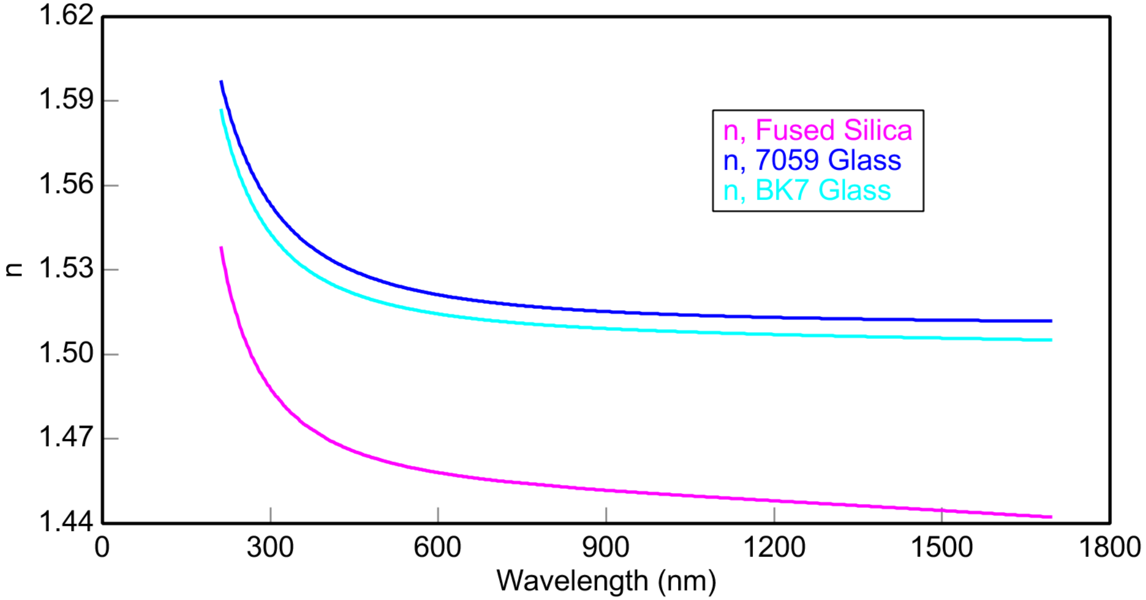
\+ **Urbach Absorption Parameters**

Glass Substrates

Key Points:

- Amorphous…
  - Index varies by “type” and “batch”.
  - Index is the same in all directions.
- Ψ provides index information.
- Δ is related to surface quality.

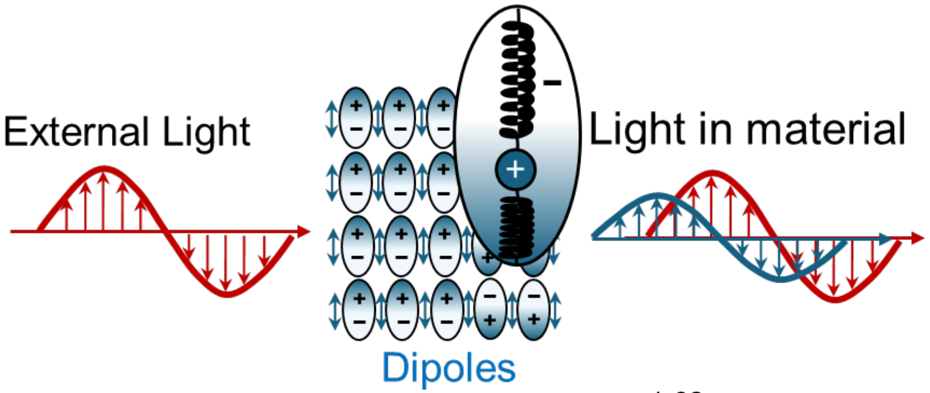


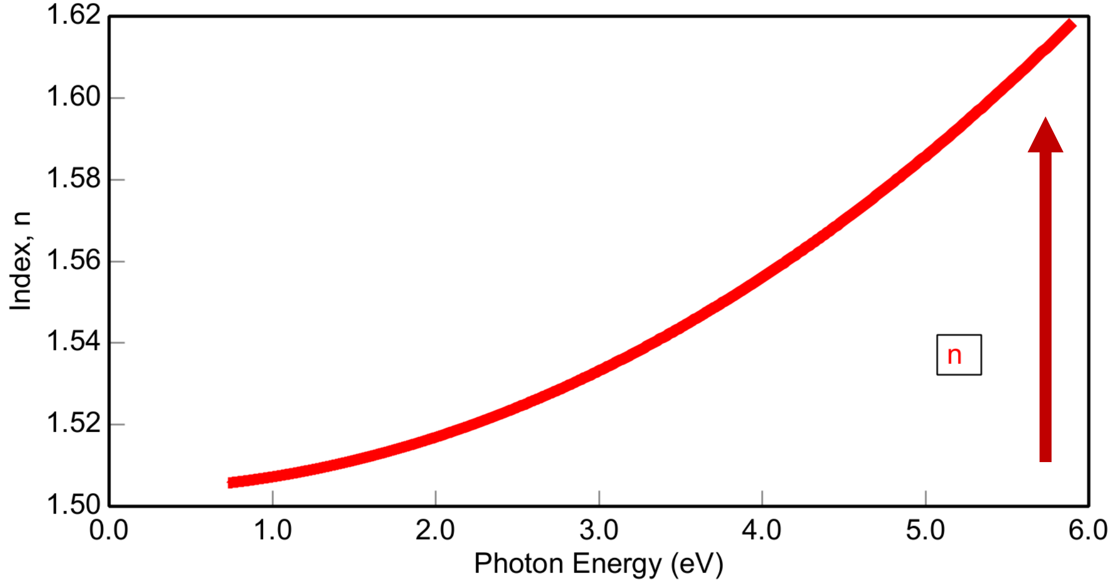


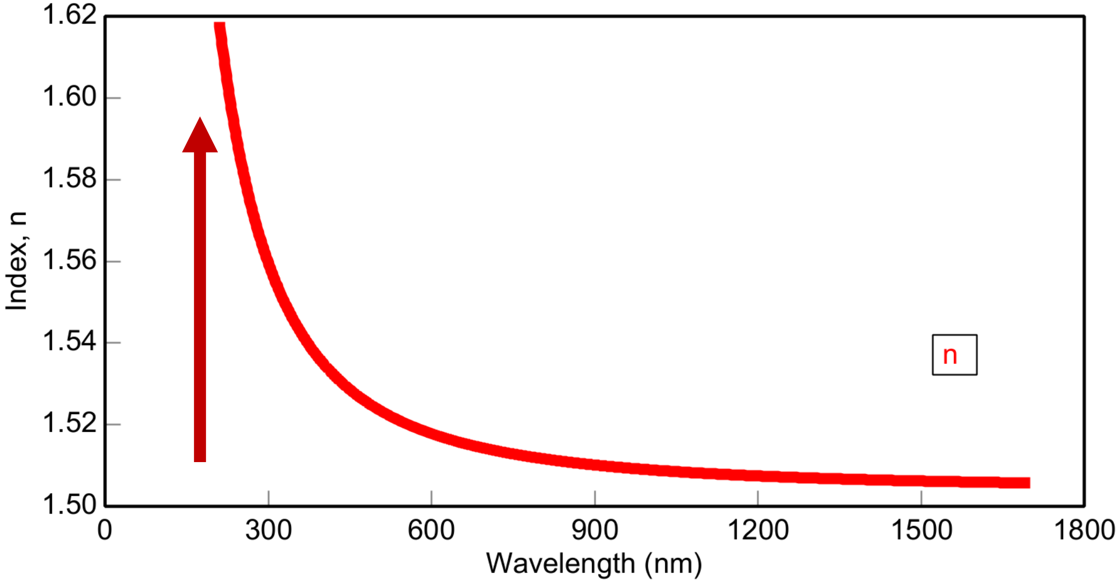
WATCH OUT!
Need to consider backside reflections since glass is transparent

Normal Dispersion

- Increasing the frequency (higher energy, shorter wavelengths) typically increases the dipole effects in the material (increases the index)



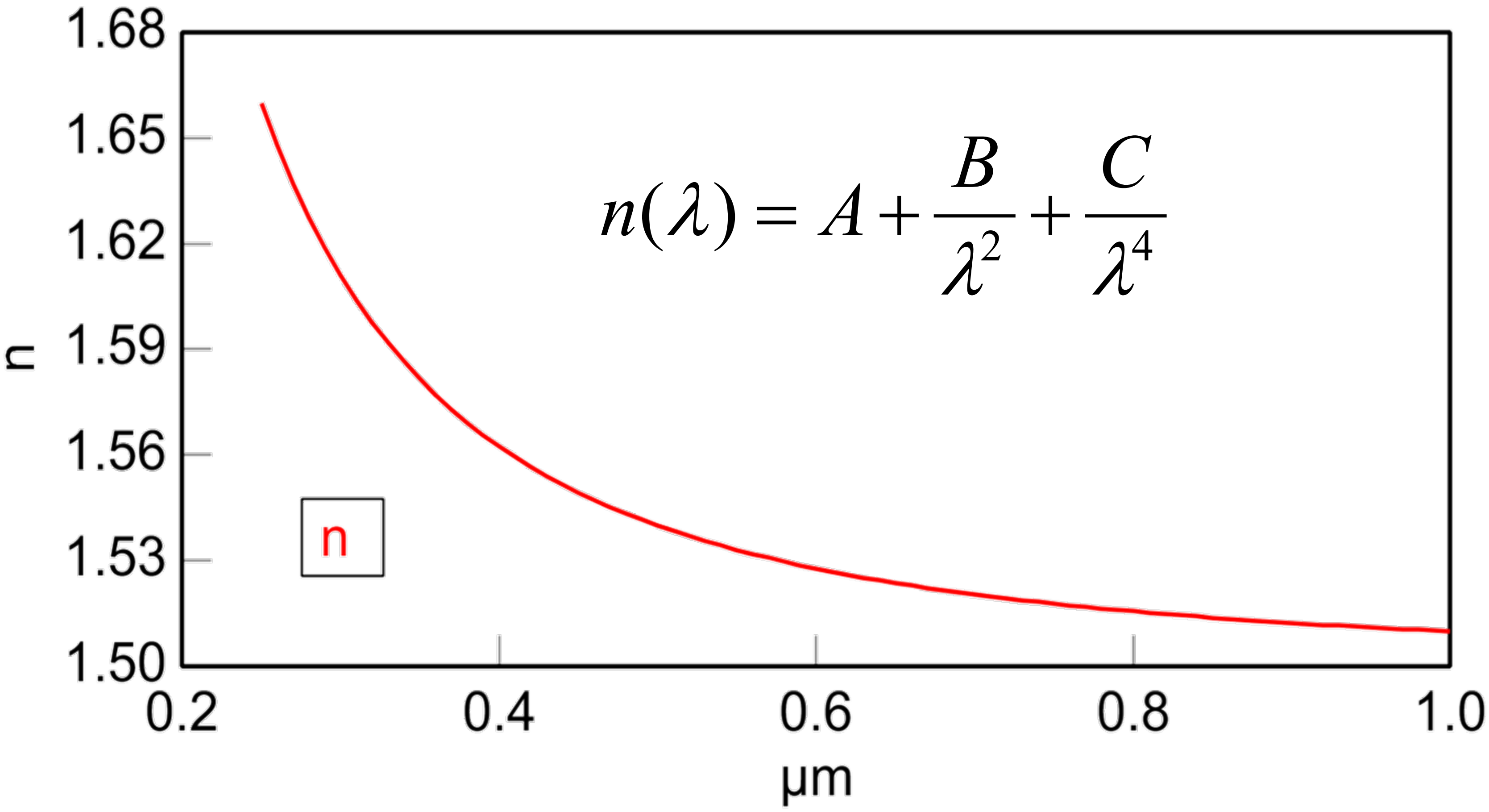




Cauchy Equation

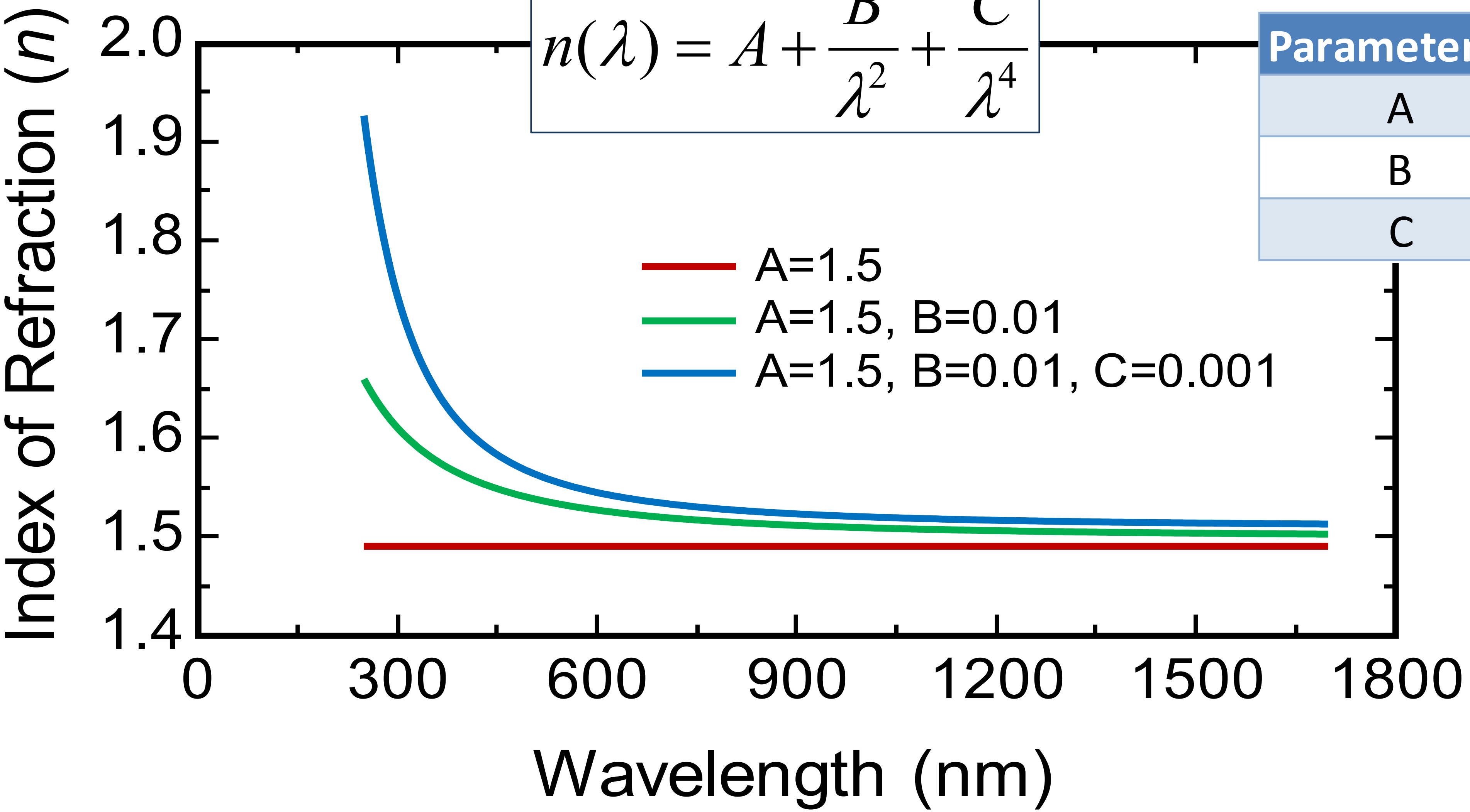
- Cauchy equation is empirical description of index dispersion n(λ) of transparent materials (k = 0 or very small)

- Substrate = Cauchy
  A = 1.450 B = 0.01000 C = 0.0000
  Show Urbach Absorption Parameters = OFF



Cauchy Parameters

$$n(\lambda) = A + \frac{B}{\lambda^2} + \frac{C}{\lambda^4}$$



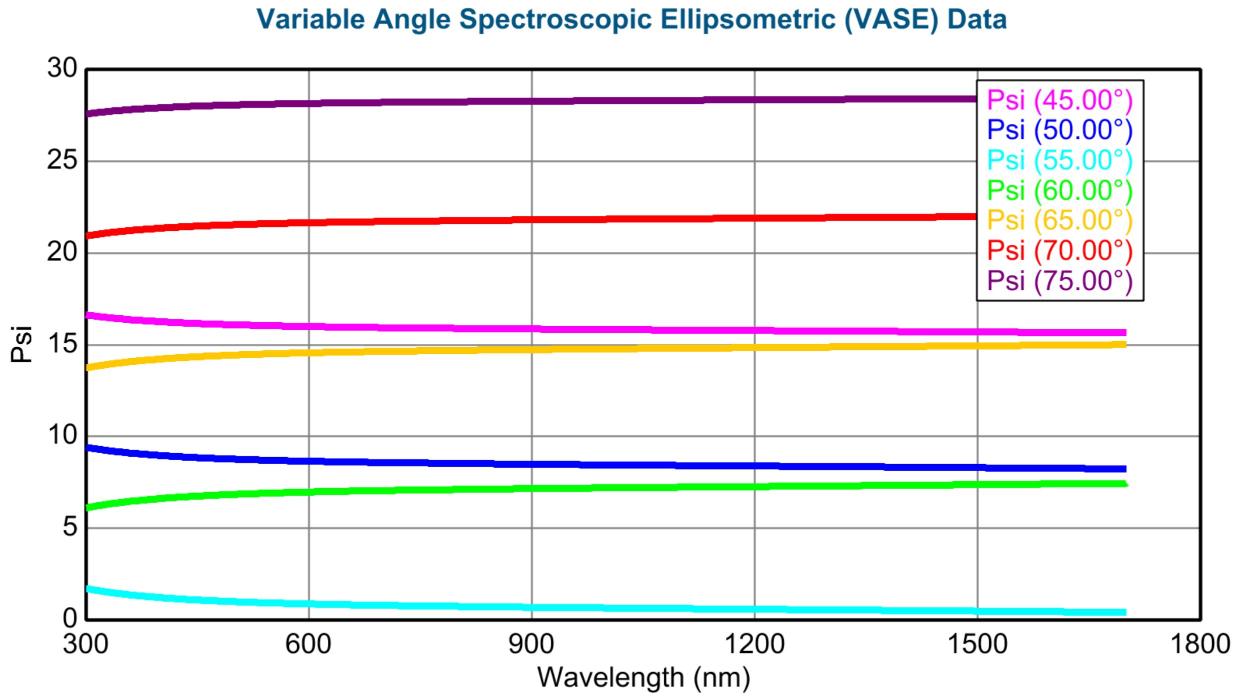
Parameter	Typical Range
A	1.3-2.5
B	0.005-0.05
C	0.0000-0.005

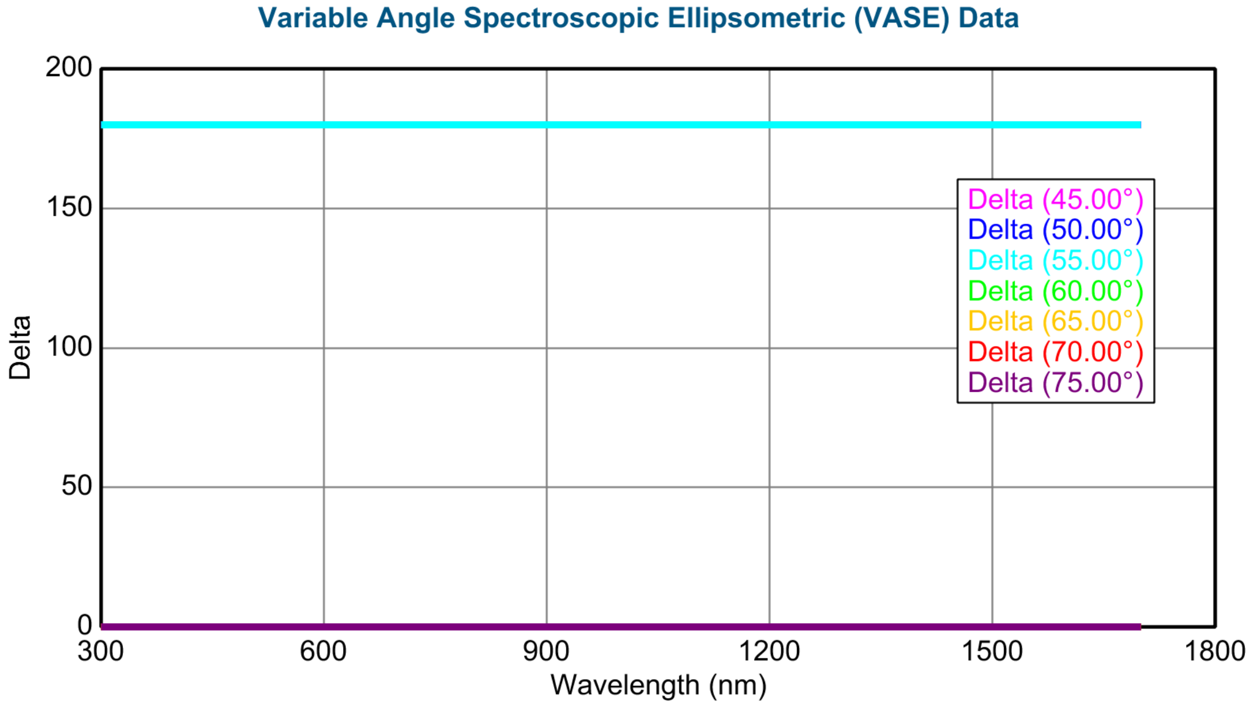
Augustin-Louis Cauchy
(1789 – 1857)

Transparent Substrates – Data Features

- Psi spectra are flat and smooth, as they follow behavior of n.
  - Psi approaches 0° at Brewster's Angle
- Delta = 0° or 180°, depending on angle (crosses at ϕ_B).
  - Only deviates if (a) absorption or (b) surface film

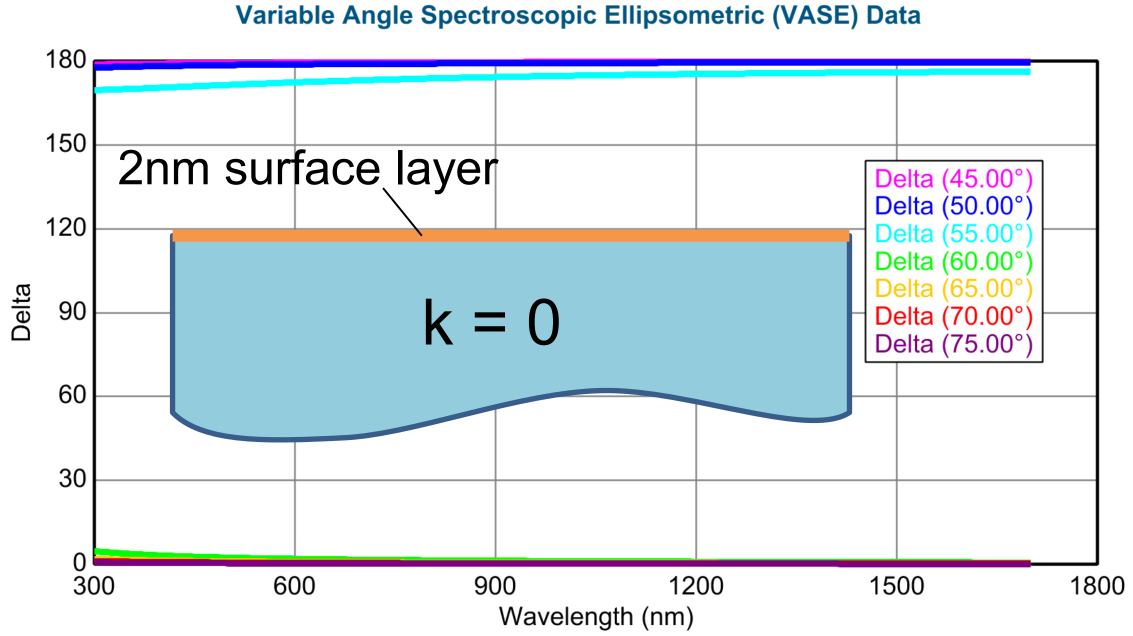
$$\phi_B = \arctan(n)$$

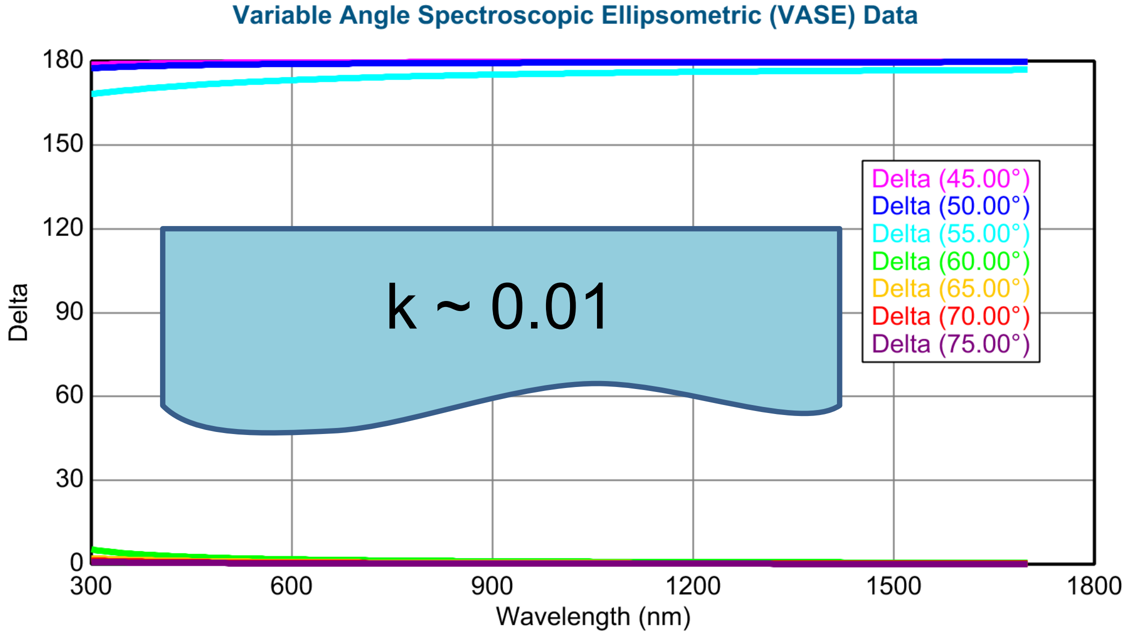




Absorption or Surface Film?

- Both surface layer and substrate absorption cause Δ to shift from 0°, 180°.

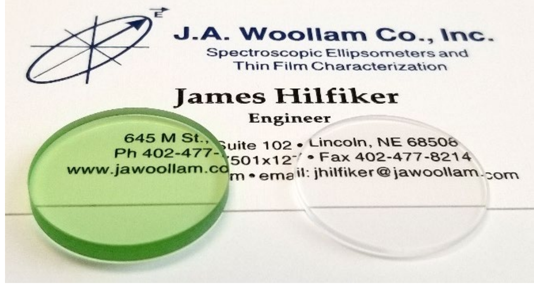


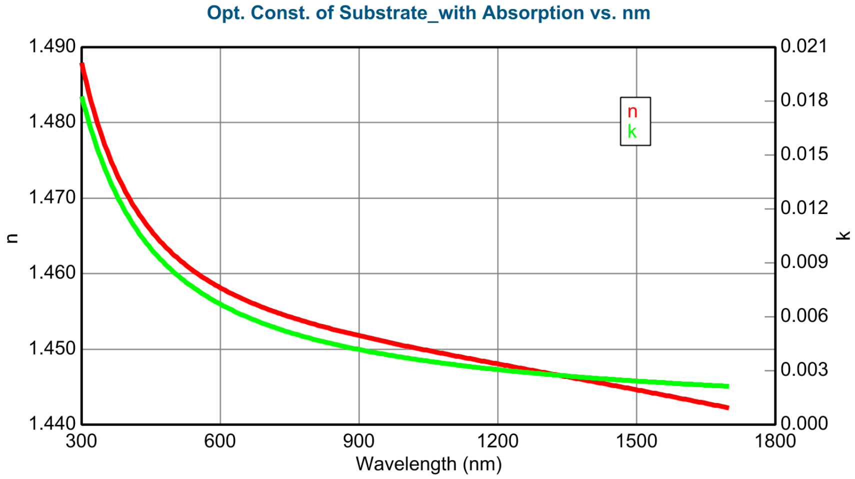


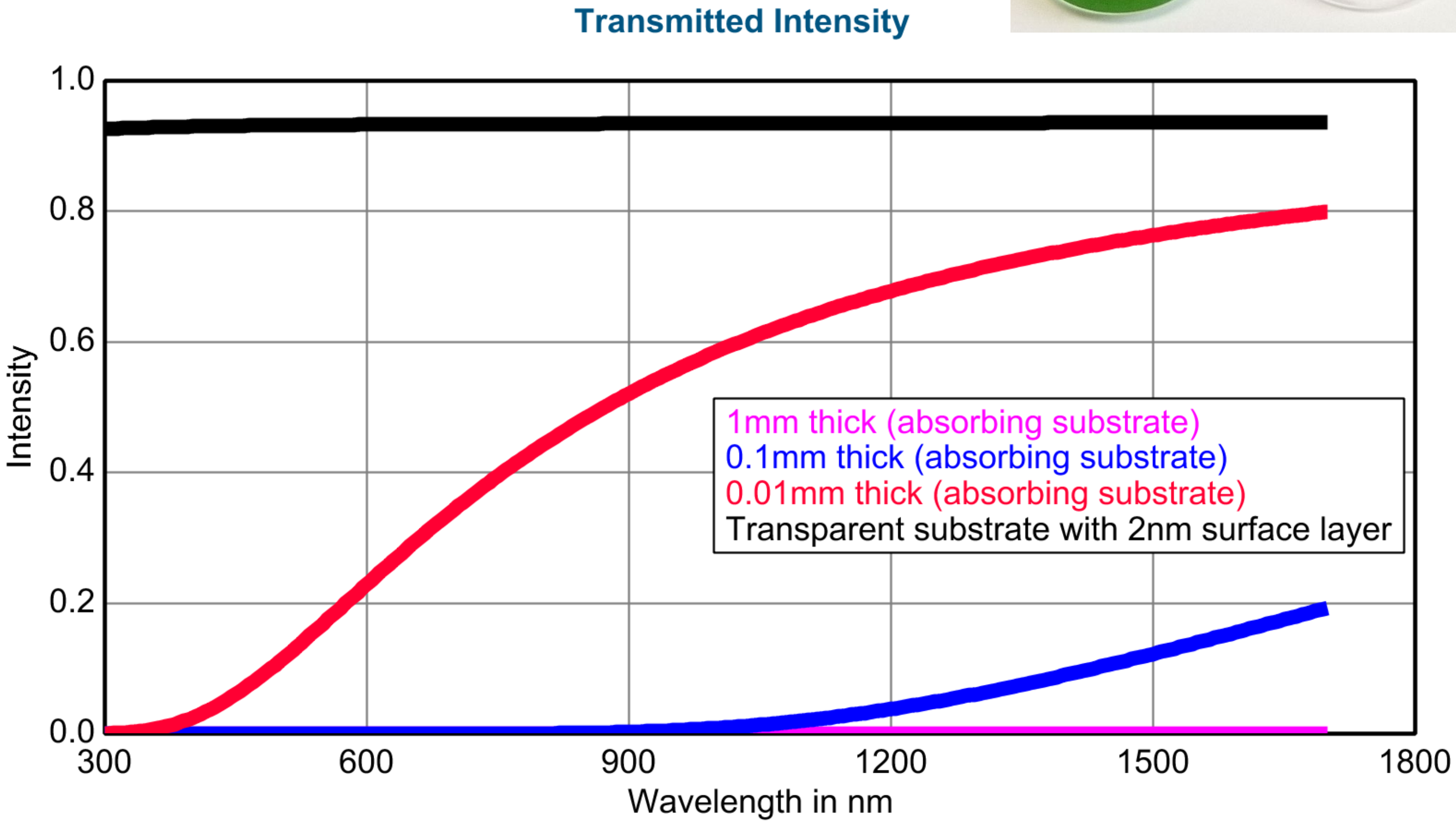
Transparency tells us the CORRECT answer

Transmission Intensity

- Absorption and surface layers can be distinguished by considering light transmission.







Modeling Transparent Substrates

- Add Cauchy for substrate, fit A, B, C to match Ψ
- Turn 'on' roughness to match Δ
- Avoid backside reflections or add correction
- Save material file for later use

Roughness is used to approximate any surface film with lower index than substrate

Include Surface Roughness = ON Roughness = **0.00 nm** (fit)

- Substrate = Cauchy

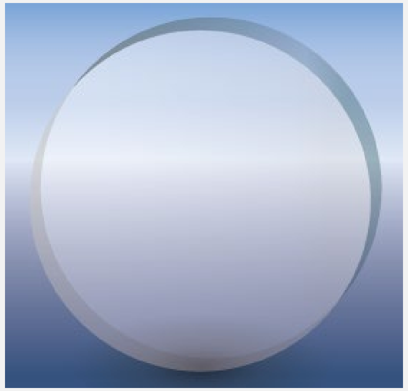
A = **1.450** (fit) B = **0.01000** (fit) C = **0.0000** (fit)

+ **Urbach Absorption Parameters**

If roughness has *negative* thickness, the math is trying to tell you that your surface has higher index than substrate.

1-6: N-BK7 Substrate

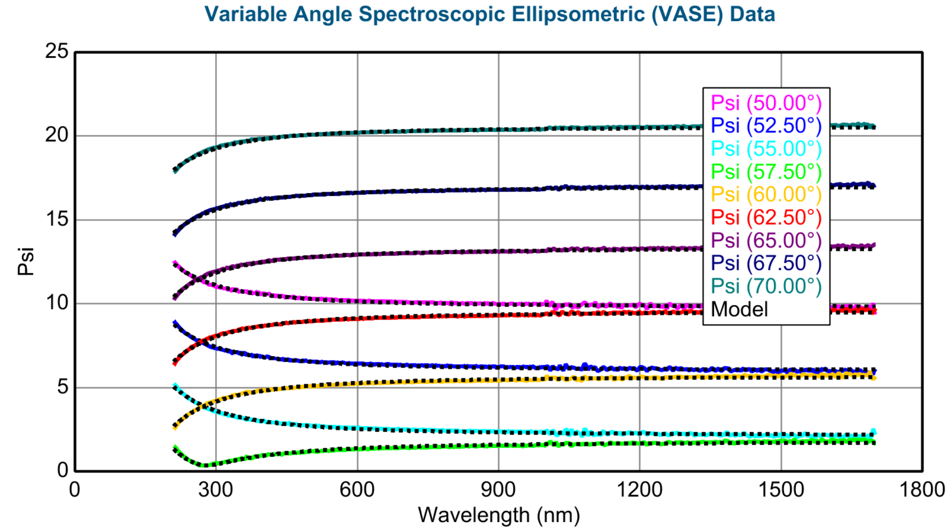
- Determine index from high-quality borosilicate Schott glass



- Fit Cauchy A, B, C and surface roughness
- Roughness is used to approximate any surface film with a lower index than the substrate.

If roughness has *negative* thickness,
the math is trying to tell you that your surface has
higher index than substrate.

1-6 N-BK7 RESULTS



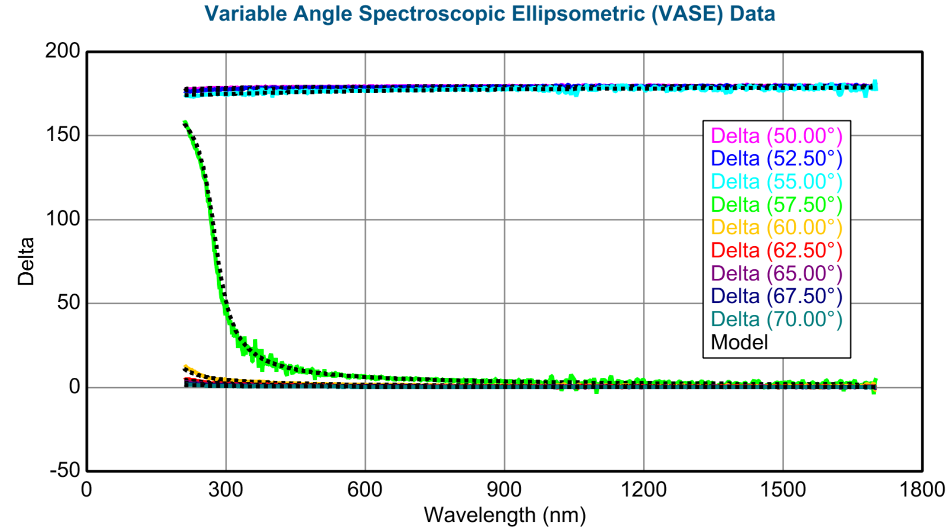
Roughness = 13.44 Å (fit)

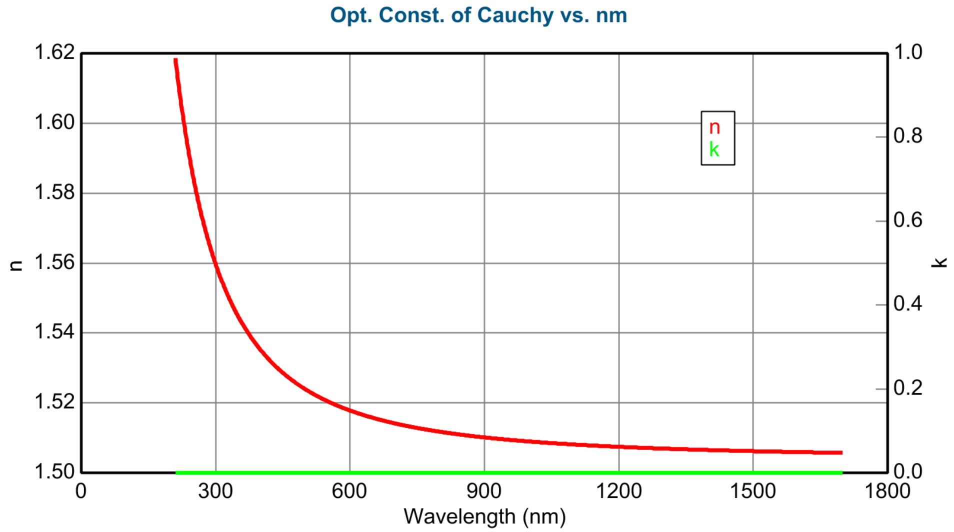
\- Substrate = Cauchy

A = 1.504 (fit) B = 0.00496 (fit) C = 4.1078E-06 (fit)

+ Urbach Absorption Parameters

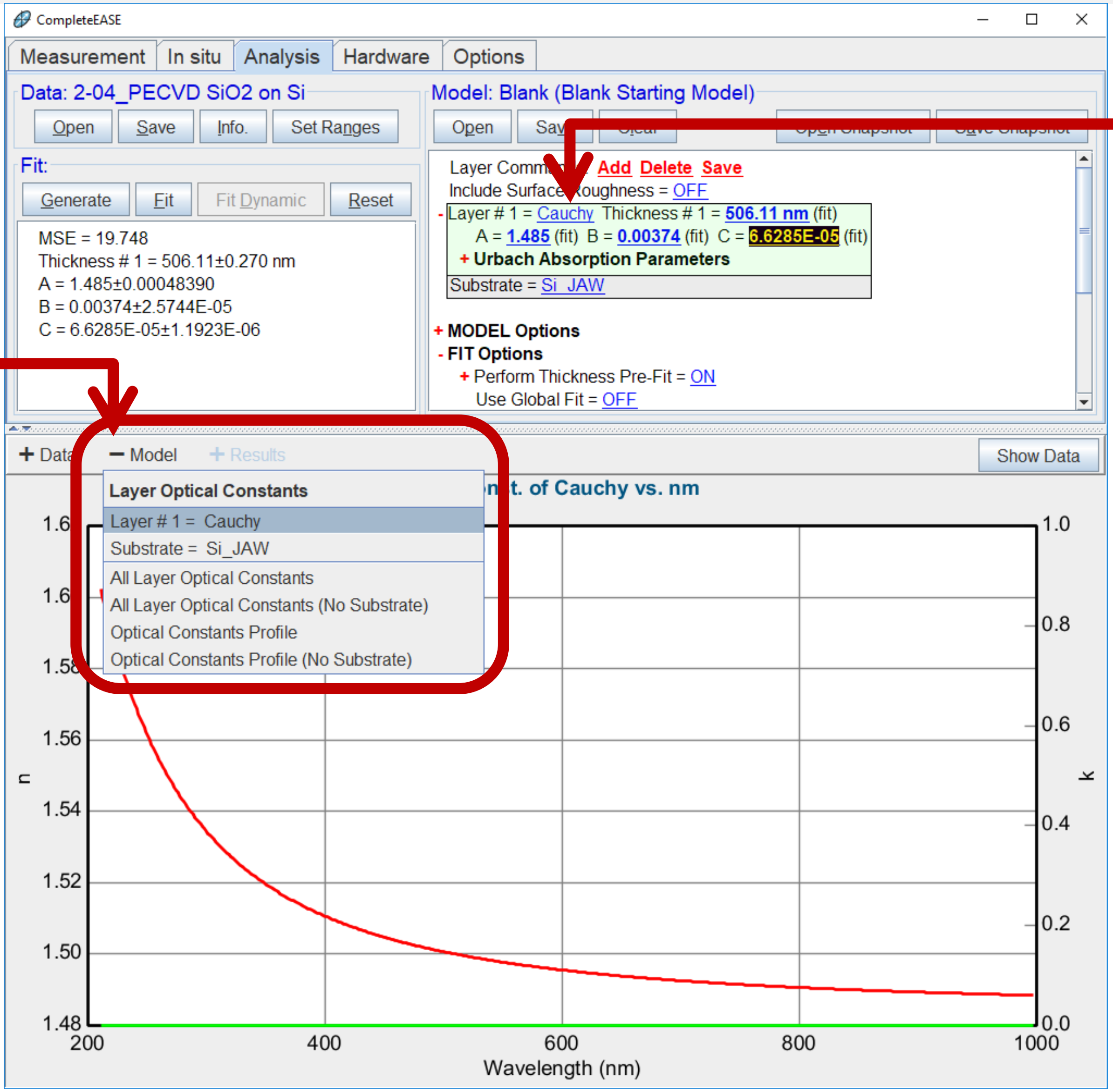
MSE = 1.536
Roughness = 13.44 ± 0.057 Å
A = 1.504 ± 4.8207E-05
B = 0.00496 ± 2.0016E-05
C = 4.1078E-06 ± 1.1437E-06
n of Cauchy @ 632.8 nm = 1.51641



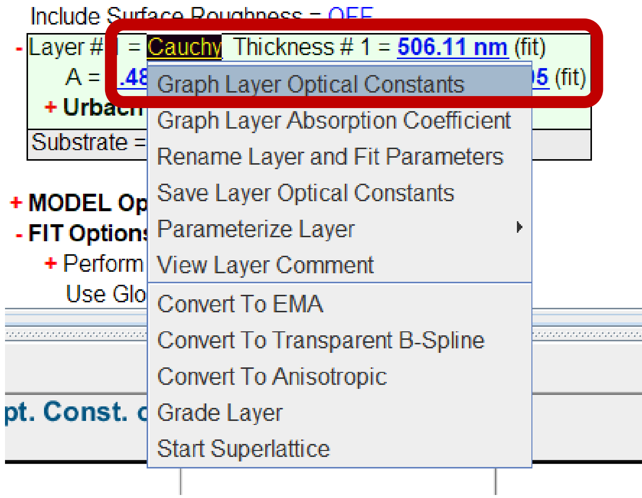


Viewing Optical Constants

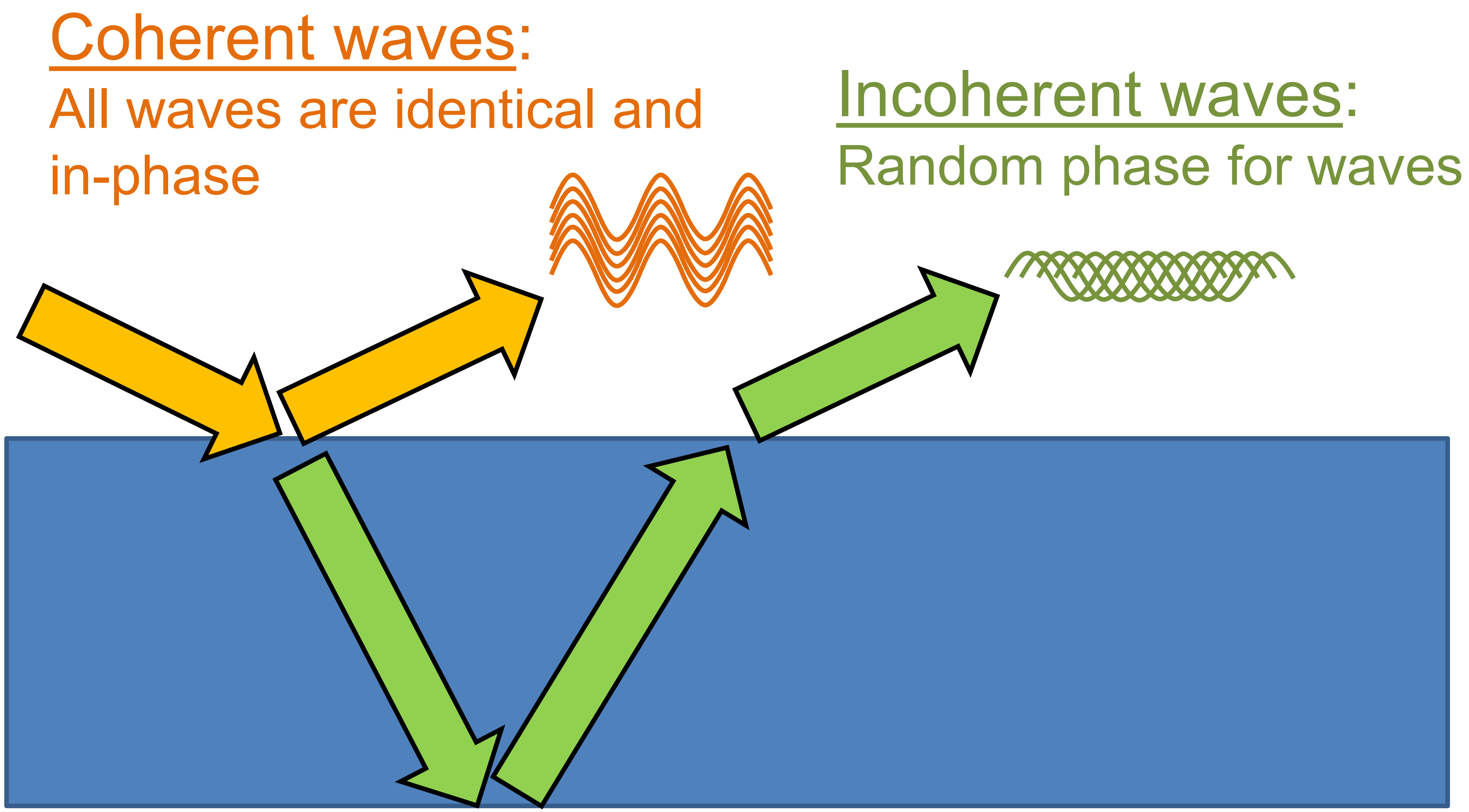
Left-Click on Model menu, choose Layer



Right-Click on Layer Name

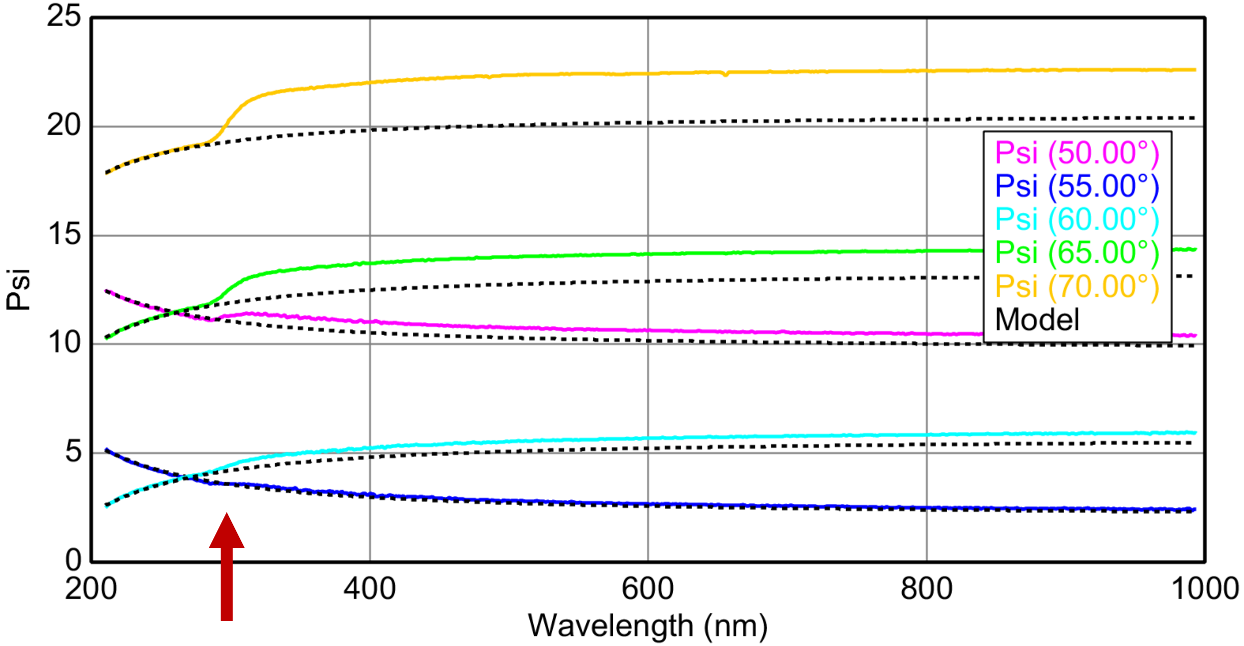


Substrate Backside Reflections



Backside reflections for Glass

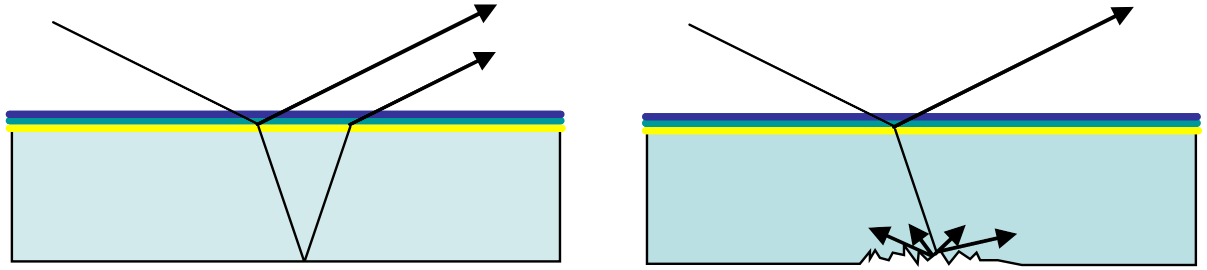
- Identifying data by "step" in UV when glass becomes absorbing, or because Psi curves versus angle are "shifted"
- How to handle:
  - Roughen/tape substrate backside
  - Model "backside reflections"



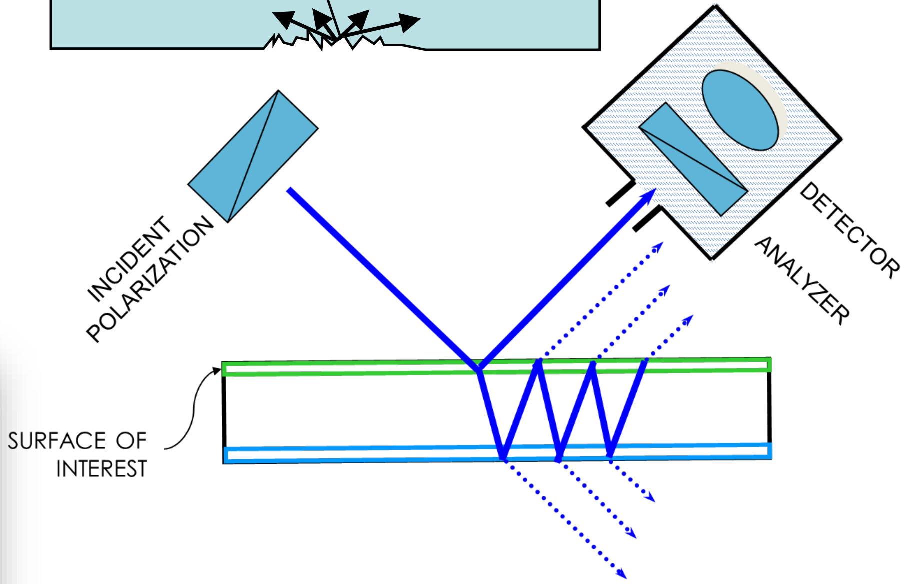
Glass transparent above this λ

Avoiding Backside Reflections

1. Roughen backside.



2. Spatially separate front & back reflections.



3. Scatter/absorb light with index-matching material.

R.A. Synowicki, "Suppression of backside reflections from transparent substrates", *Phys. Stat. Sol. (c)* **5**, (2008) 1085.

Translucent Scotch tape works very well

Modeling backside reflections

Built-in Model

Glass Substrate (With backside reflection).mod

Layer Commands: **Add** **Delete** **Save**

Include Surface Roughness = ON Roughness = **0.08 nm** (fit)

- Substrate = Cauchy Substrate Thickness = 1.0000 mm

  A = **1.500** (fit) B = **0.00743** (fit) C = **-0.00031985** (fit)

  + Urbach Absorption Parameters

- MODEL Options

Angle Offset = 0.00

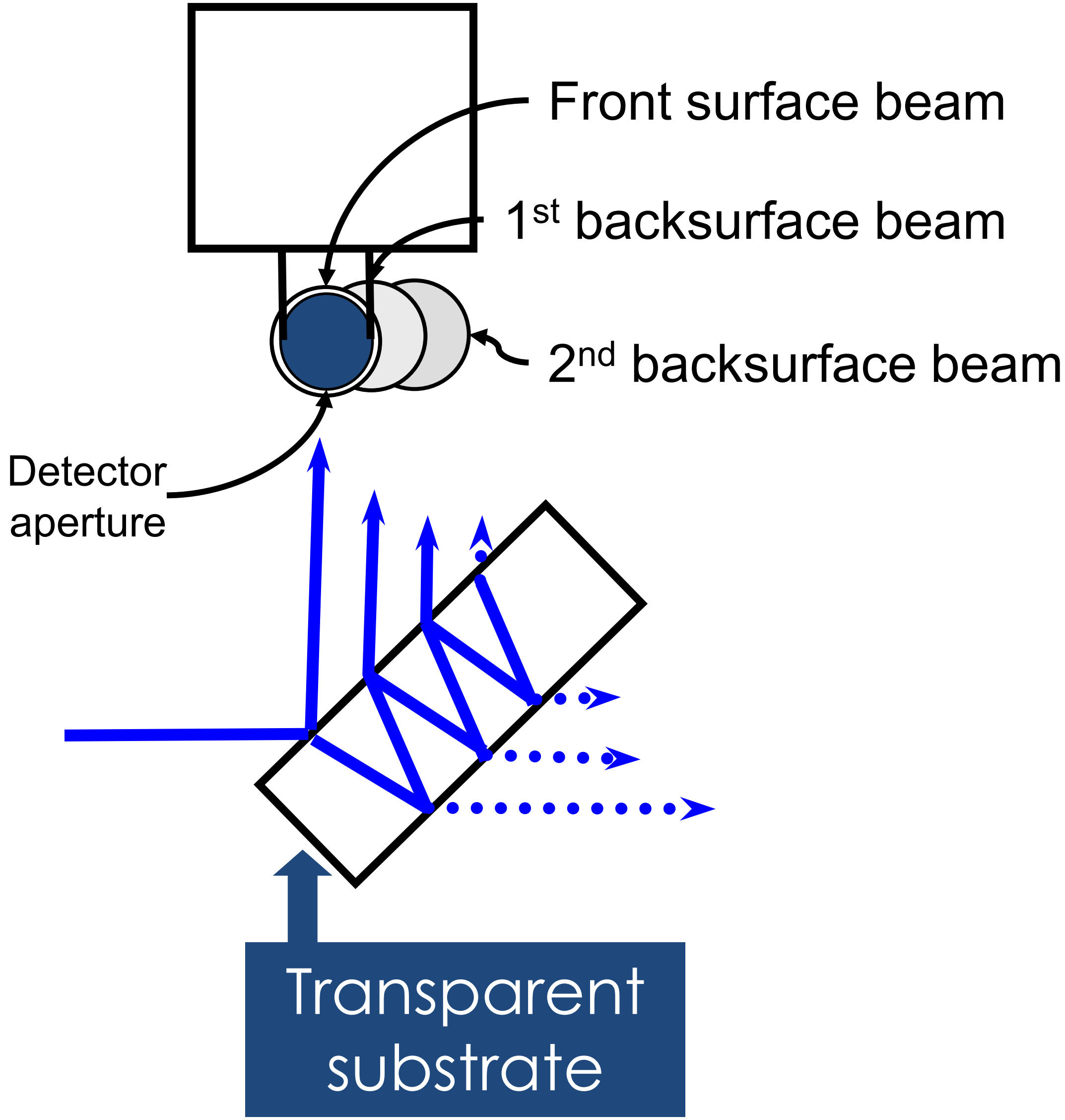
Include Substrate Backside Correction = ON

Transmission SE Data = OFF Reverse Direction = OFF

Back Reflections = **0.881** (fit)

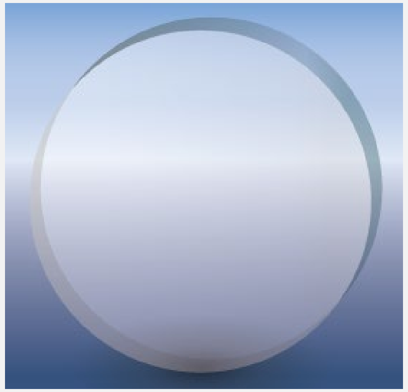
% 1st Reflection = 100.00

Model Calculation = Ideal



1-7: N-BK7 substrate with backside reflection

- Double-side polished high-quality borosilicate Schott glass
- Determine refractive index with backside reflection.



<u>Hints</u>:

Restrict the wavelengths to the region where the glass is transparent!

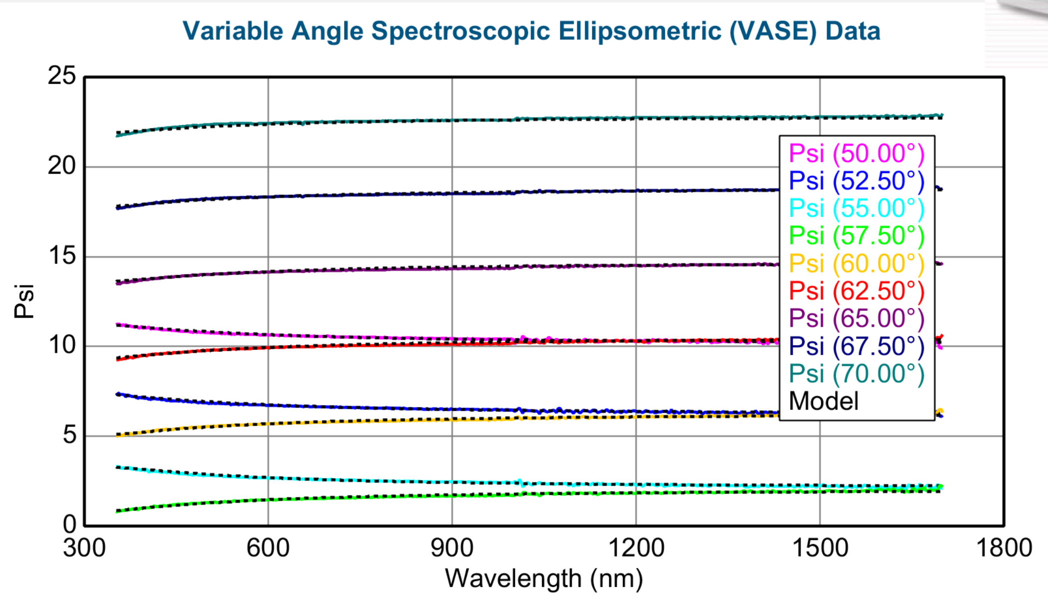
Fit the “# Back Reflections” – starting near 1.

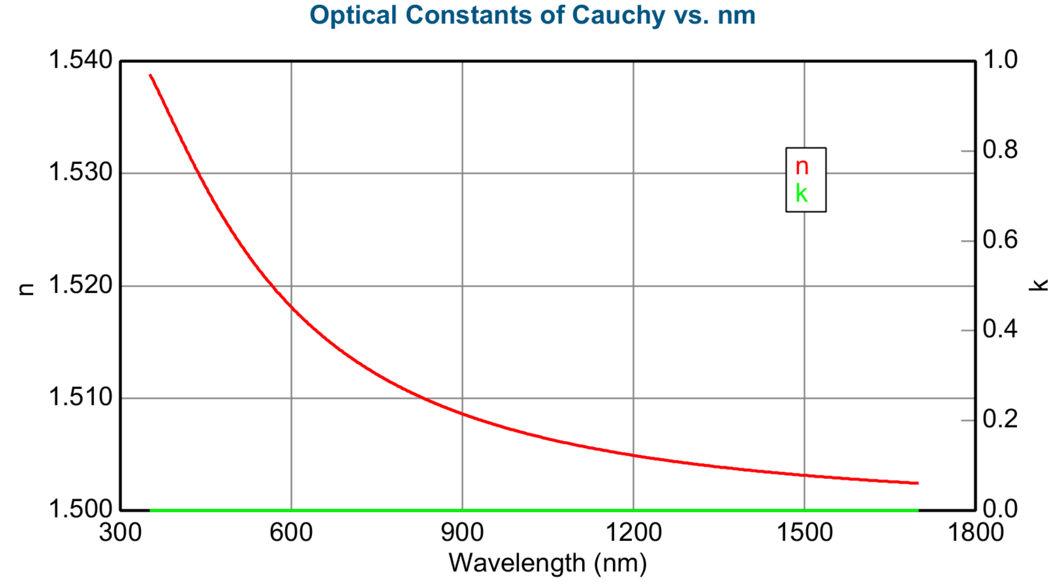
1-7 N-BK7 Substrate with BR RESULTS

MSE = 1.230
Roughness = 0.77 ± 0.116 Å
A = 1.500 ± 5.7173E-05
B = 0.00747 ± 4.4746E-05
C = -0.00032814 ± 6.3405E-06
# Back Reflections = 0.881 ± 0.00091610
n of Cauchy @ 632.8 nm = 1.51649

Layer Commands: **Add** **Delete** **Save**
Include Surface Roughness = ON Roughness = **0.77 Å** (fit)
- Substrate = Cauchy Substrate Thickness = 1.0000 mm
  A = **1.500** (fit) B = **0.00747** (fit) C = **-0.00032814** (fit)
  + **Urbach Absorption Parameters**

- **MODEL Options**
  Angle Offset = 0.00
  Include Substrate Backside Correction = ON
  Transmission SE Data = OFF Reverse Direction = OFF
  # Back Reflections = **0.881** (fit)
  % 1st Reflection = 100.00

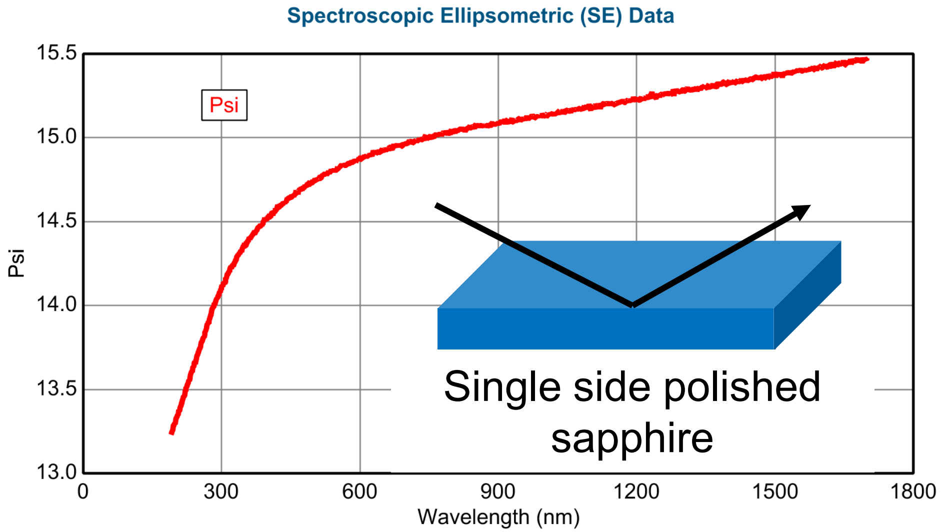


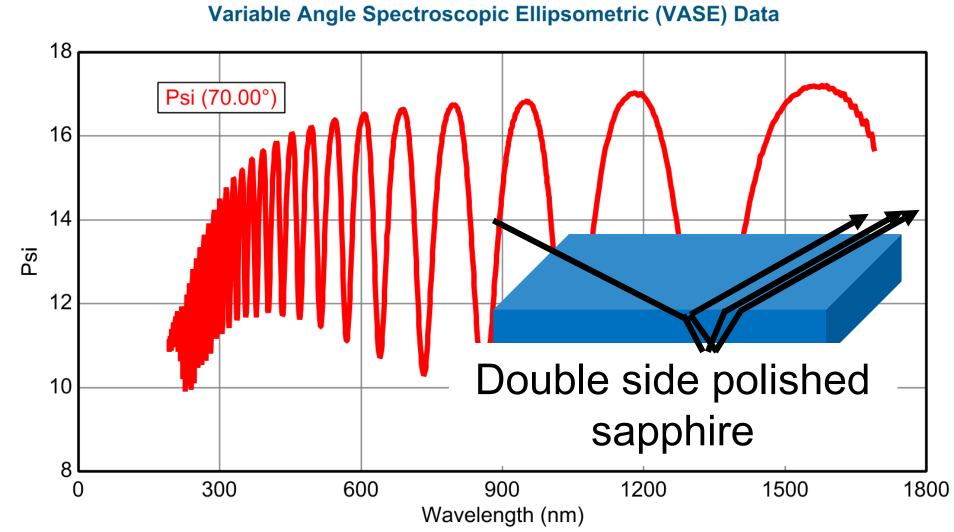


Transparent Substrate Considerations

- Light reflection
  - Low-index results in low reflected intensity
  - Backside reflection
- Surface quality
  - Surface roughness or contamination
- Anisotropy (not covered)
- Small absorption (Session 5)

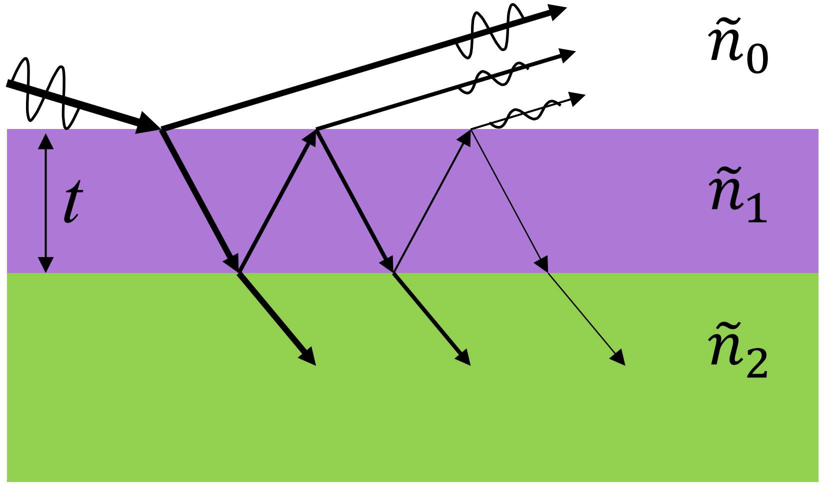
Avoid anisotropic effects by collecting only the top-surface reflection.



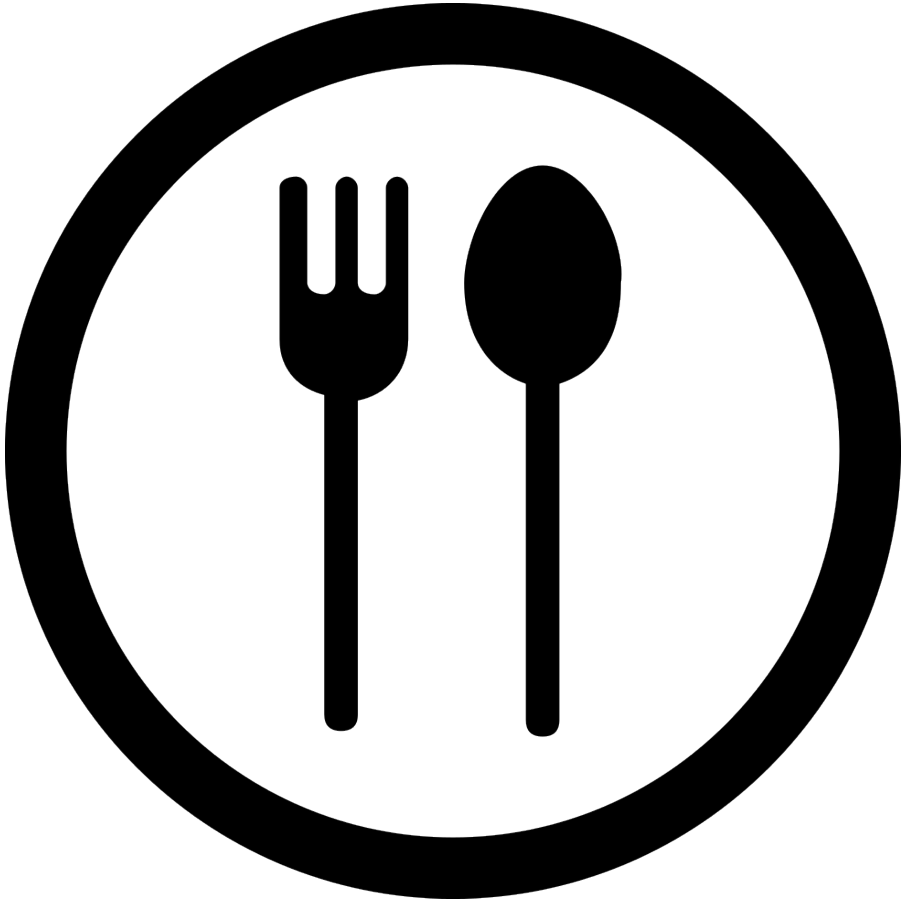


Course Outline

- **Session 1: Theory, Substrates (Si and Glass)**
- Session 2: Transparent Films
- Session 3: Absorbing & Semi-Absorbing Films (B-Spline)
- Session 4: Semi-Absorbing Films (Gen-Osc)
- Session 5: Thin Absorbing Films and Multilayers
- Session 6: Advanced Topics



LUNCH time



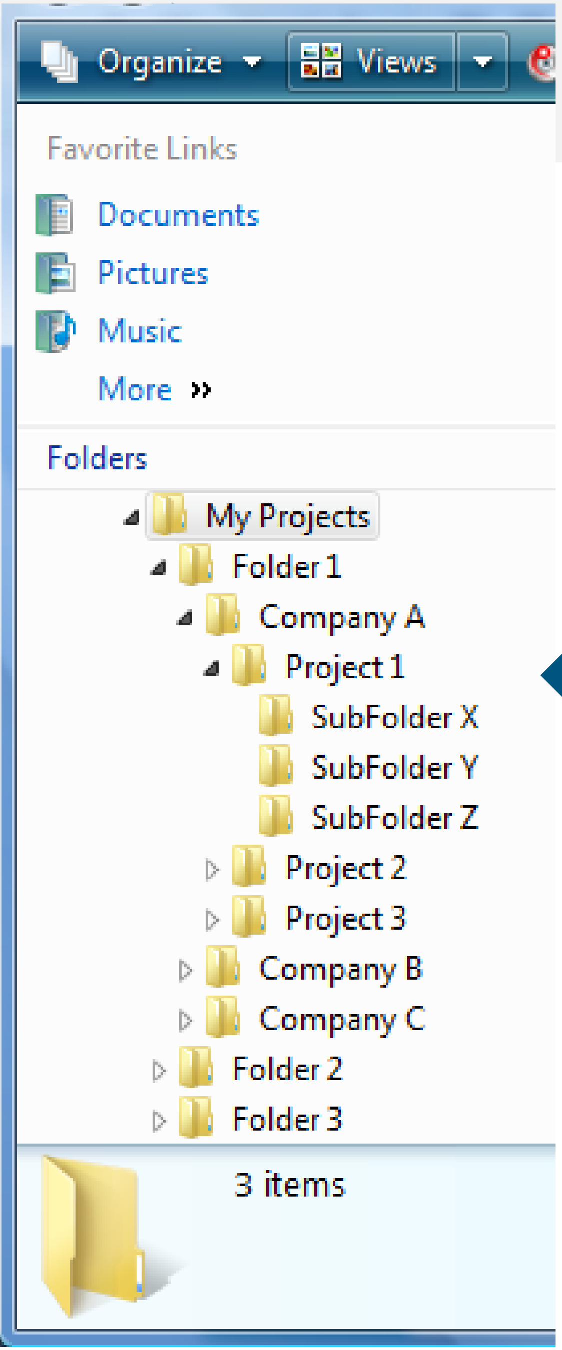
J.A. Woollam
Ellipsometry Solutions

Extra Slides

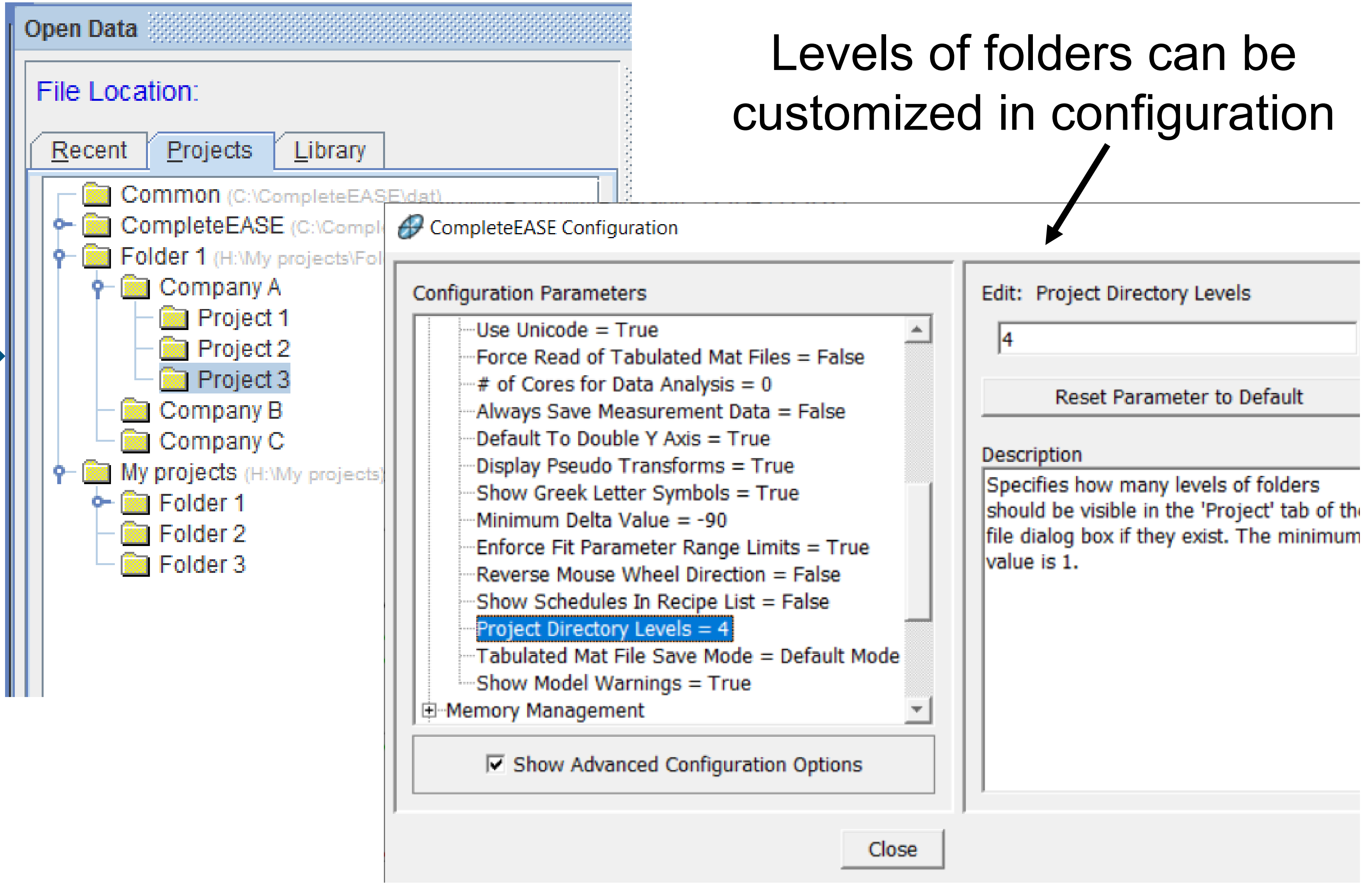
CompleteEASE File Extensions

Type	Extension
Experimental Ψ, Δ data	*.SE
Model	*.mod
Material file (optical constants)	*.mat
Snapshot (Exp. data, model and fit results)	*.SEsnap
Data Acquisition Parameters	*.parms
Mapping Pattern	*.scan
Recipe points to i) Acquisition Parms., ii) Pattern & iii) Model	*.recipe

File Structure



Levels of folders can be customized in configuration

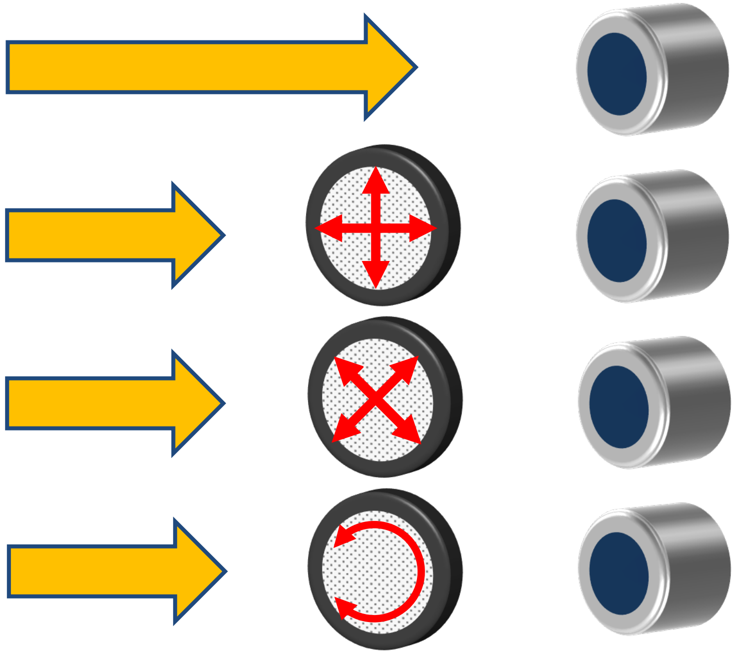


Describing Polarization: Stokes Parameters

- Describes light based on "observables"
- Often called "Stokes Vector" even though not an actual vector

$$S = \begin{bmatrix} S_0 \\ S_1 \\ S_2 \\ S_3 \end{bmatrix} = \begin{bmatrix} I_x + I_y \\ I_x - I_y \\ I_{+45°} - I_{-45°} \\ I_R - I_L \end{bmatrix}$$

Light beam **Optic** **Detector** **What is Measured**



S_0 = *Total intensity*

S_1 = *Horizontal – Vertical polarized intensity*

S_2 = *+45° – (-45°) polarized intensity*

S_3 = *Right Hand – Left Hand circular polarized intensity*