

J.A. Woollam

TRANSPARENT MATERIALS

SESSION 2

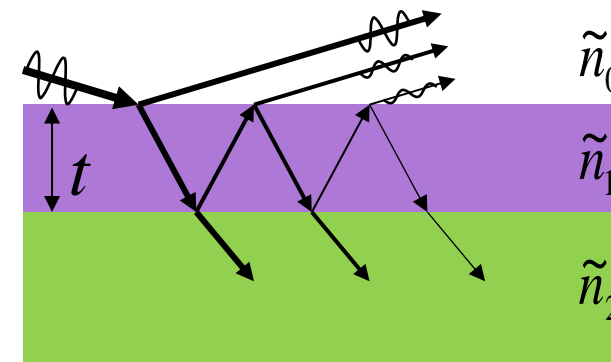
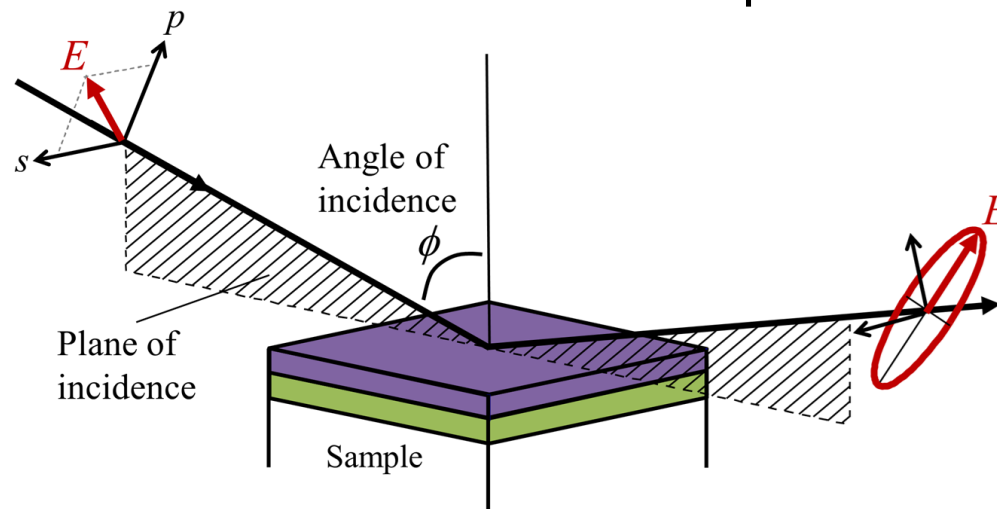
Jianing Sun

Yale University
March 2025



Course Outline

- Session 1: Introduction to Ellipsometry
- **Session 2: Transparent Materials**
- Session 3: Absorbing Materials using B-Spline
- Session 4: Semi-absorbing films using Gen-Osc
- Session 5: Thin Absorbing Films & Multi-Sample Analysis
- Session 6: Advanced Topics and Review





Material Optical Category

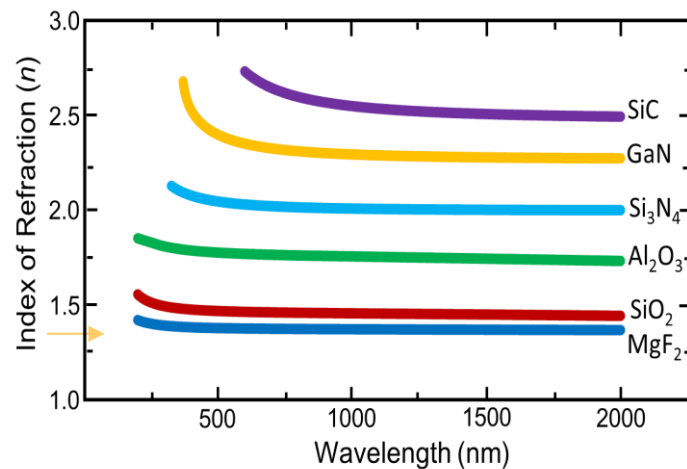
$$\tilde{n} = n - ik$$

$$\tilde{\epsilon} = \epsilon_1 - i\epsilon_2$$

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

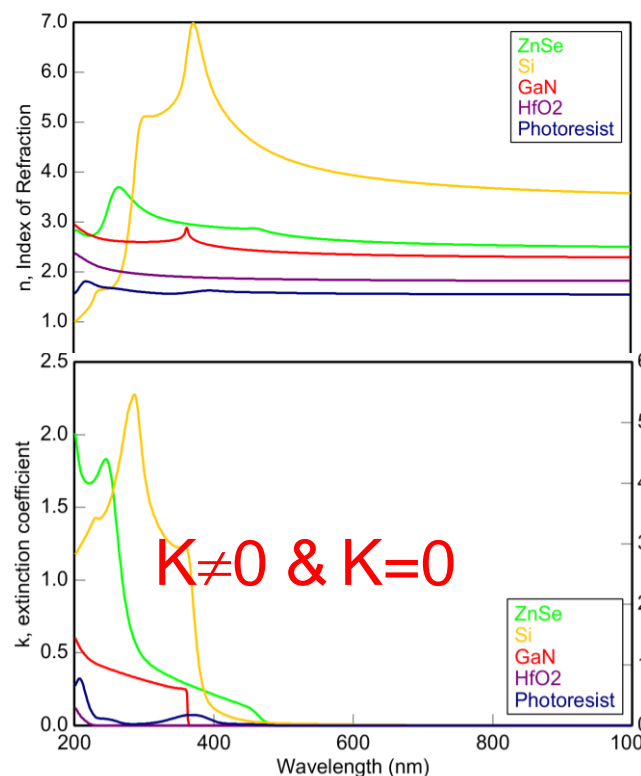


Transparent

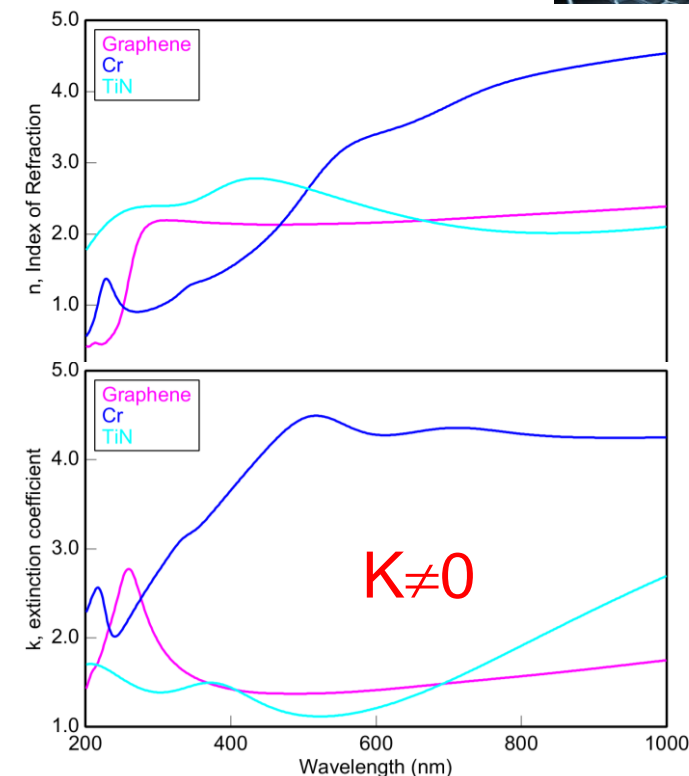


$K=0$

Semi-absorbing



Absorbing





Session 2: Transparent Films

A. Transparent Thin Films

- Built-in Model
- Ultra-thin films
- Identify transparent region

B. Thin Film Complexities



2A: Transparent Thin Films



- Identify wavelengths where the film is transparent.
- Determine thickness and index (n) for any transparent film.
- Create model for similar samples.

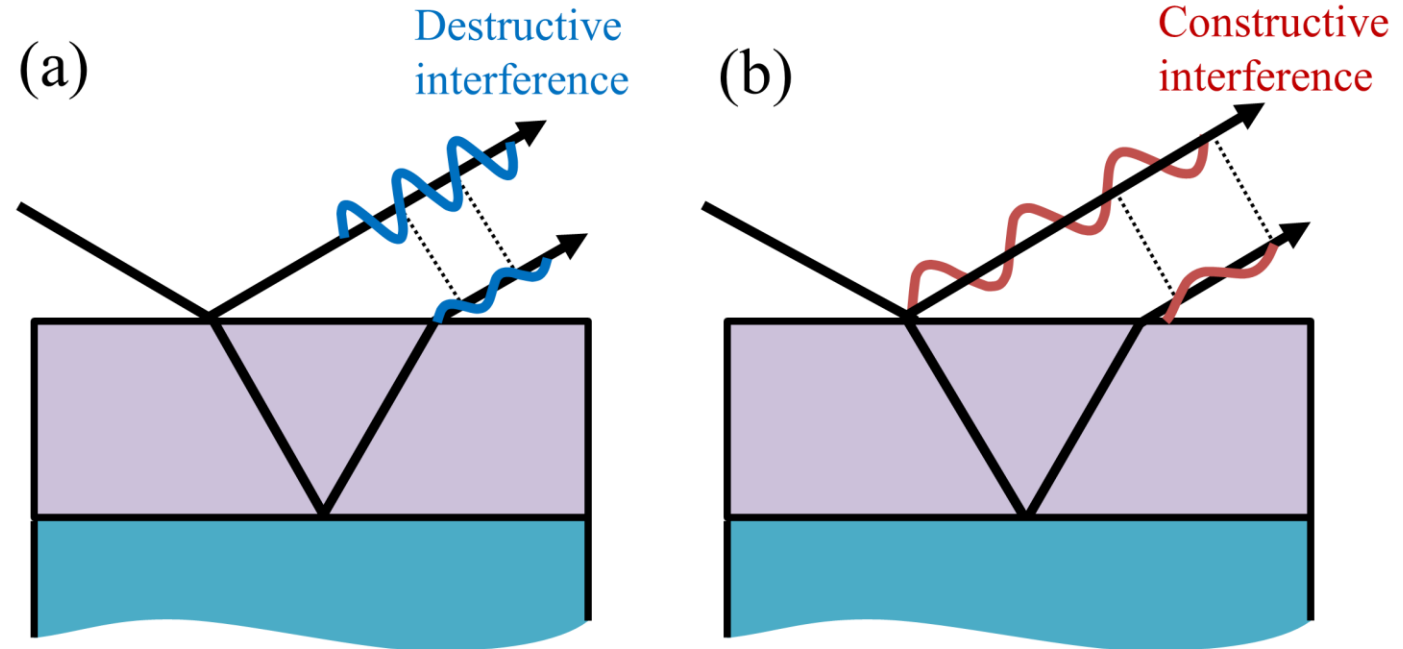
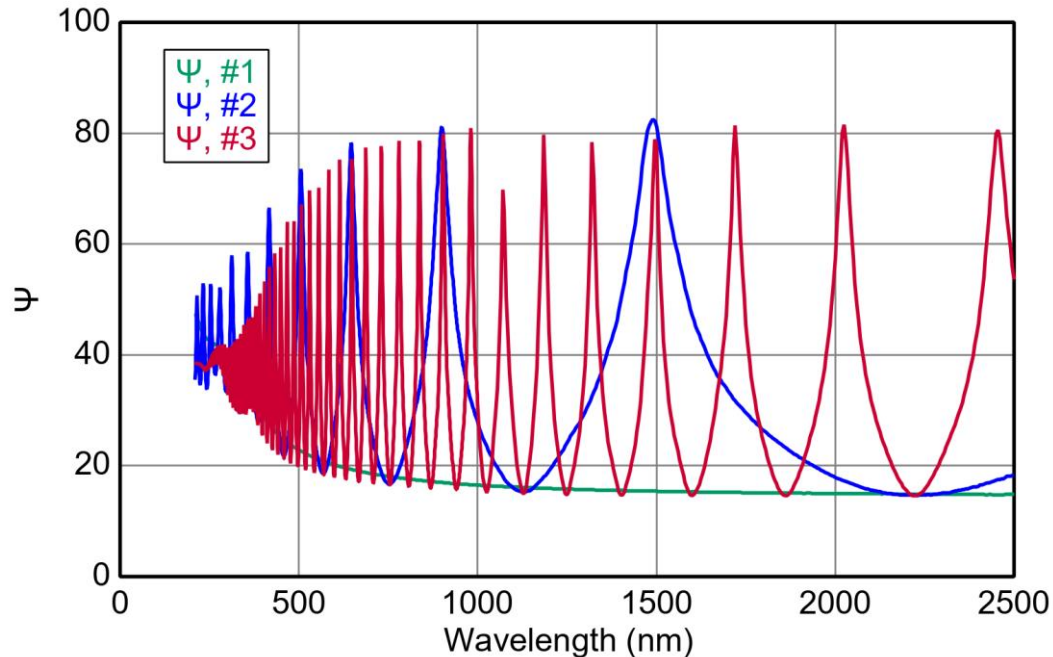
- Data Features
- Modeling and Automation
 - Cauchy Dispersion Equation
 - Built-in model
- Saving Results



Data Features – Transparent Films

- Data curves oscillate resulting from interference effect.
 - The mixing of light from top and bottom of film with different path lengths causes interference that results in peaks and valleys in data.

Spectroscopic Ellipsometric (SE) Data

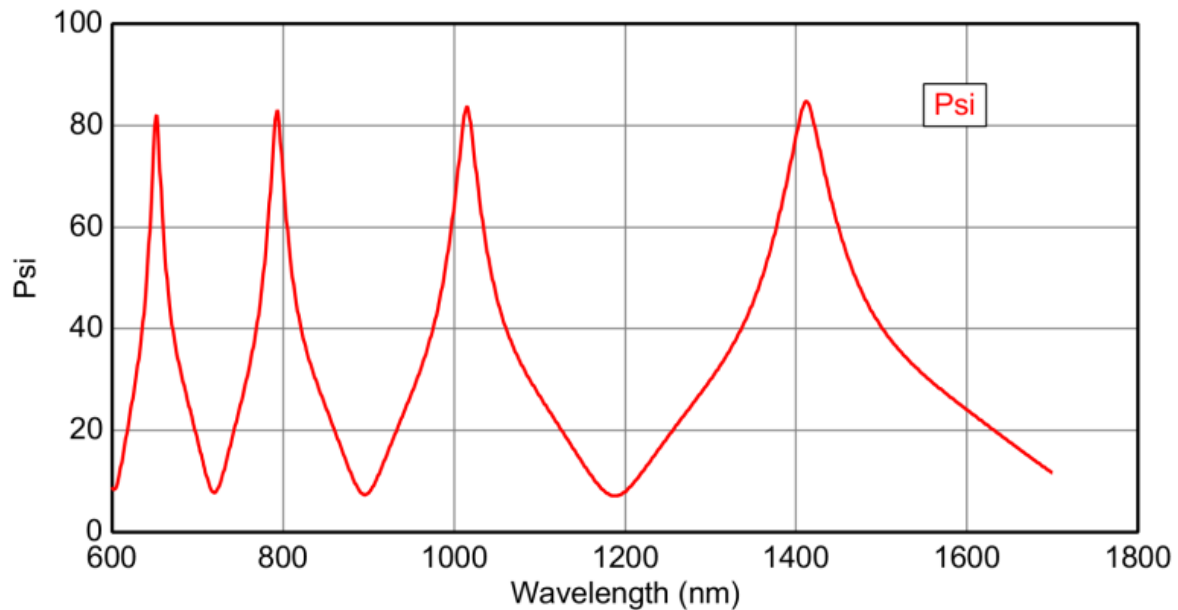




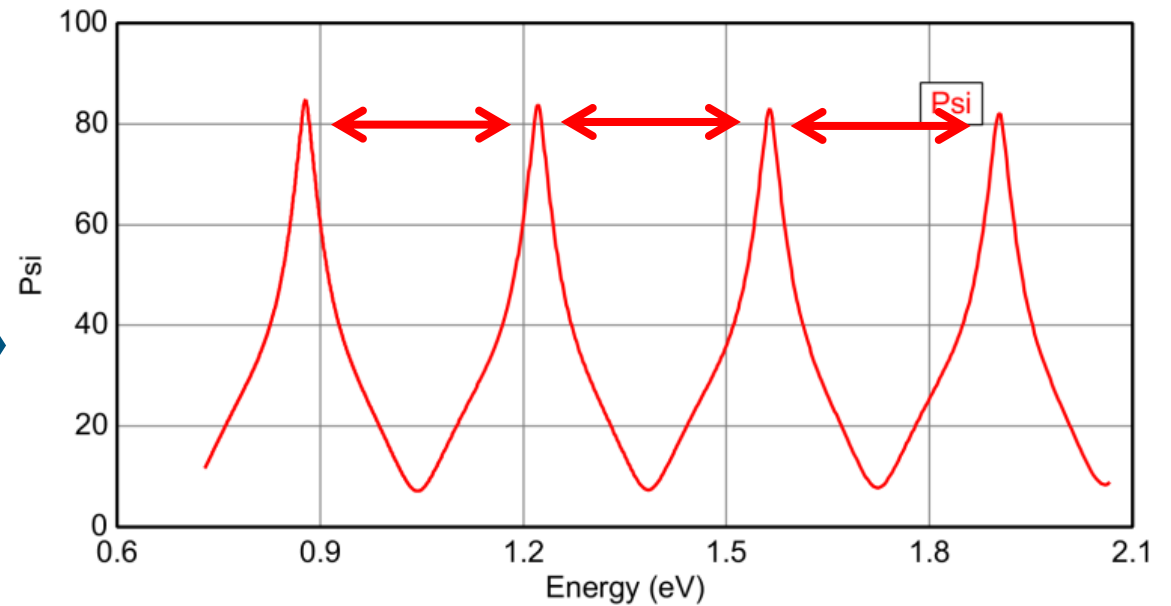
Thin Film Interference

- Pattern affected by thickness and index of refraction (n).

Spectroscopic Ellipsometric (SE) Data



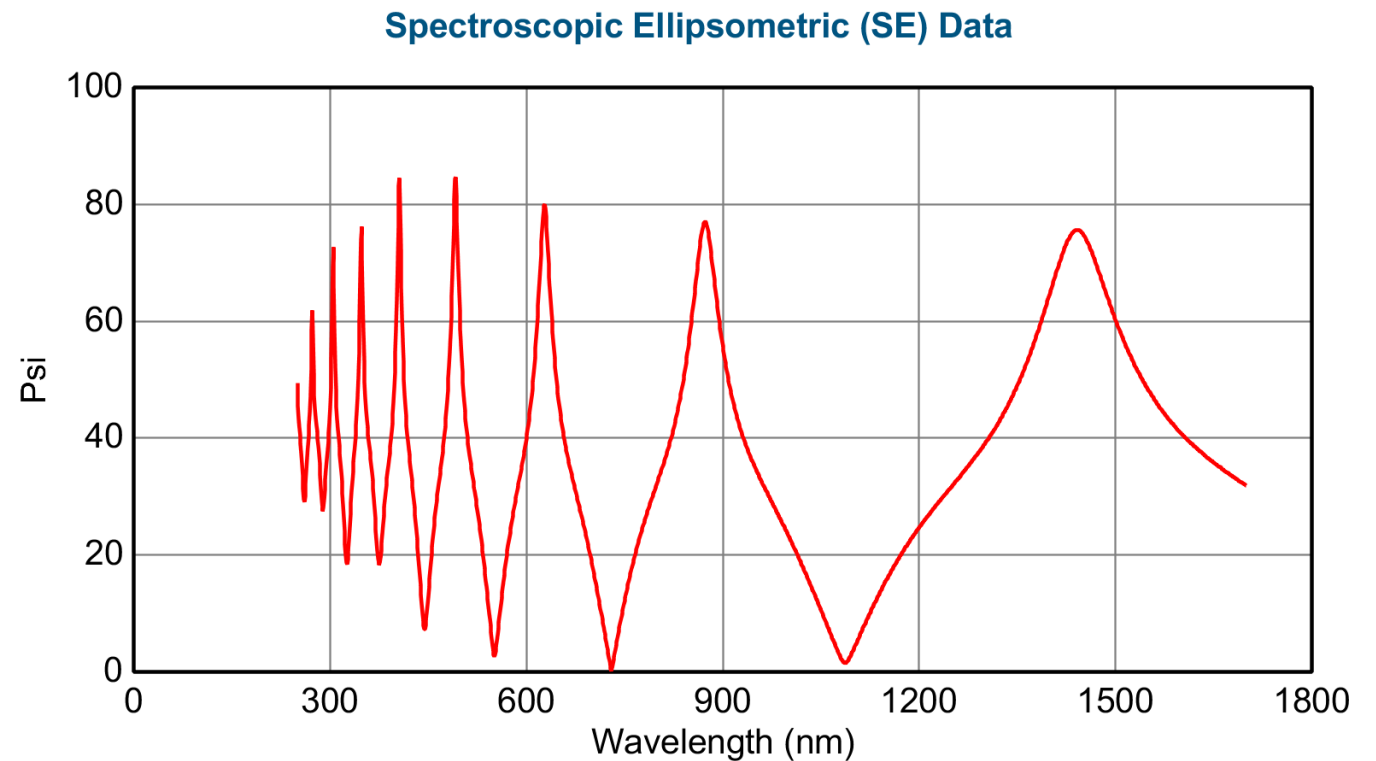
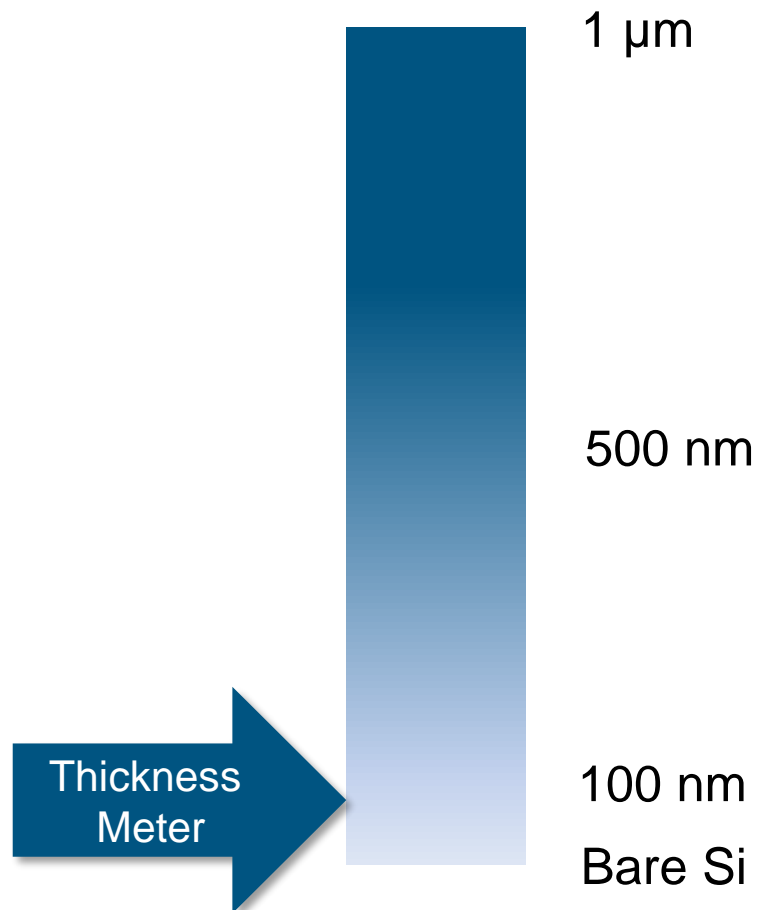
Spectroscopic Ellipsometric (SE) Data





Thickness Effects

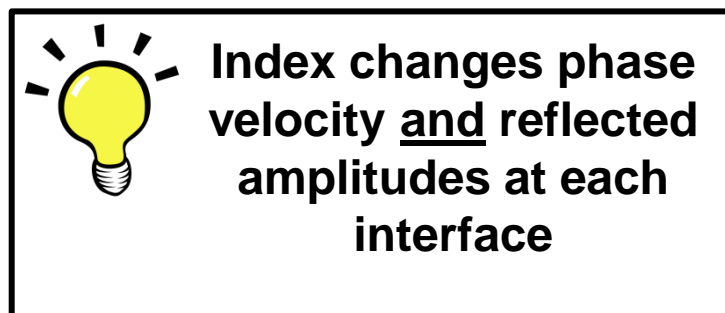
- # of oscillations ~ thickness
- Thicker films = more interference oscillations



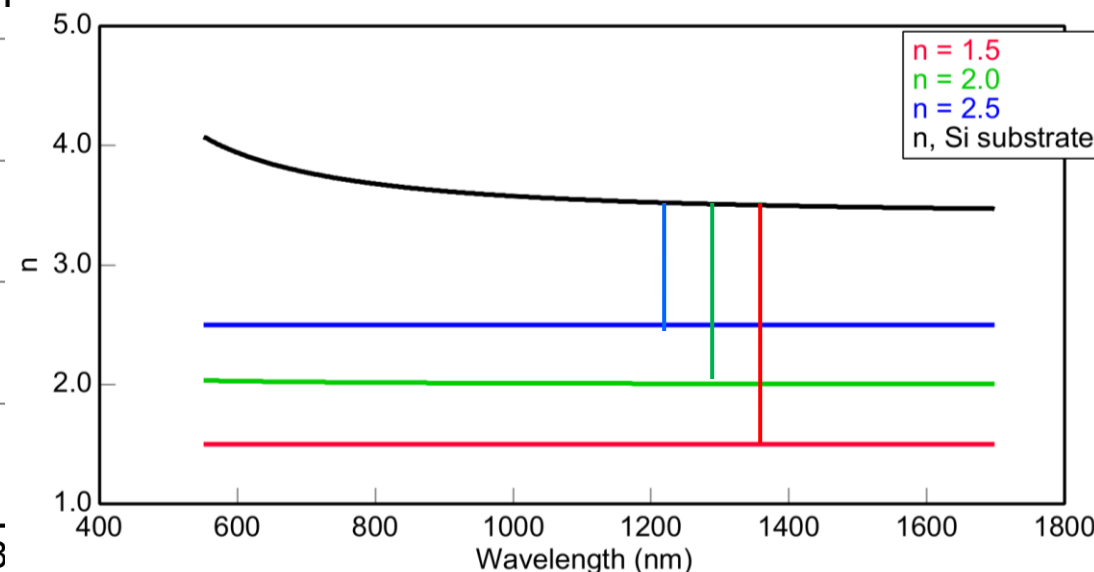
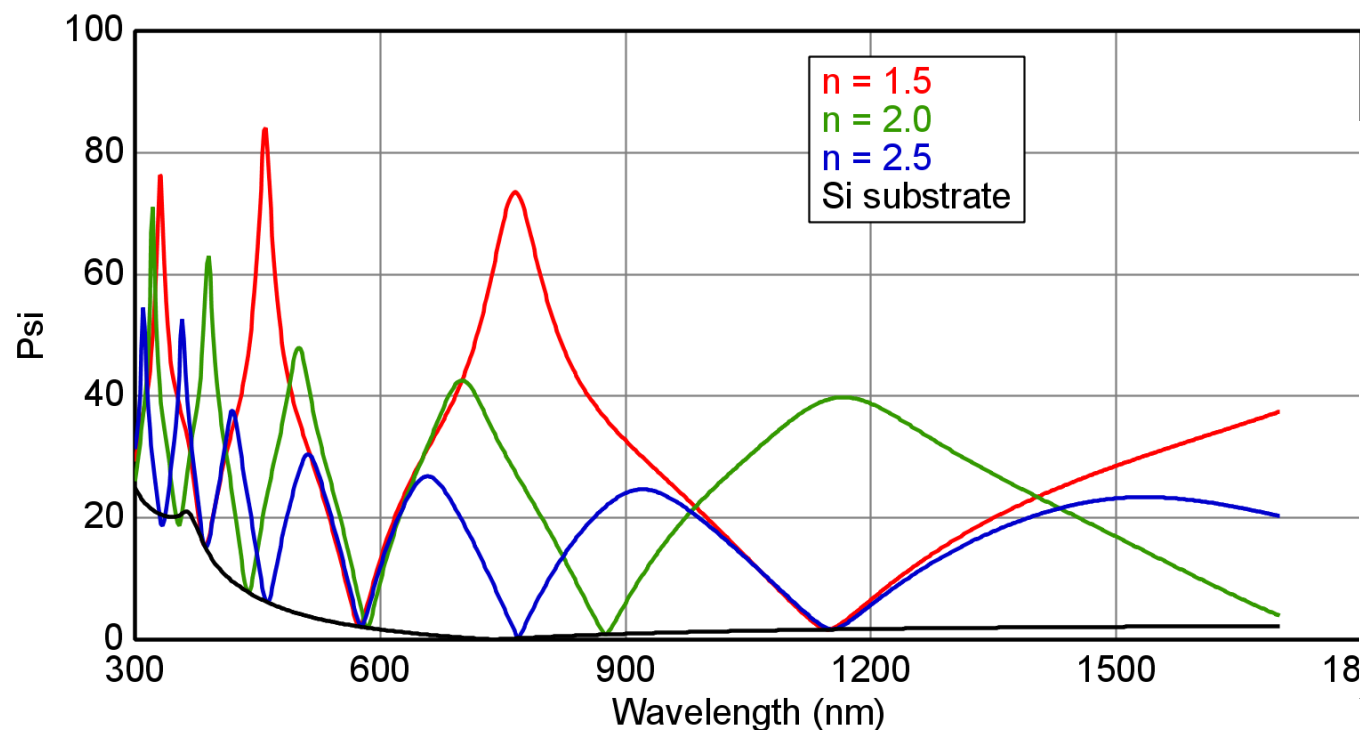


Index Effects

- Psi magnitude \sim index difference between film & substrate.
- Greater index difference = greater amplitude.
- Index also affects # of oscillation fringes.



Spectroscopic Ellipsometric (SE) Data





Fitting Transparent Thin Films

I

Use Existing
MATERIAL files

II

Use CAUCHY

III

Use
AUTOMATED
MODEL





Using Existing Mat files

- Refractive index of a film is fixed to predetermined values.
- Determine ONLY thickness.
- Works well when layer is stable and consistent, such as Si or silicon thermal oxide.
- Useful when ellipsometry lacks sensitivity to refractive index, such as ultra-thin films or in multi-layer stack.

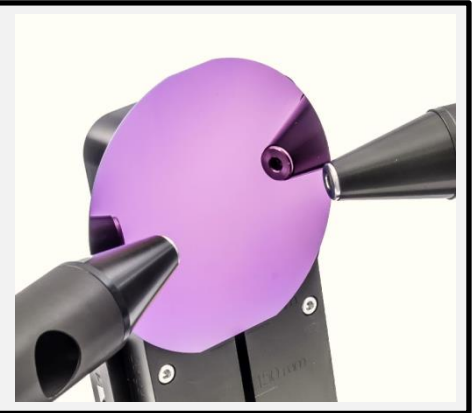


Use Existing
MATERIAL files

[2-01] Thermal SiO₂ on Si

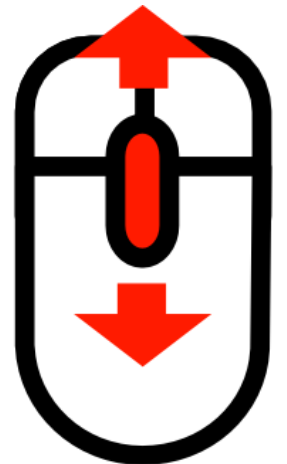
- Determine thickness using existing optical constants.

Use Existing
MATERIAL files



- Use “Si_JAW.mat” for substrate
- Add “SiO2_JAW.mat” for layer.
- Adjust thickness and fit.

Use Roller-Wheel
over the thickness
SHIFT X10
or
CTRL-SHIFT X1

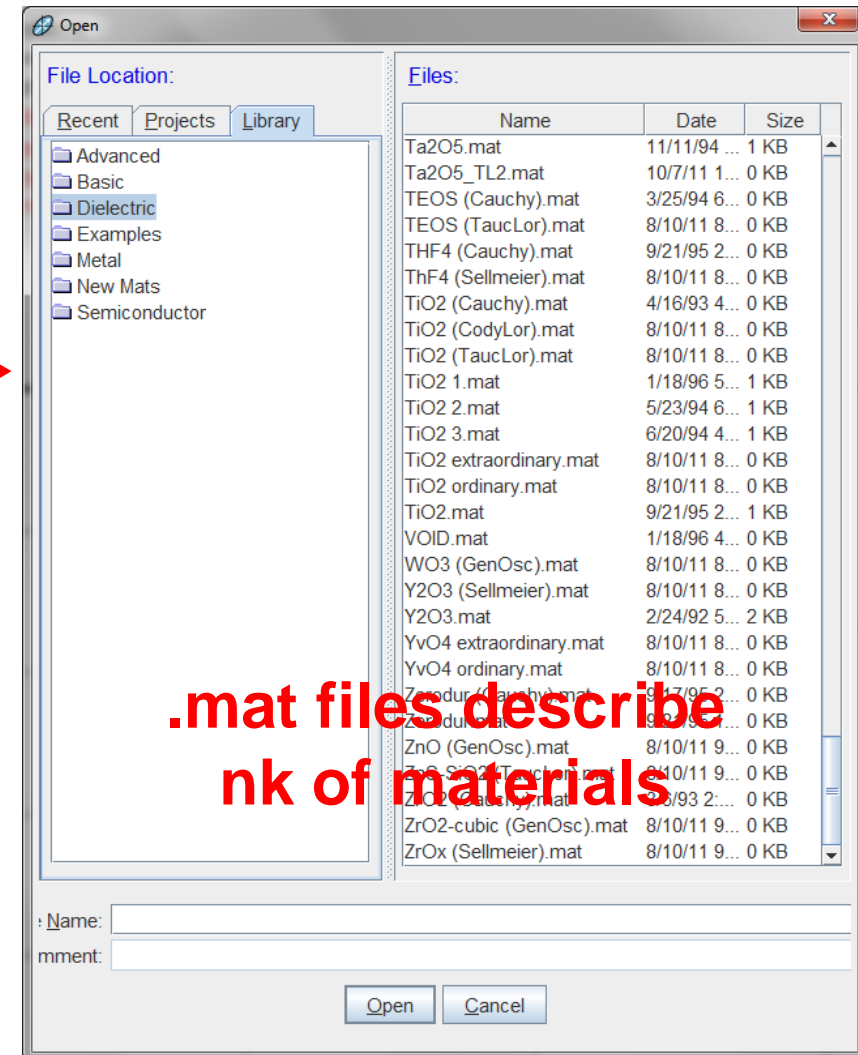
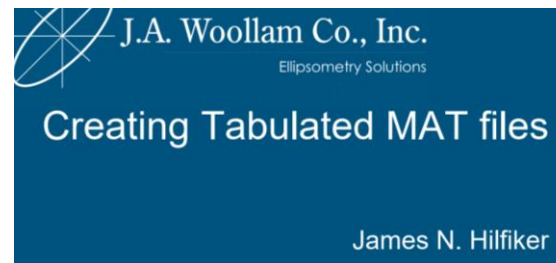
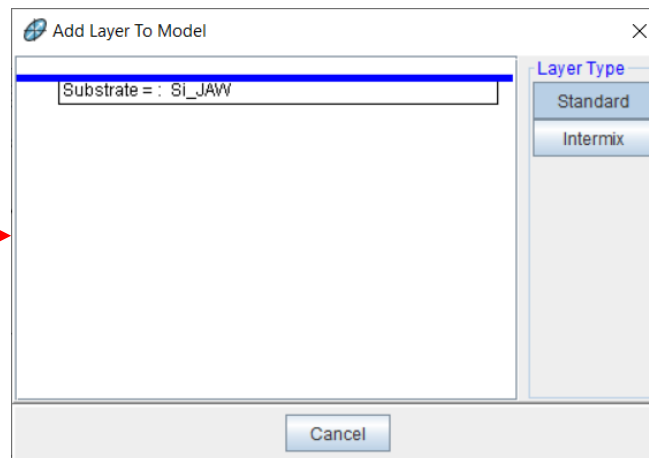




Existing Material Files

Use Existing
MATERIAL files

Layer Commands: **Add Delete Save**
Include Surface Roughness = **OFF**
Substrate = **Si_JAW**



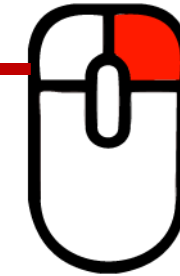
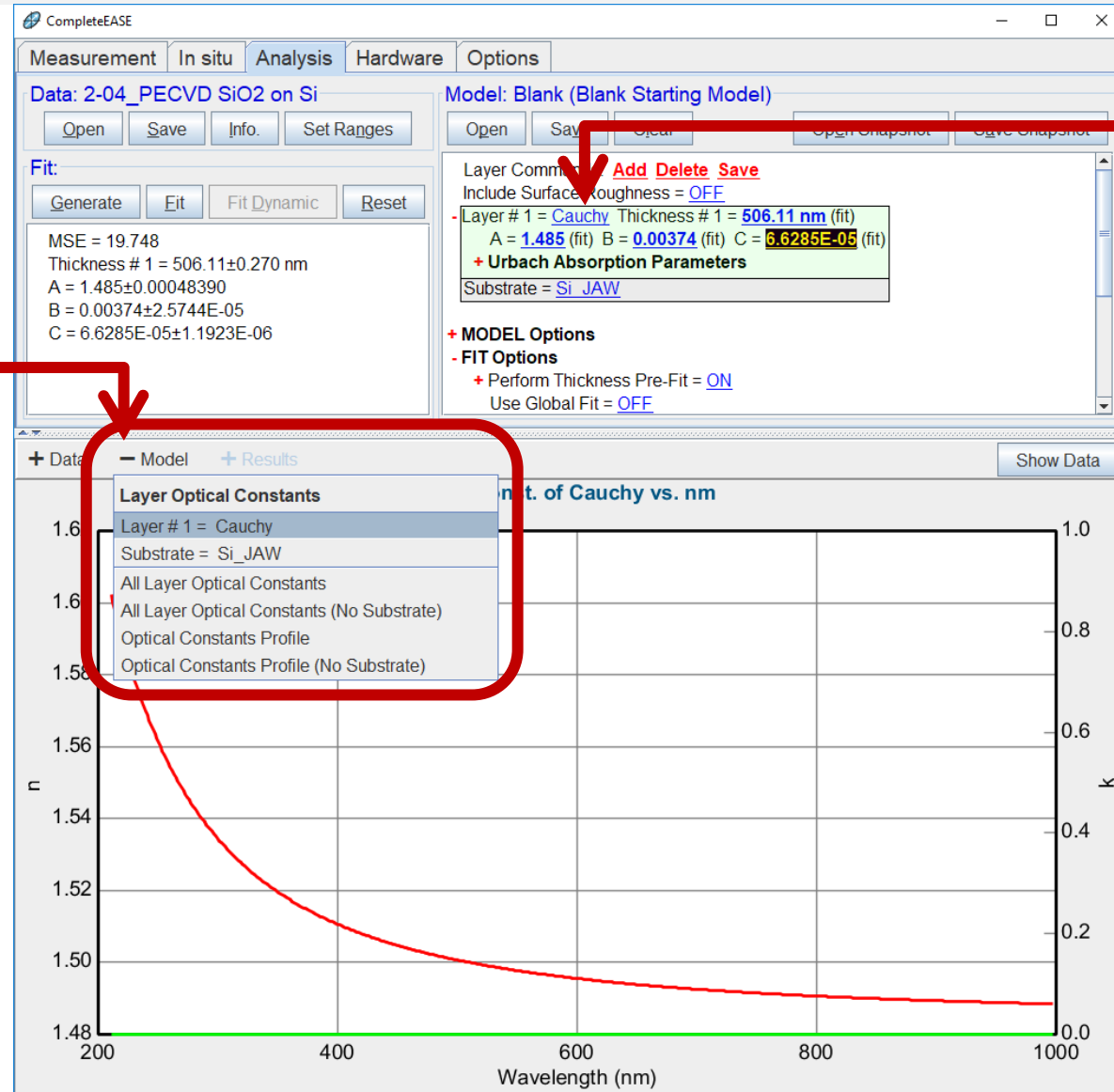
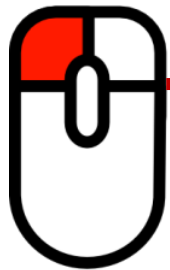
.mat files describe
bank of materials

Palik, E. D. Handbook of Optical Constants of Solids
(3 Volumes) Academic Press, San Diego, 1998.

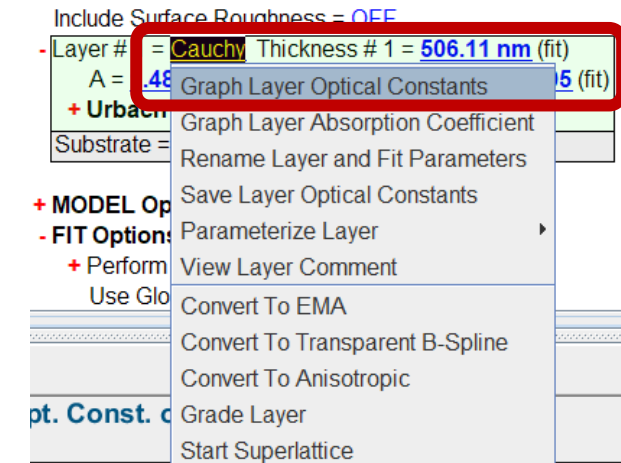


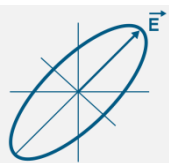
Viewing Optical Constants

Left-Click on
Model menu,
choose Layer



Right-Click on
Layer Name





2-01 Thermal SiO₂ on Si: Results



Fit Results

MSE = 9.439

Thickness # 1 = 188.72 ± 0.011 nm

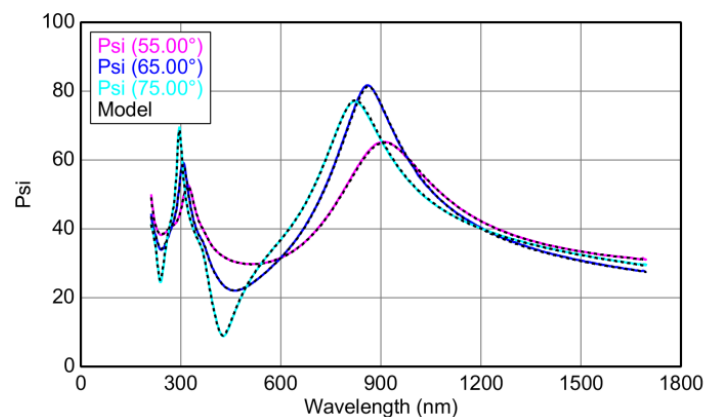
Optical Model

Layer # 1 = SiO₂_JAW Thickness # 1 = 188.72 nm (fit)

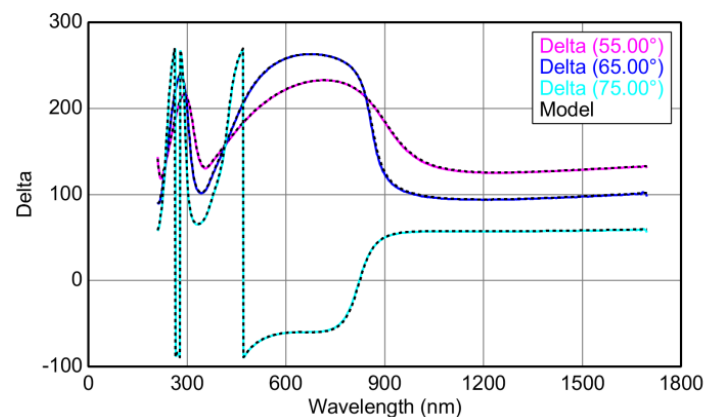
Substrate = Si_JAW

Experimental and Model Generated Data Fits

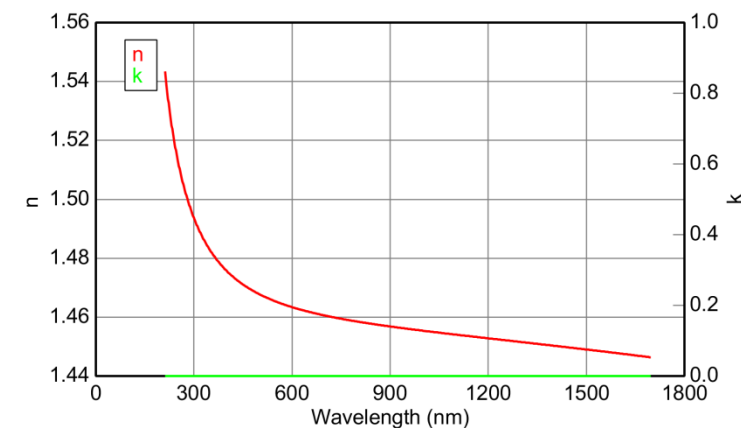
Variable Angle Spectroscopic Ellipsometric (VASE) Data



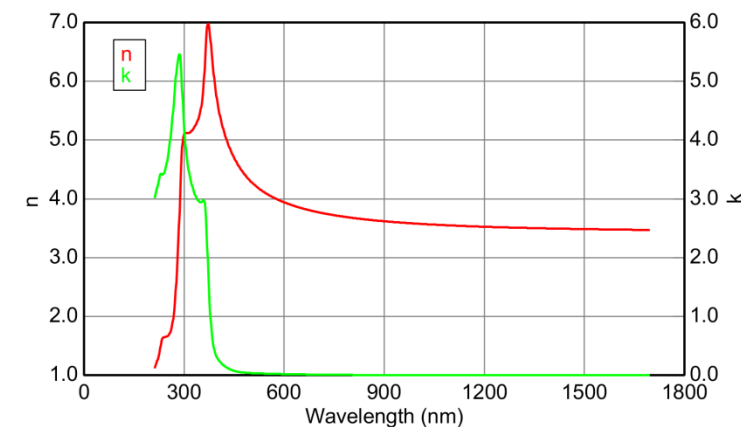
Variable Angle Spectroscopic Ellipsometric (VASE) Data

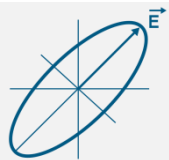


Opt. Const. of SiO₂_JAW vs. nm



Opt. Const. of Si_JAW vs. nm





Si with Thermal Oxide Built-in Models

Systems with wvls up to 1700nm

Layer # 2 = SIO2_JAW Thickness # 2 = 100.00 nm (fit)
Layer # 1 = INTR_JAW Thickness # 1 = 1.00 nm
Substrate = SI_JAW

- MODEL Options

Angle Offset = [0.00](#) (fit)

- Built for silicon with thermal oxide samples
 - Backside reflection not included.
- Recommend to use for system health check
- Angle offset is a hardware parameter and should not be sample-dependent for ex-situ systems
 - Only be validated with calibration wafers

RC2 XNIR Systems (wvls up to 2500nm)

+ Layer # 2 = SiO2_uniaxial_JAW3 Thickness # 2 = 1000.00 nm (fit)
Layer # 1 = Intr_JAW3 Thickness # 1 = 1.00 nm
Substrate = Si_JAW3

- MODEL Options

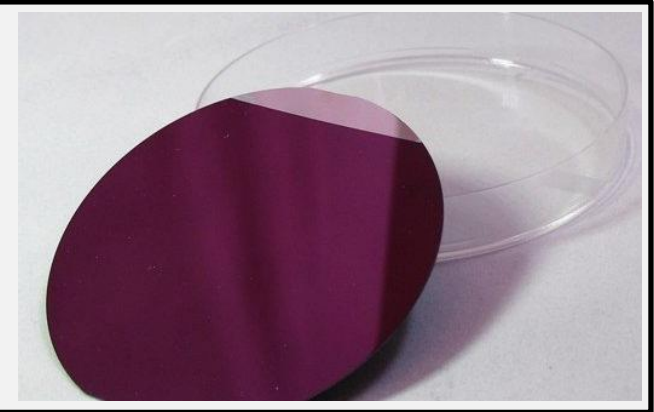
Angle Offset = [0.00](#) (fit)

*C. M. Herzinger et al, *Ellipsometric determination of optical constants for silicon and thermally grown silicon dioxide via a multi-sample, multi-wavelength, multi-angle investigation*, Journal of Applied Physics, 83,6,3323 (1998)

[2-02] Ta_2O_5 on Si

- Fit data using Ta2O5.mat

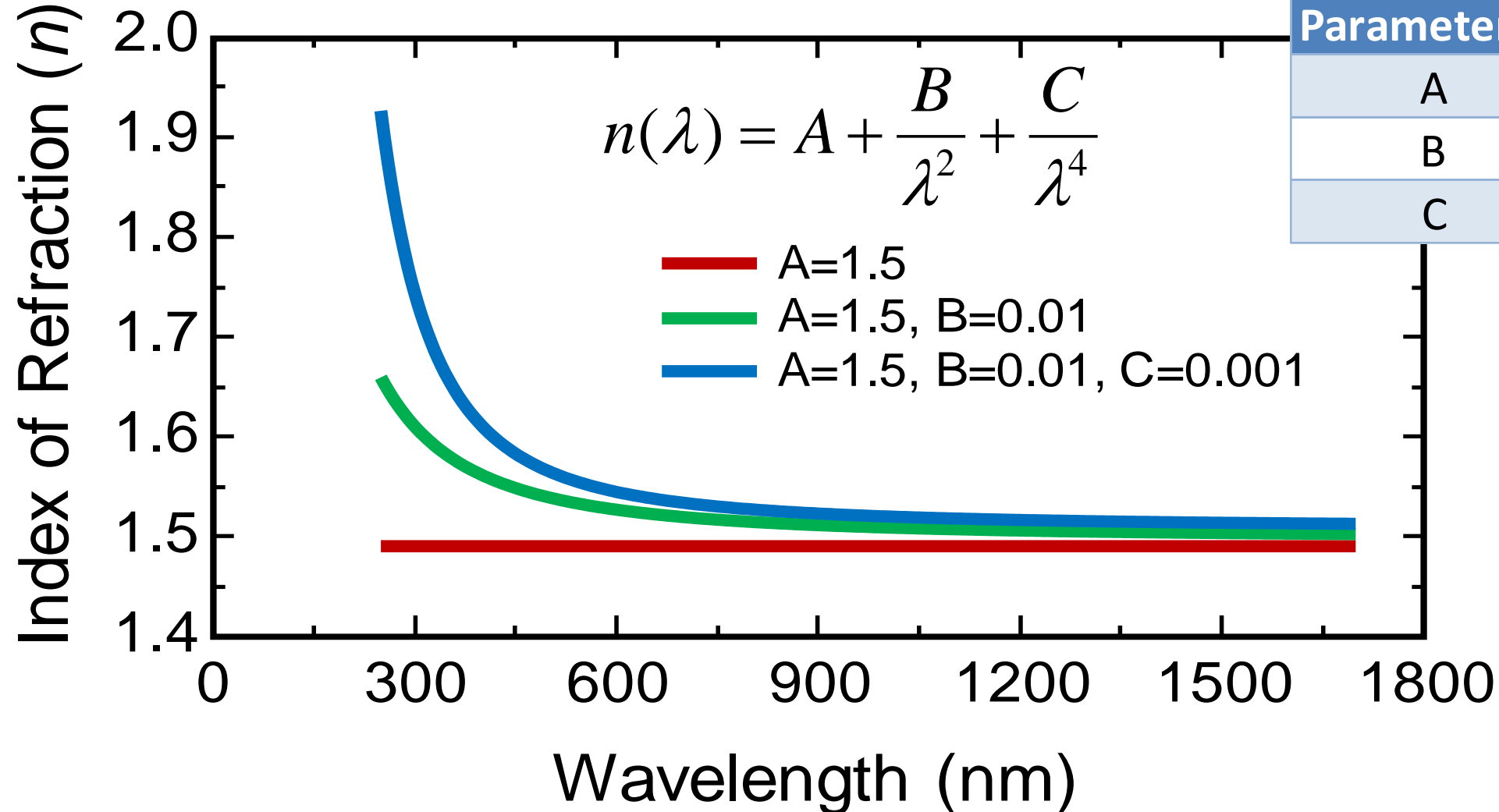
Use Existing
MATERIAL files



- Copy index of refraction to Graph Scratchpad
- What can be done to further improve the fit?



Cauchy Parameters



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

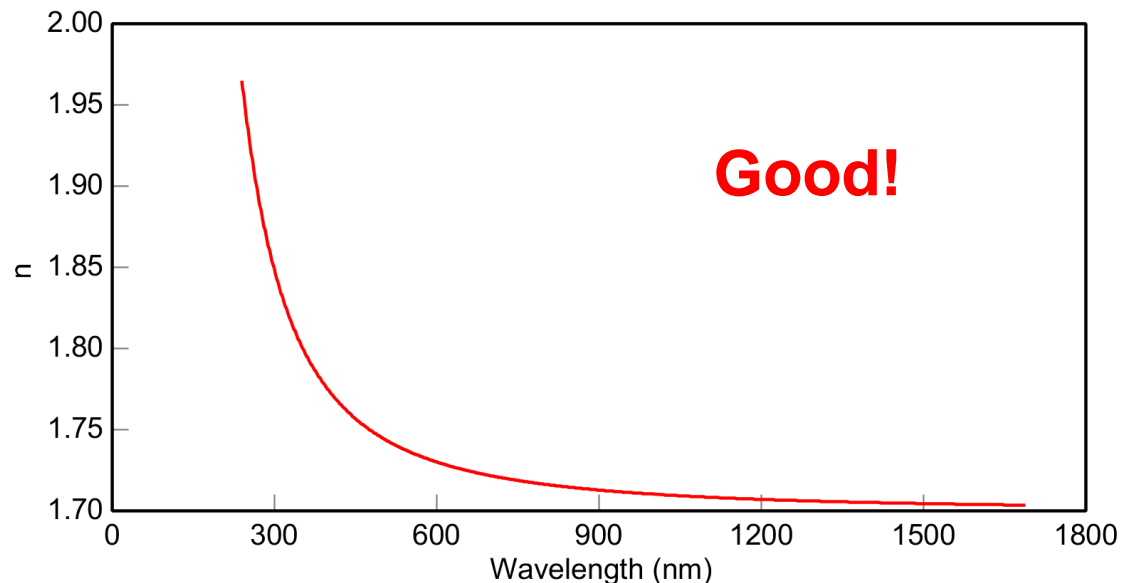


Physicality of Cauchy Dispersion

Physical

- Transparent index of refraction must increase with decreasing wavelengths (referred to as **normal dispersion**)

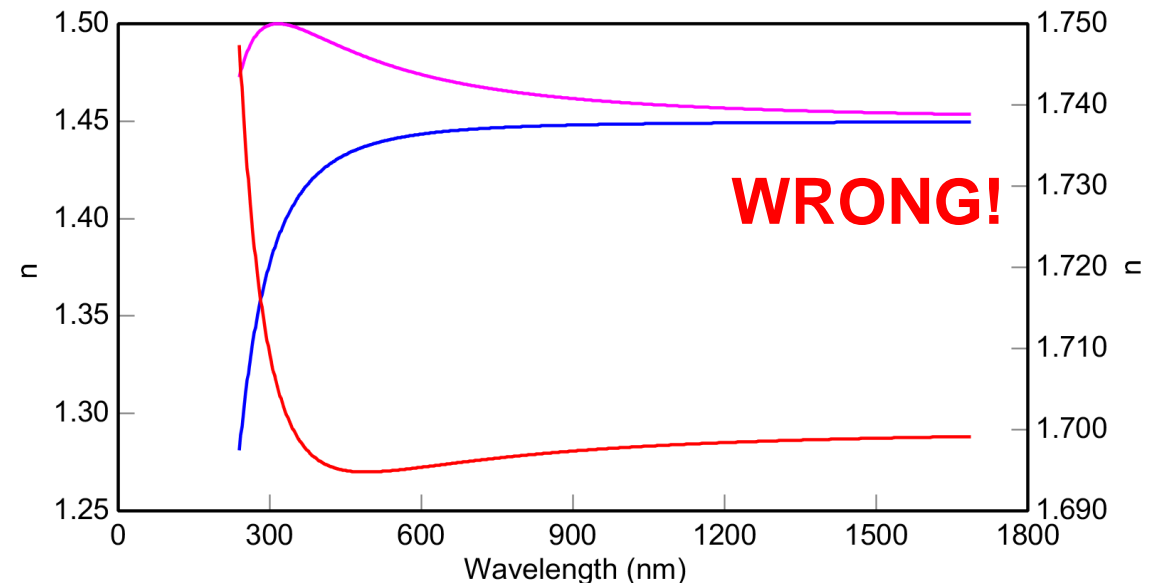
Physical Cauchy Index of Refraction

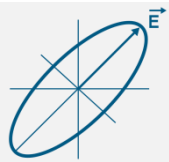


Unphysical

- If transparent index of refraction (n) decreases towards shorter wavelengths.
- Possible solutions
 - Reset $C=0$
 - Reduce the wavelength range
 - Add absorption

Unphysical Cauchy Index of Refraction





Which results are physical?

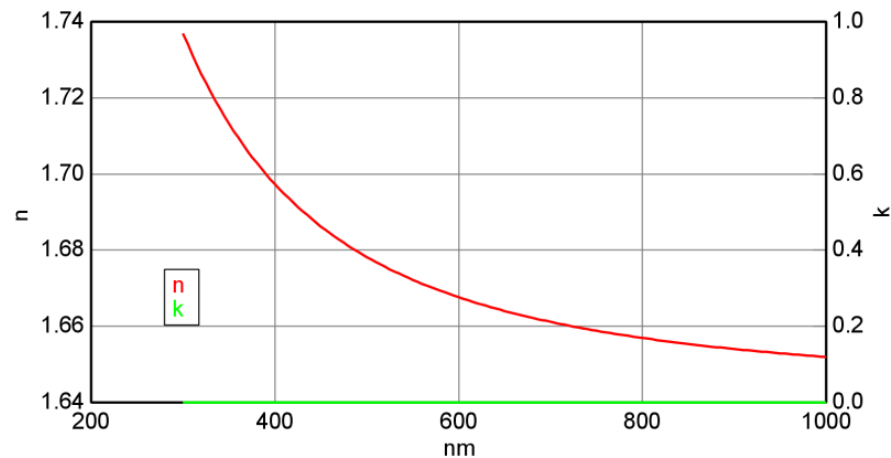
A

Opt. Const. of Cauchy vs. nm

$$A = 1.643$$

$$B = 0.009$$

$$C = -4.8600\text{E-}05$$



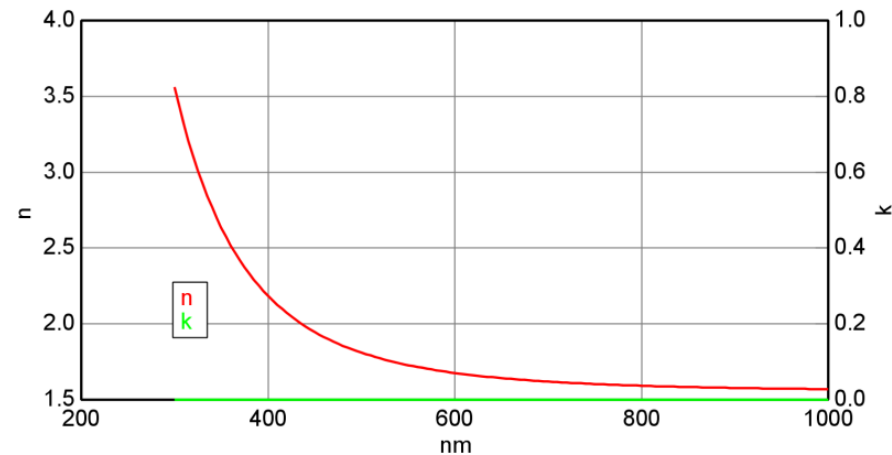
B

Opt. Const. of Cauchy vs. nm

$$A = 1.555$$

$$B = -0.00177$$

$$C = 0.01640$$



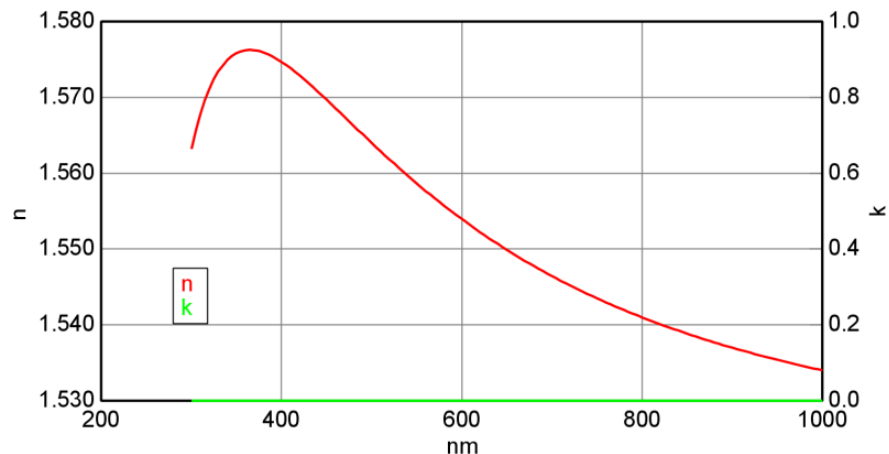
C

Opt. Const. of Cauchy vs. nm

$$A = 1.520$$

$$B = 0.015$$

$$C = -0.001$$



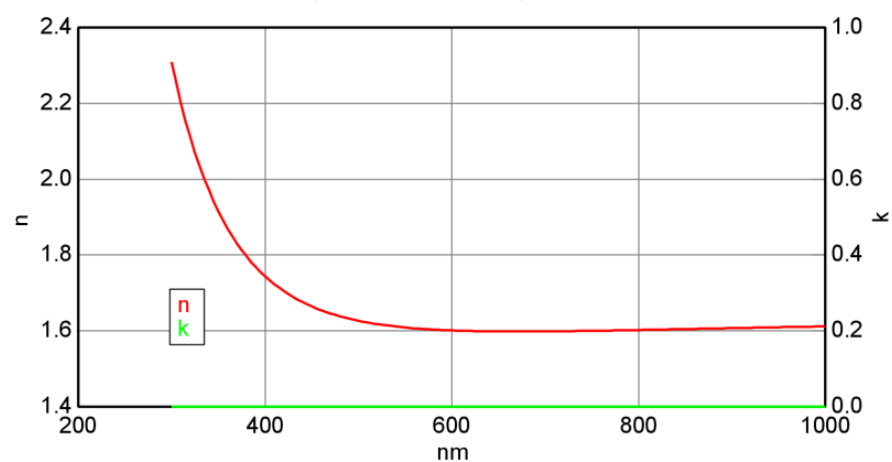
D

Opt. Const. of Cauchy vs. nm

$$A = 1.643$$

$$B = -0.04009$$

$$C = 0.009$$





Cauchy Procedure

Use CAUCHY

Estimate Index
(Cauchy-A)



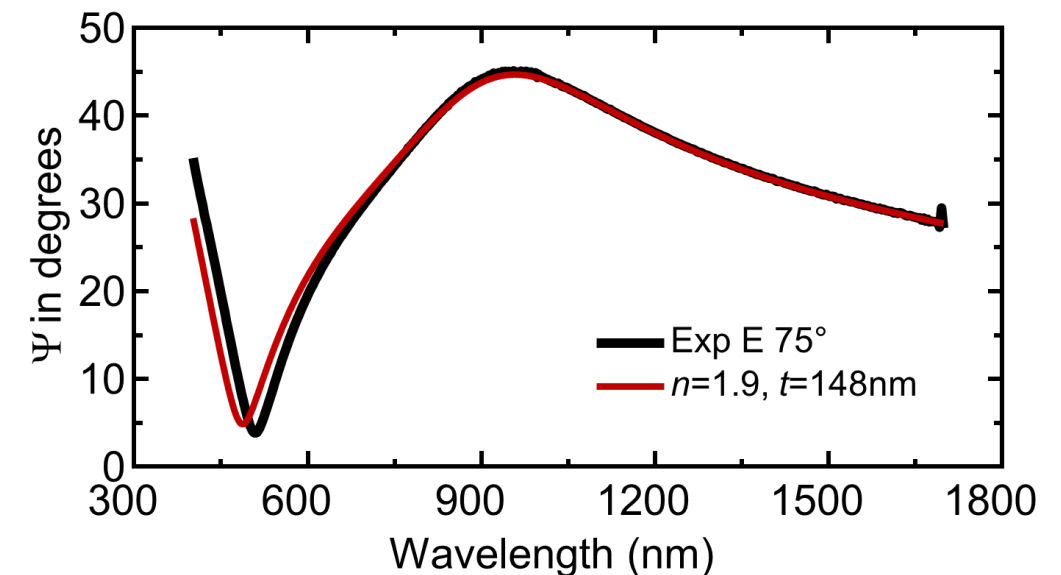
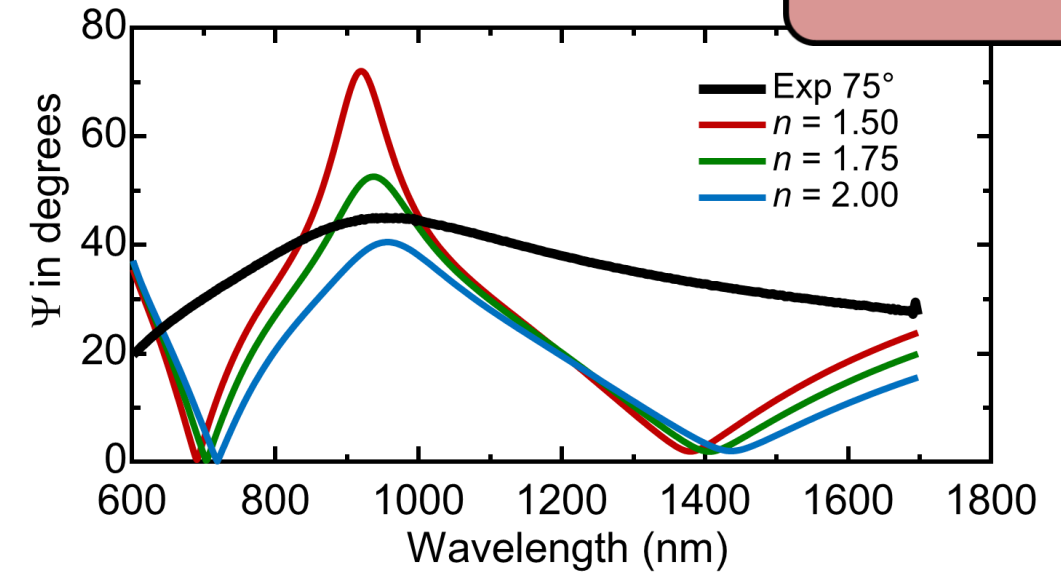
Estimate Thickness



Fit Thickness & Cauchy Parameters

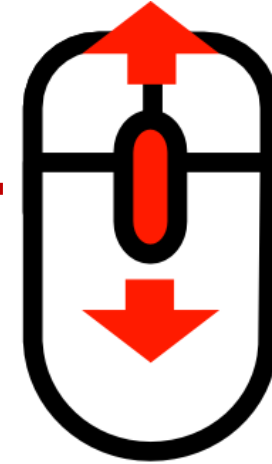
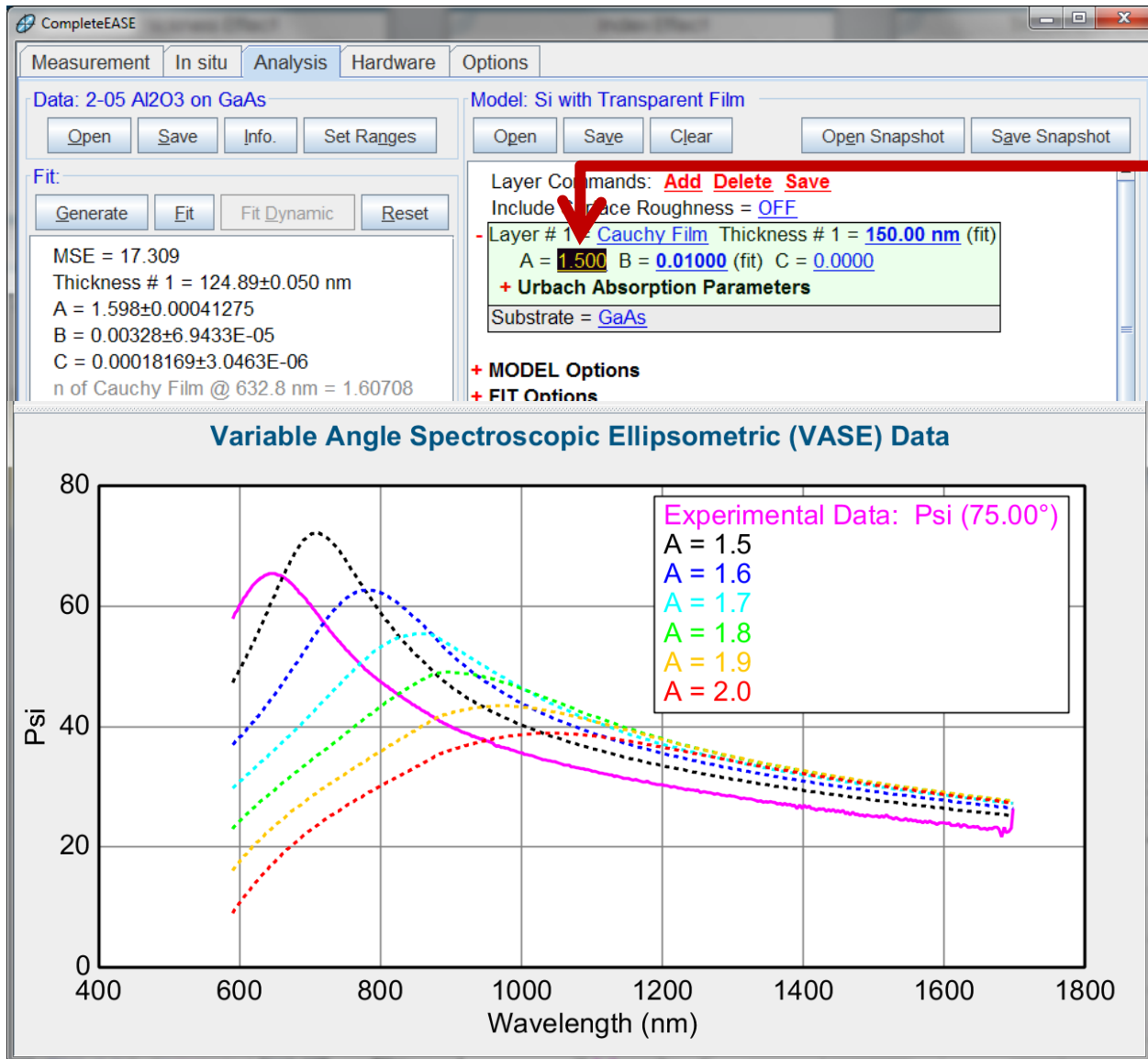


Start with $B = 0.01$ and $C=0$,
only add at end if needed



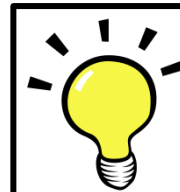


Estimating the Index



SHIFT
or
CTRL-SHIFT

Roll the 'A' parameter until Psi peaks / valleys have same amplitude as data curves.

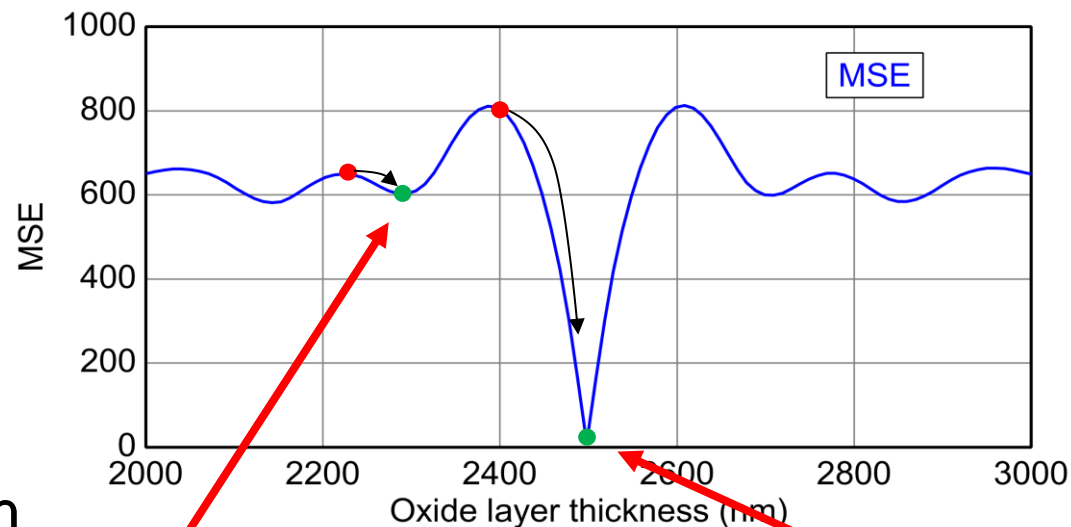


Keep B = 0.01, C=0
Range of 'A' between 1.3 and 2.5



Start Values Matter

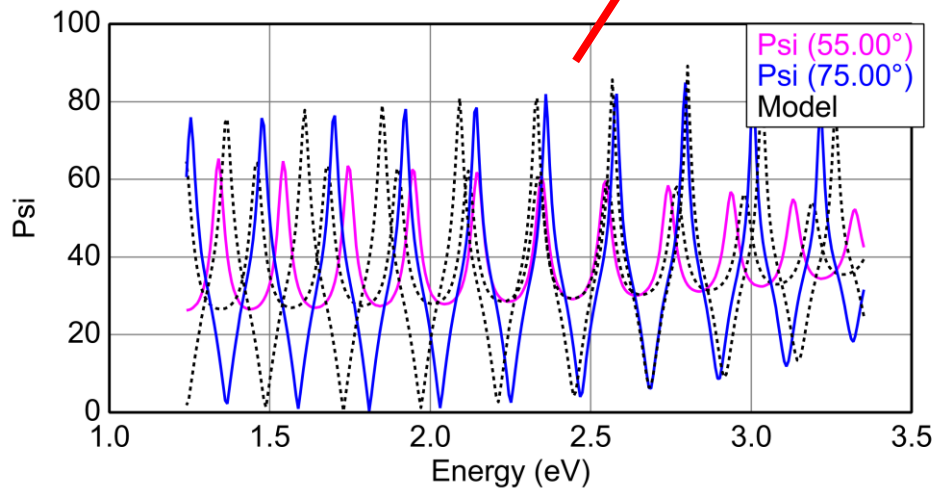
Parameter Uniqueness Fit



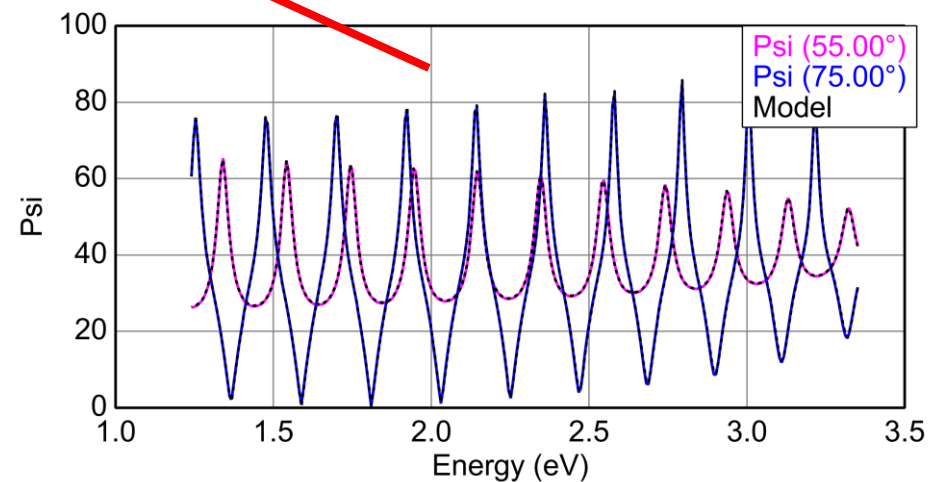
AVOID Local Minimum

Global Minimum

Variable Angle Spectroscopic Ellipsometric (VASE) Data



Variable Angle Spectroscopic Ellipsometric (VASE) Data





“Auto” Cauchy Procedure

III

Use
AUTOMATED
MODEL

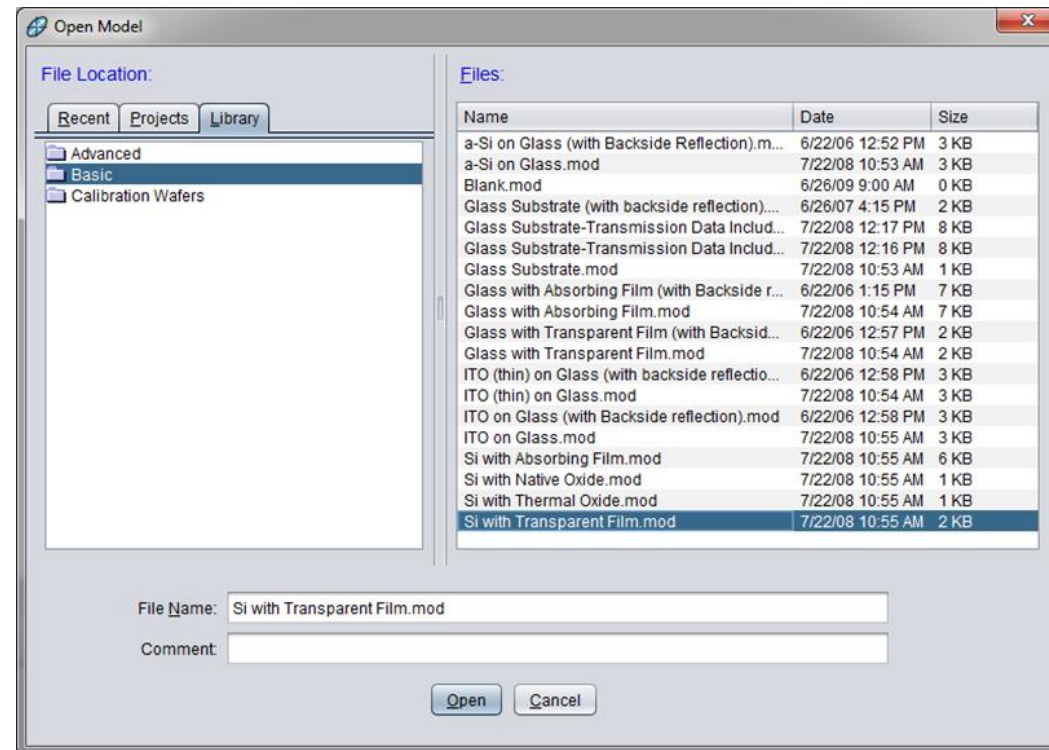
Estimate
Thickness & Index



Fit Thickness &
Cauchy Parameters

Si with Transparent Film.mod

(uses Thickness Pre-Fit & Global Fit)





Si with Transparent Film.mod

Include Surface Roughness = [OFF](#)

- Layer # 1 = [Cauchy Film](#) Thickness # 1 = [100.00 nm](#) (fit)

A = [1.500](#) (fit) B = [0.0000](#) (fit) C = [0.0000](#) (fit)

+ [Urbach Absorption Parameters](#)

Substrate = [SI_JAW](#)

+ MODEL Options

- FIT Options

- + Perform Thickness Pre-Fit = [ON](#)
- Use Global Fit = [ON](#)
 - # of Data Points = [20](#) # of Iterations = [5](#)
 - Parm #1 = [A](#)
 - Min. = [1.300](#) Max. = [3.000](#) # Guesses = [30](#)
 - Parm #2 = [\(none\)](#)
 - Parm #3 = [\(none\)](#)
 - Include Wvl. Range Expansion Fits = [OFF](#)

Fit Weight = [N.C.S](#)

Limit Wvl. for Fit = [OFF](#)

Limit Angles for Fit = [OFF](#)

Max. Acceptable MSE = [100.000](#)

- Include Derived Parameters = [ON](#)

[Add Derived Parameter](#)

1: Type = [n](#) Layer # = [1](#) Wavelength = [632.8 nm](#) Name = [n @ 632.8 nm](#) Hide = [OFF](#)

of Decimal Places = [5](#)

Low Spec. = [0.00](#) High Spec. = [0.00](#)

+ OTHER Options

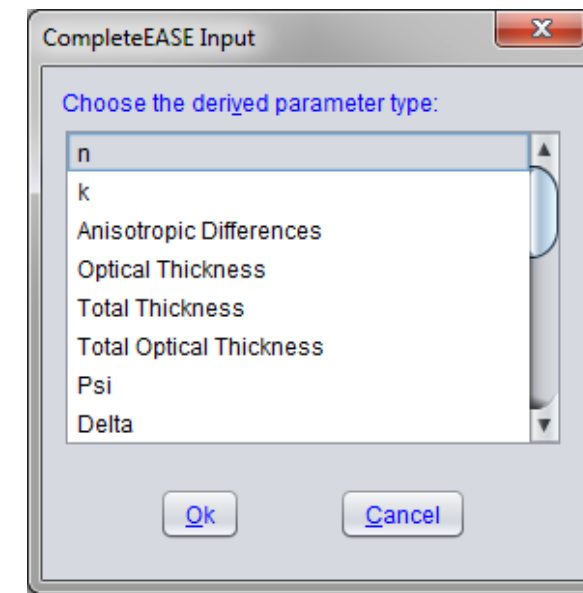
[Configure Options](#)

[Turn Off All Fit Parameters](#)

- Valid for Si substrate with transparent film, **NO backside reflections**
- Cauchy A, B, C and thickness already ON
- Includes Thickness Pre-Fit, Global Fit for Cauchy A, derived parameter $n@632.8\text{nm}$



Use for Preliminary Search. Turn OFF when close to answer



Always remember to check if the refractive index is physical!

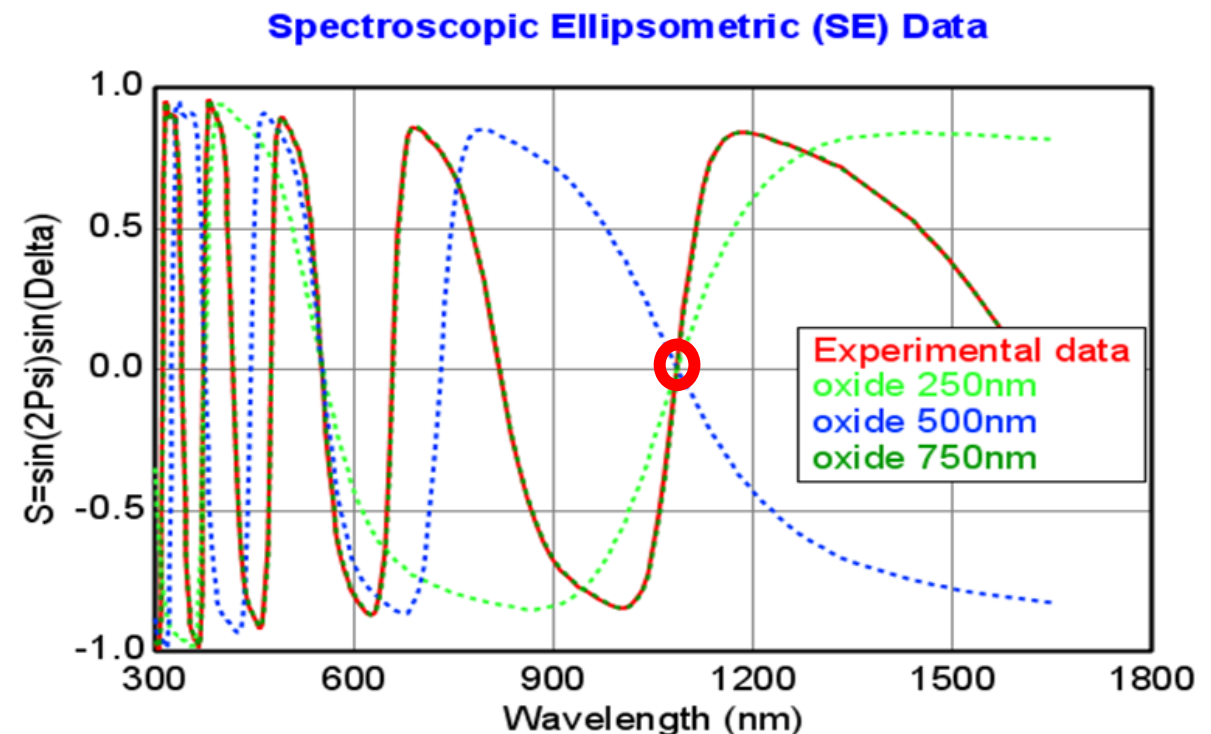


Thickness Prefit

- **Very Fast** algorithm to identify possible thickness values
 - Useful in built-in model, unknown start values, thick films and mapping data
 - Need correct index, since index also affects interference.



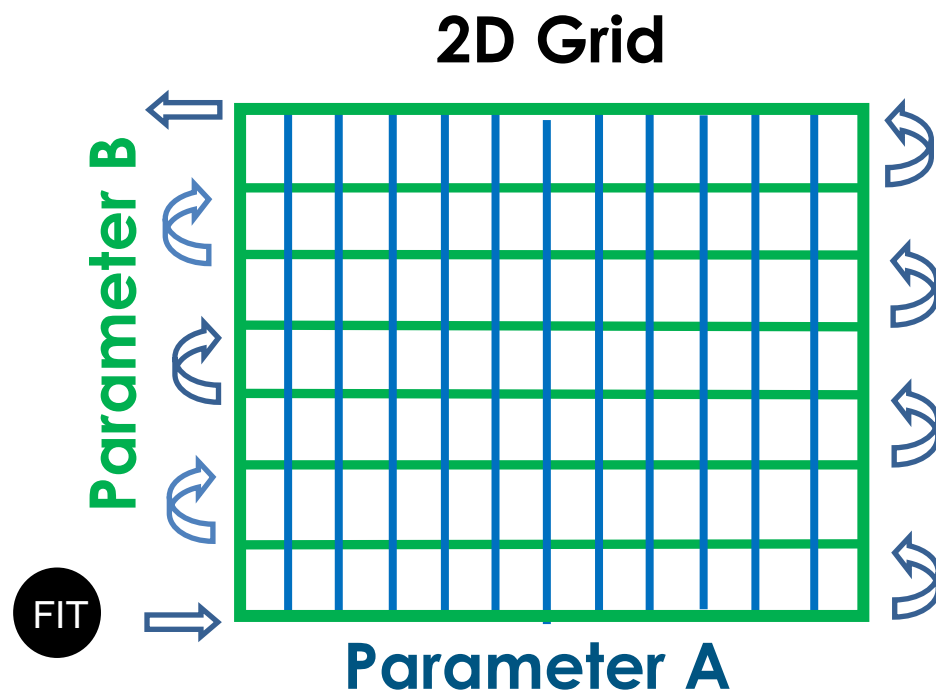
Combine with Global Fit for Index to improve search.





Global Fit

- Search any fit parameter using a grid of possible values
- Helps avoid “local” MSE minimums



Layer Commands: **Add Delete Save**

Include Surface Roughness = **ON** Roughness = **6.67 nm** (fit)

+ Layer # 1 = **Cauchy Film** Thickness # 1 = **118.11 nm** (fit)
Substrate = **SI_JAW**

+ MODEL Options

- FIT Options

+ Perform Thickness Pre-Fit = **ON**

- Use Global Fit = **ON**

Parameters: **Add Delete All**

x Param. #1 = **A**

Min. = **1.300** Max. = **3.000** # Guesses = **30**

+ Customize Global Fit

Fit Weight = **N,C,S**

Limit Wvl. for Fit = **OFF**

Limit Angles for Fit = **OFF**

Max. Acceptable MSE = **100.000**

+ Include Derived Parameters = **ON**

+ OTHER Options

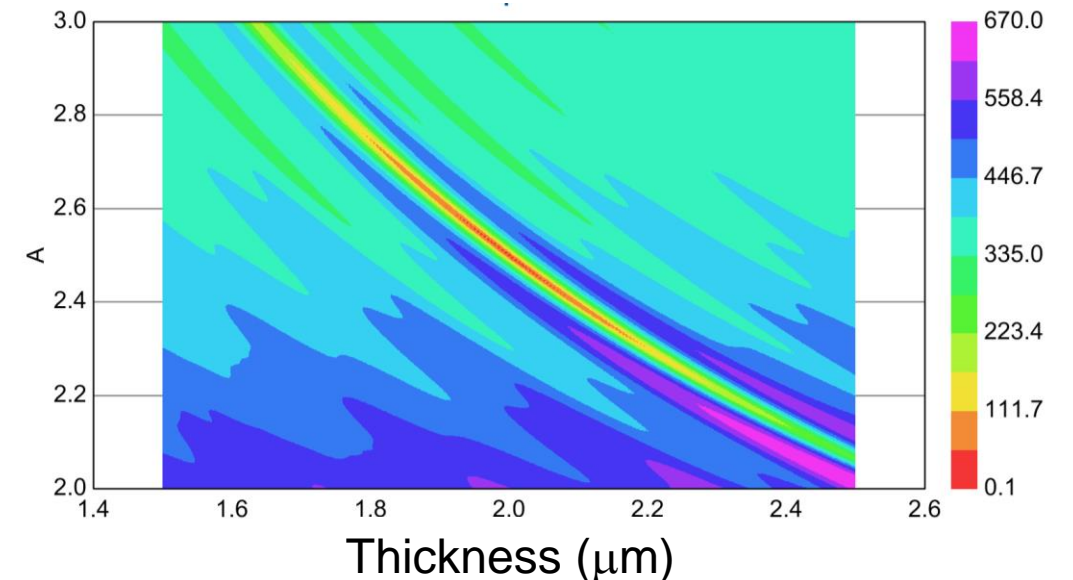
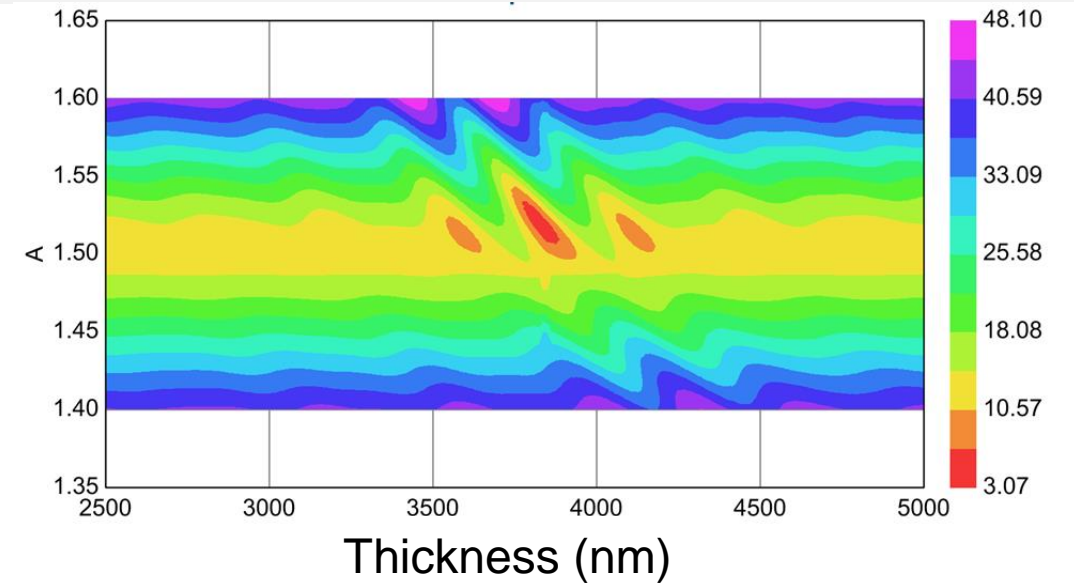
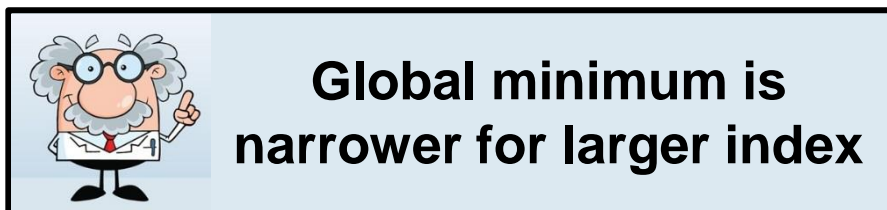
Configure Options

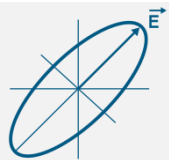
Turn Off All Fit Parameters



Global Fit “Guidelines”

- Search every 50 nm thickness.
 - 20 guesses for every 1 micron.
- Search every 0.05 index.
 - 20 guesses for every n range of 1.
- Limit total “# guesses” to avoid long fitting times.
 - Avoid fitting Cauchy “B” and “C”





Derived Parameters

Calculates or reports user-selected values based on Fit Results

Layer Commands: [Add](#) [Delete](#) [Save](#)

Include Surface Roughness = [OFF](#)

+ Layer # 1 = [Cauchy](#) Thickness # 1 = [1000.00 Å](#) (fit)
Substrate = [SI_JAW](#)

+ MODEL Options

- FIT Options

+ Perform Thickness Pre-Fit = [ON](#)

+ Use Global Fit = [ON](#)

Fit Weight = [N.C.S](#)

Limit Wvl. for Fit = [OFF](#)

Limit Angles for Fit = [OFF](#)

Max. Acceptable MSE = [100.000](#)

- Include Derived Parameters = [ON](#)

[Add Derived Parameter](#)

1: Type = [n](#) Layer # = [1](#) Wavelength = [632.8 nm](#) Name = [n @ 632.8 nm](#) Hide = [OFF](#)

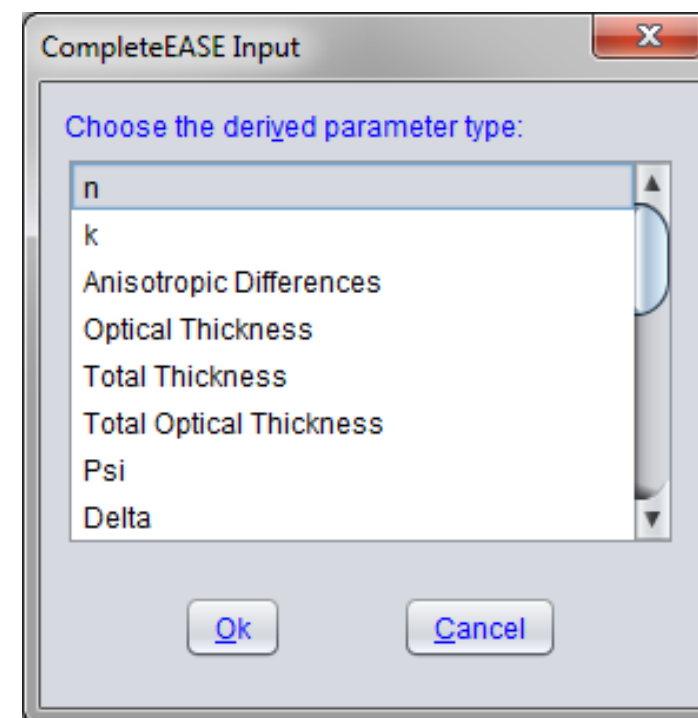
of Decimal Places = [5](#)

Low Spec. = [0.00](#) High Spec. = [0.00](#)

+ OTHER Options

[Configure Options](#)

[Turn Off All Fit Parameters](#)





2-02 Ta₂O₅ on Si: Results



Fit Results

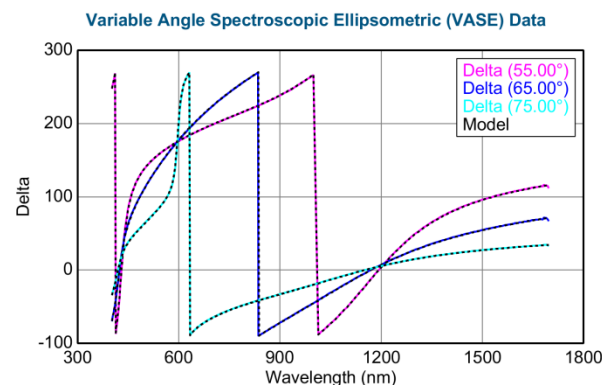
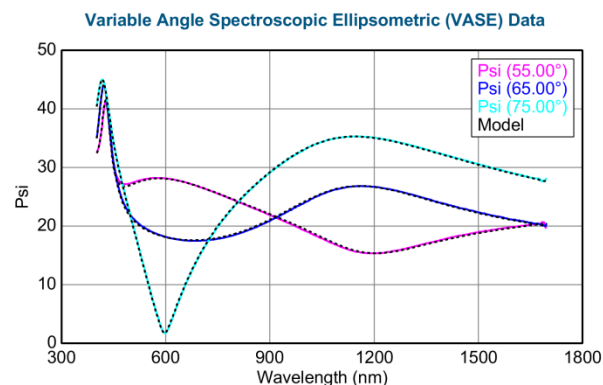
MSE = 5.117
Thickness # 1 = 152.34 ± 0.019 nm
A = 2.106 ± 0.00024121
B = 0.02241 ± 0.00023662
C = $0.00124 \pm 3.4986\text{E-}05$

Optical Model

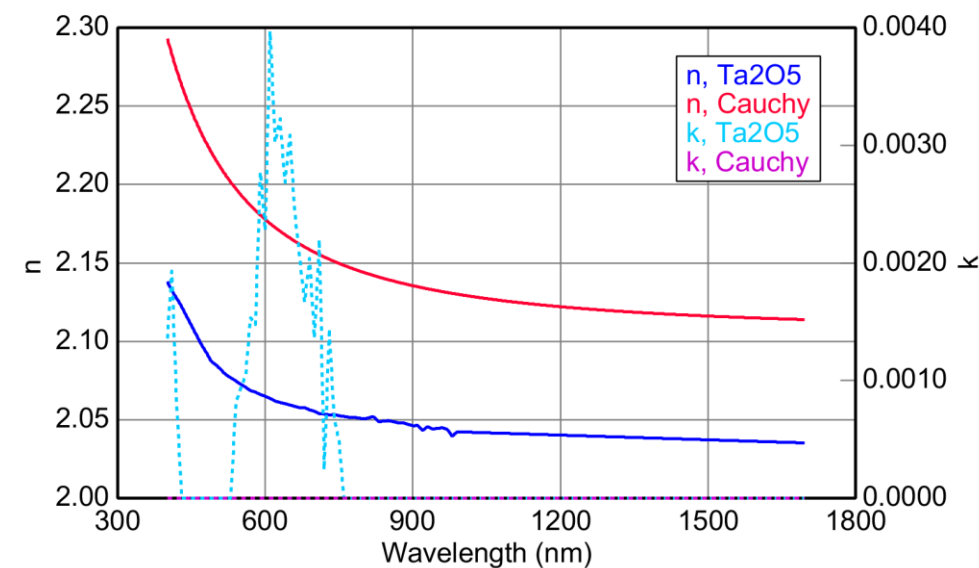
- Layer # 1 = Cauchy Thickness # 1 = 152.34 nm (fit)
A = 2.106 (fit) B = 0.02241 (fit) C = 0.00124 (fit)
+ Urbach Absorption Parameters
Substrate = Si_JAW

	MSE	Ta2O5 Thickness (nm)	n @ 632.8 nm
Ta2O5	77.416	163.64	2.061
Cauchy	5.117	152.34	2.170

Experimental and Model Generated Data Fits

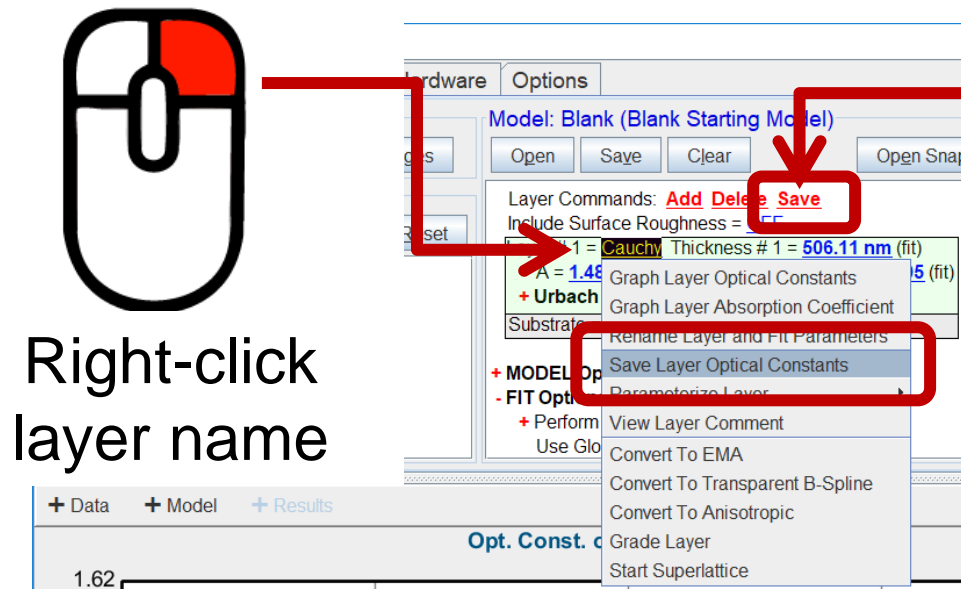


Opt. Const. of Ta2O5



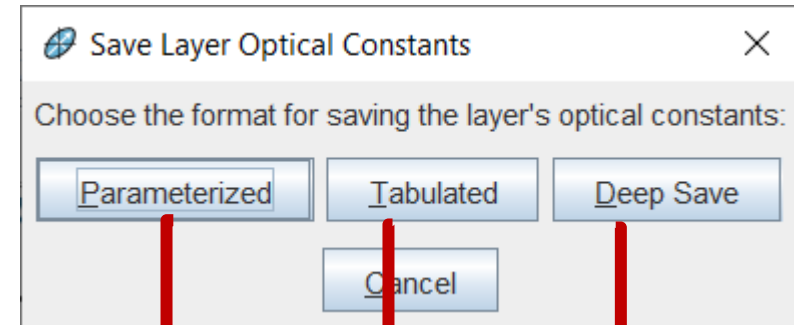


Saving Material Files



Right-click
layer name

Left-click Save Layer Command
Choose Format



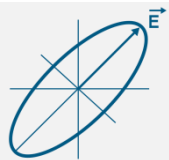
- Layer # 3 = MgF2_Parm_c Thickness # 3 = 0.00 nm
A = 1.378 B = 0.00309 C = -7.6324E-06
+ Urbach Absorption Parameters
- Layer # 2 = MgF2_Tab Thickness # 2 = 0.00 nm
- Layer # 1 = MgF2_Deep_c Thickness # 1 = 0.00 nm (fit)
A = 1.378 (fit) B = 0.00309 (fit) C = -7.6329E-06 (fit)
+ Urbach Absorption Parameters
- Substrate = SI_JAW

Save parameters

Fixed table

Save parameters, range and will
be default as fit parms

ANGSTROMS	n	k
1900.0000	2.1254433	0.0000000
1910.0000	2.1231935	0.0000000
1920.0000	2.1209763	0.0000000
1930.0000	2.1187910	0.0000000
1940.0000	2.1166372	0.0000000
1950.0000	2.1145141	0.0000000
1960.0000	2.1124213	0.0000000
1970.0000	2.1103582	0.0000000
1980.0000	2.1083243	0.0000000
1990.0000	2.1063190	0.0000000
2000.0000	2.1043410	0.0000000



Quick “Analysis Report”

- Copy data analysis details to clipboard.

1. Get model ready

OTHER Options:

“Add Opt. Const. to Report”

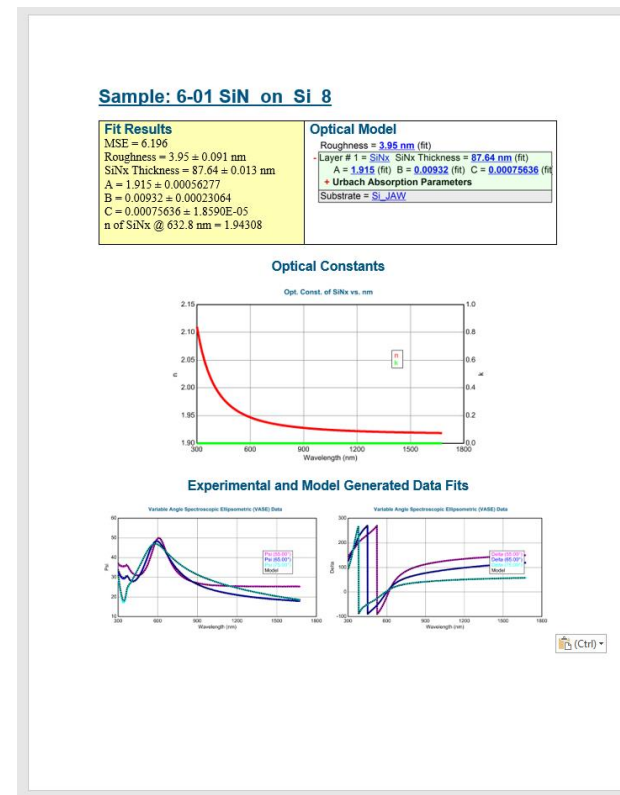
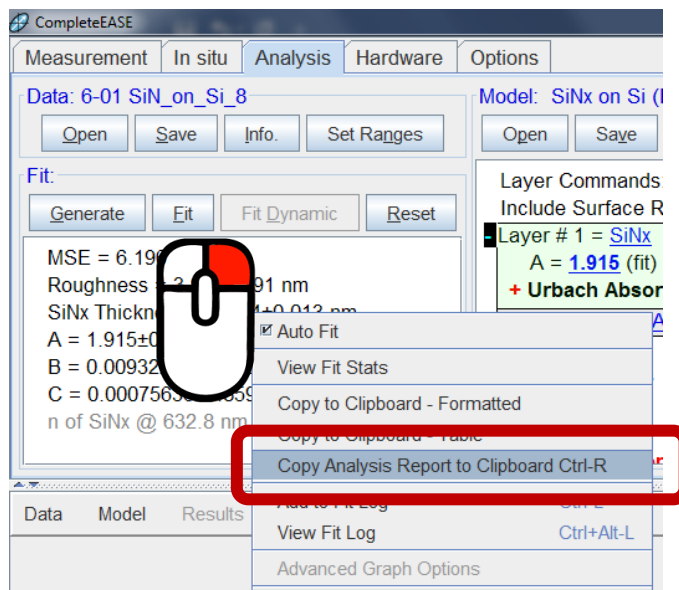
2. Right-click in Fit panel:

“Copy Analysis Report to Clipboard”

3. Paste

Layer Commands: **Add Delete Save**
 Include Surface Roughness = **ON** Roughness = **3.95 nm** (fit)
 - Layer # 1 = **SiNx** SiNx Thickness = **87.64 nm** (fit)
 A = **1.915** (fit) B = **0.00932** (fit) C = **0.00075636** (fit)
 + Urbach Absorption Parameters
 Substrate = **Si_JAW**

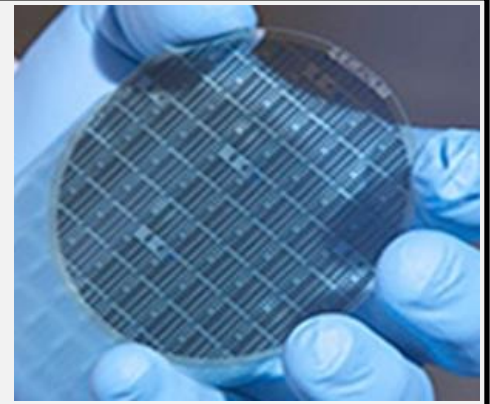
- + **MODEL Options**
 - + **FIT Options**
 - **OTHER Options**
 - Wvl. Range Expansion Fit** Increment (eV) = **0.50** **Graph**
 - Try Alternate Models** MSE Improvement Threshold = **25** %
 - Fit Parameter Uniqueness**
 - Fit Parameter Error Estimation**
- Add Opt. Const. to Report = **ON** Layer # = **1**
- Configure Options**
Turn Off All Fit Parameters



2-02 2-03 2-04 Built-in Models

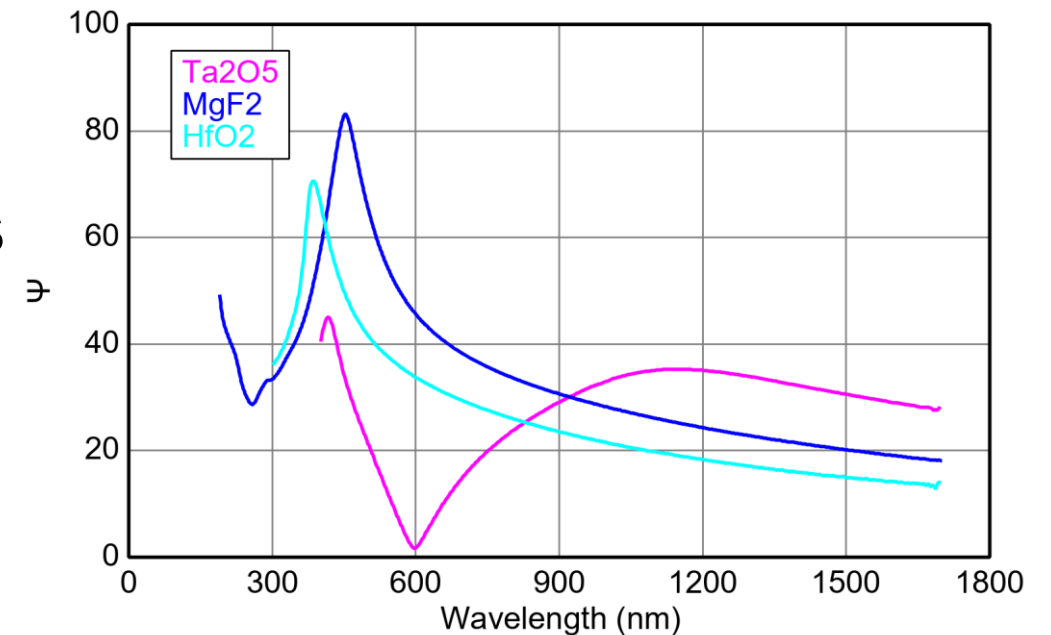
- Ta_2O_5 on Si
- MgF_2 on Si
- HfO_2 on Si

Use
AUTOMATED
MODEL



- Practice Built-in Model
- Save refractive index and snapshots

Variable Angle Spectroscopic Ellipsometric (VASE) Data



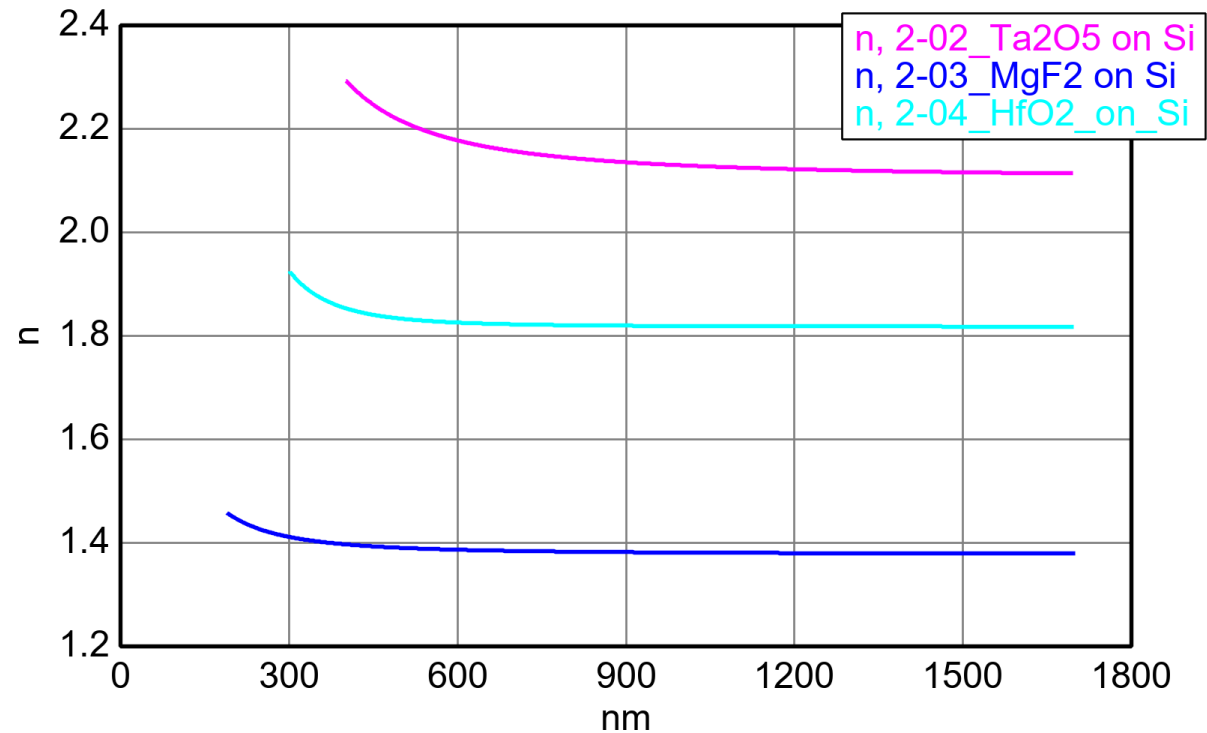


Built-in Model Practice Data Results



	MSE	Thickness	A	B	C	n @ 632.8 nm
2-02_Ta2O5 on Si	5.117	152.34	2.106	0.02242	0.00124	2.16961
2-03_MgF2 on Si	5.442	112.12	1.378	0.00309	-7.63E-06	1.38586
2-04_HfO2_on_Si	6.375	61.29	1.818	0.000604	0.000824	1.8243

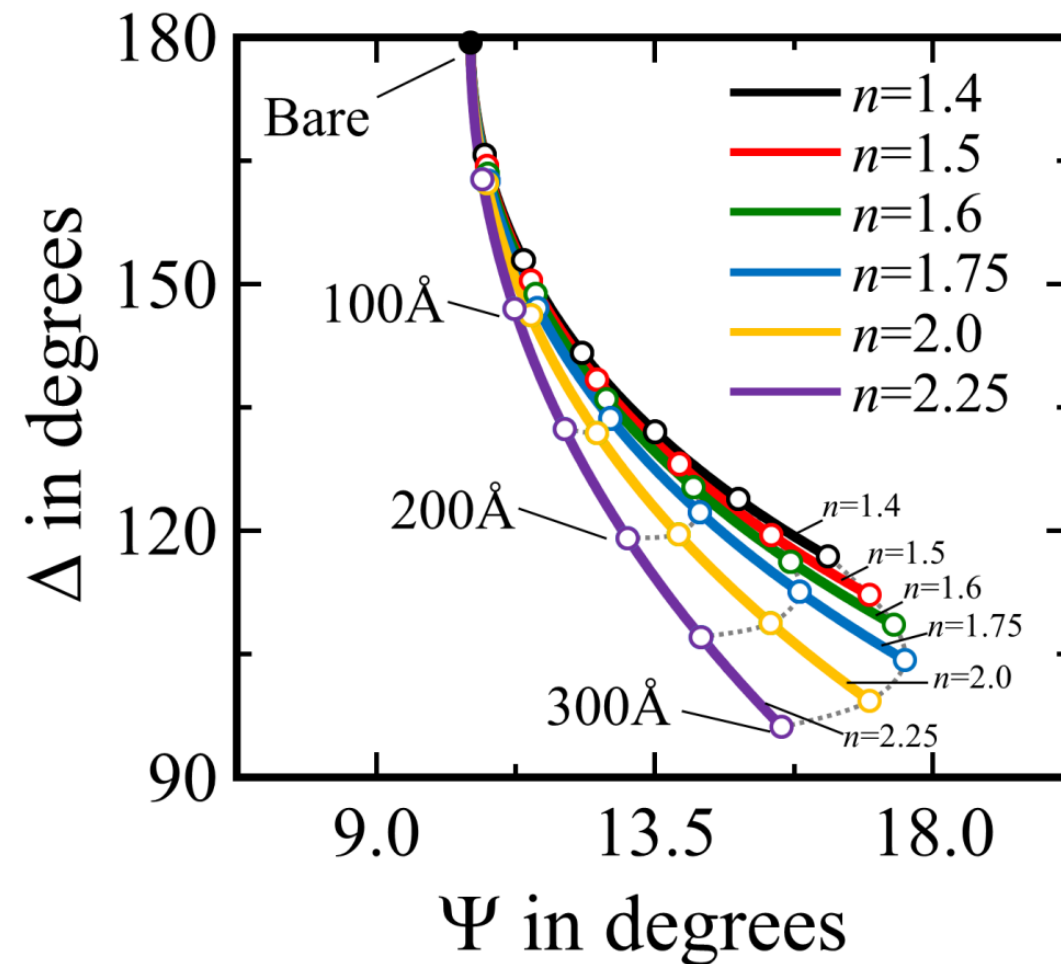
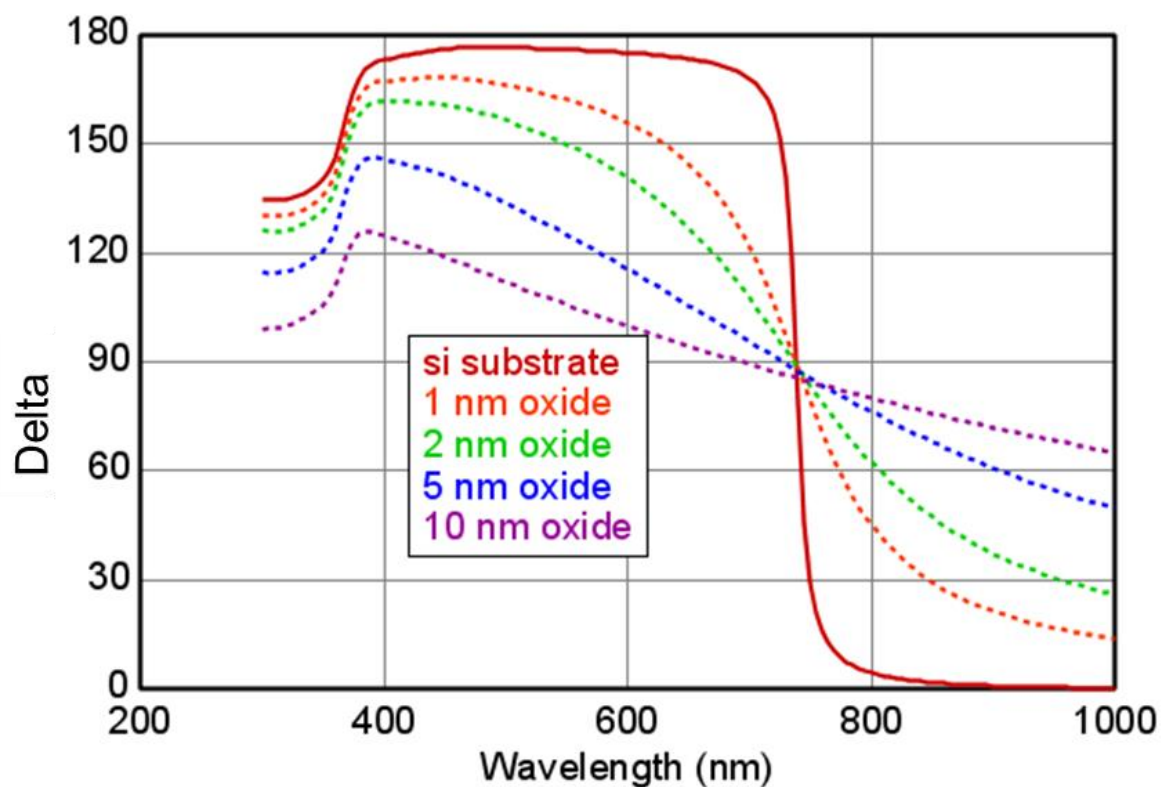
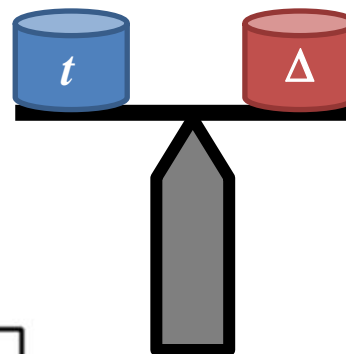
Optical Constants





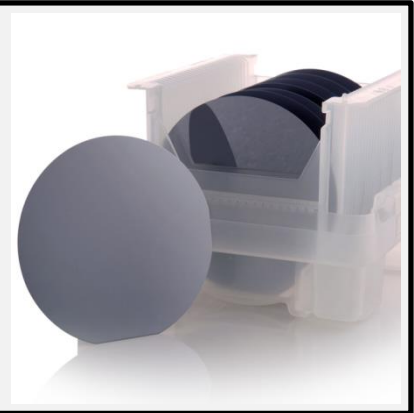
Ultra-Thin Films

- Only Δ changes significantly with thickness.
- Can't determine index.

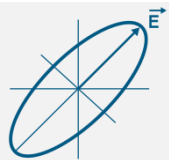


(2-05) SAM film on Si_A_post

- Use “Si with transparent film.mod”
- Test sensitivity to Cauchy A parameter



- Does the optical model have good sensitivity to the index of refraction of ultra-thin film?
- How important is the surface layer on substrate?



Parameter Uniqueness Test

Layer Commands: **Add Delete Save**

Include Surface Roughness = **OFF**

- Layer # 1 = **Cauchy Film** Thickness # 1 = **152.34 nm** (fit)

A = **2.106** (fit) B = **0.02242** (fit) C = **0.00124** (fit)

+ **Urbach Absorption Parameters**

Substrate = **SI_JAW**

+ **MODEL Options**

+ **FIT Options**

- **OTHER Options**

Wvl. Range Expansion Fit Increment (

Try Alternate Models MSE Improvement

Fit Parameter Uniqueness **Graph**

Fit Parameter Error Estimation

Add Optical Constants to Report = **OFF**

Parameter Uniqueness Fit

Fit Parameter Uniqueness

☒ 1-Dimensional Analysis ☐ 2-Dimensional Analysis

A

Thickness # 1

CA

B

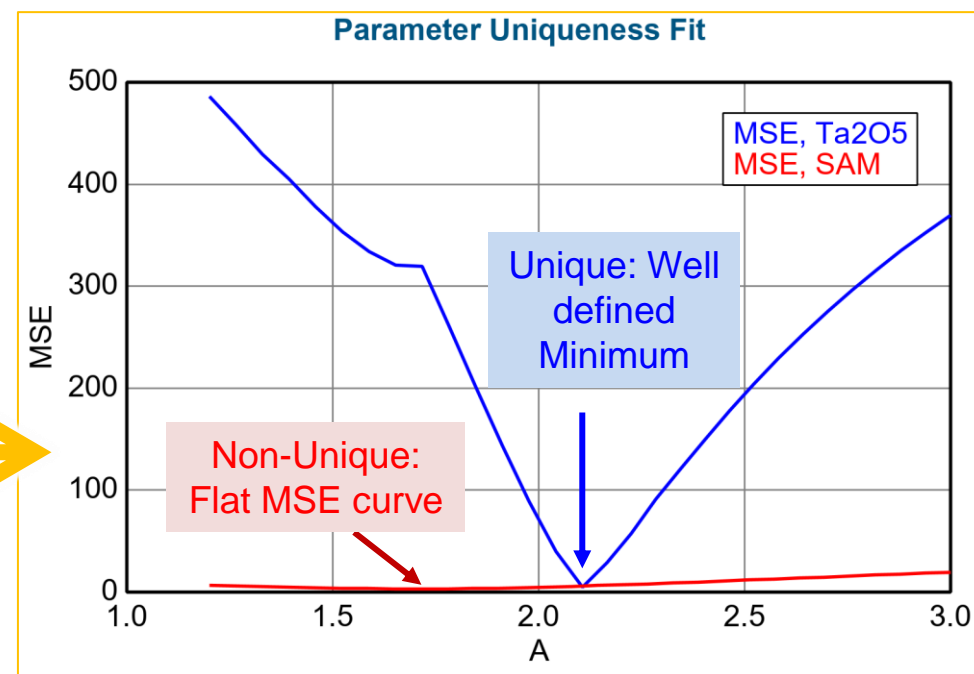
Minimum Value: Maximum Value: # of fit points:

Current Value: 3.46

Minimum Value: Maximum Value: # of fit points:

Ok Cancel

No sensitivity to index of refraction for ultra thin films!



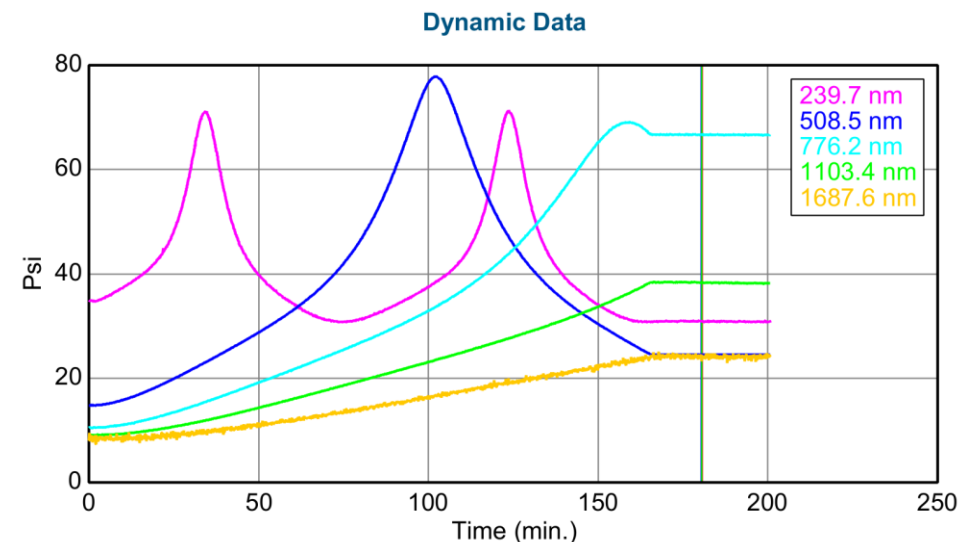
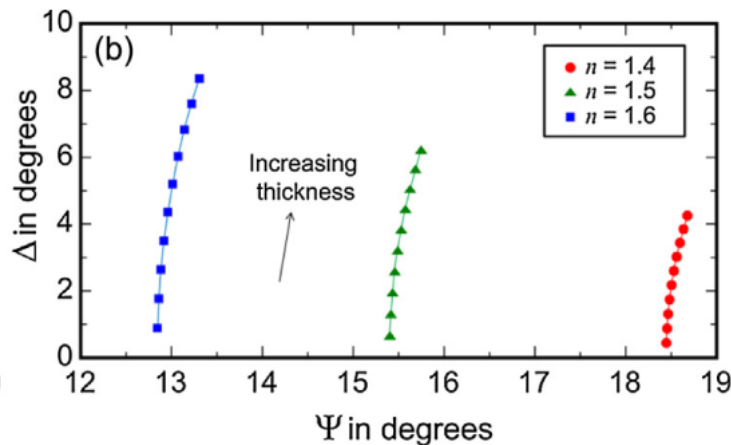
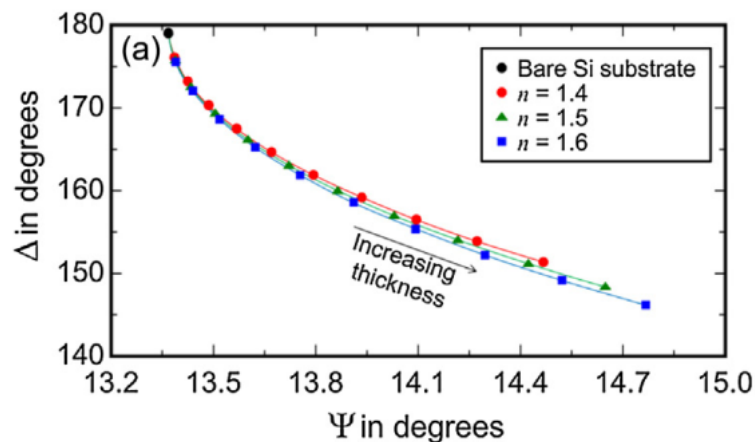
A very useful tool in testing parameter sensitivity, such as in multiple layers, ultra-thin films, and absorbing materials



Tips on Ultra-thin Film – Refractive Index

- Determine from thicker films, such as in ALD
- Use empirical values, often for organics or metal oxide
- Determine from free-standing film

J.N. Hilfiker et al. / Applied Surface Science 421 (2017) 508–512



Layer # 2 = Cauchy Thickness # 2 = 5.86 nm (fit)

A = 1.643 B = 0.00459 C = 0.00015076

+ **Urbach Absorption Parameters**

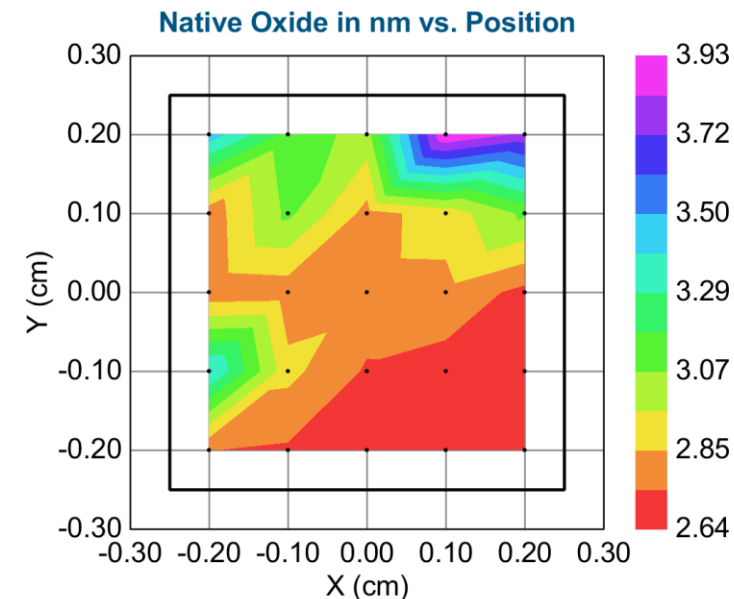
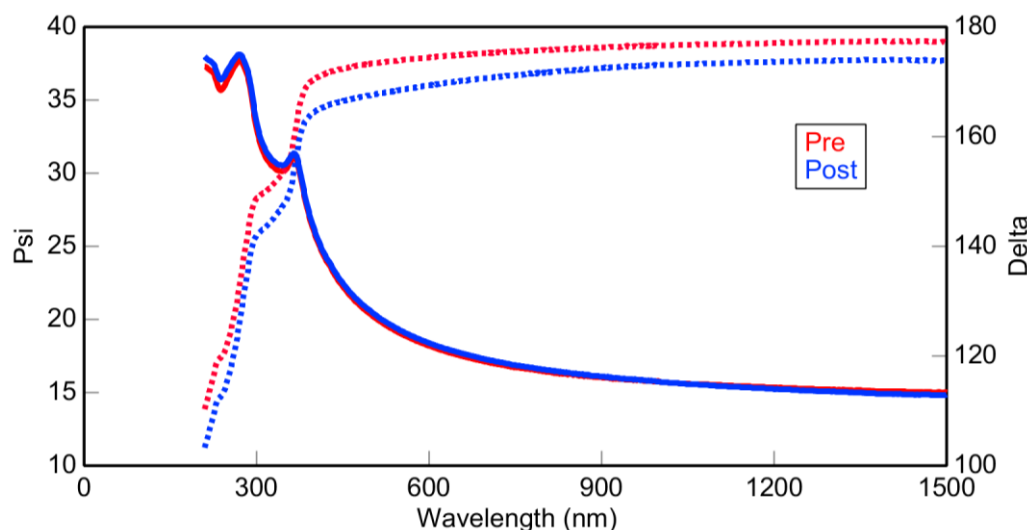
Layer # 1 = NTVE_JAW Thickness # 1 = 3.13 nm

Substrate = Si_Temp_JAW(-25_500C)



Tips on Ultra-thin Film – Surface Layer

- Important to characterize initial oxide or roughness thickness as they are crucial to the thickness accuracy of the ultra-thin films
 - Measure before and after at the same location on the same sample
 - In-situ monitoring if possible



- Layer # 2 = Cauchy Thickness # 2 = 2.68 nm (fit)
A = 1.500 B = 0.01000 C = 0.0000
+ Urbach Absorption Parameters
Layer # 1 = NTVE_JAW Thickness # 1 = 2.82 nm
Substrate = SI_JAW

Correct

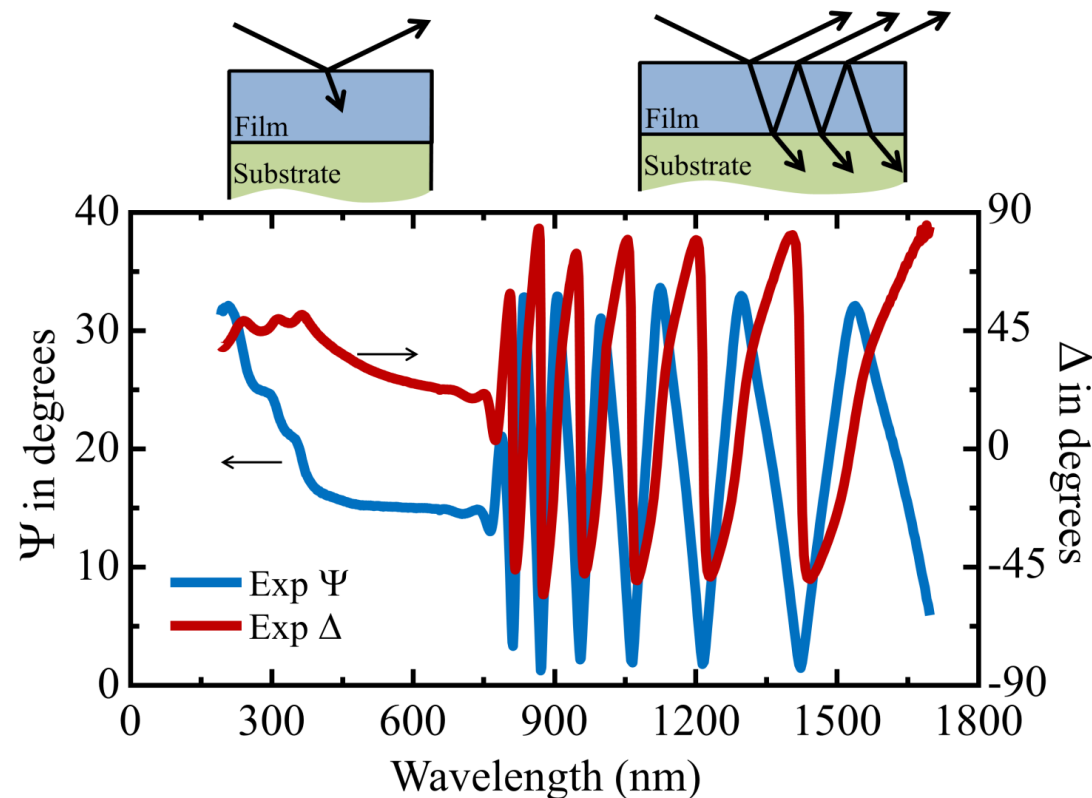
- Layer # 1 = Cauchy Thickness # 1 = 5.67 nm (fit)
A = 1.632 (fit) B = 0.00010530 (fit) C = 0.0000
+ Urbach Absorption Parameters
Substrate = SI_JAW

Wrong



Importance of Transparent Range

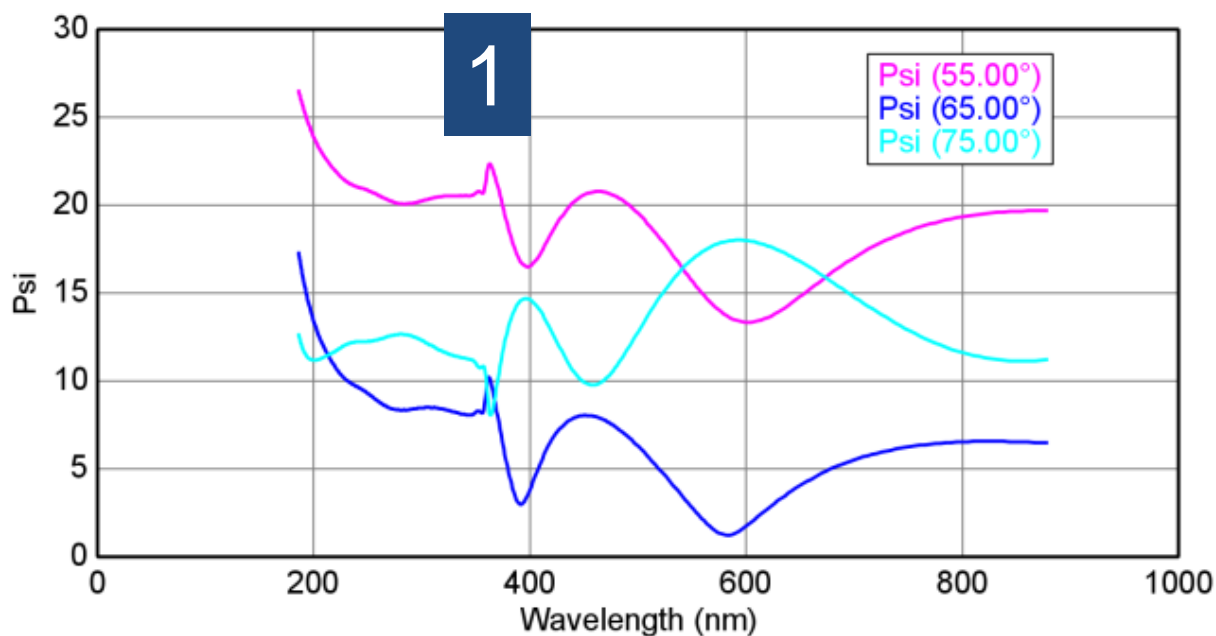
1. Needed to determine film thickness.
2. Simplified analysis by considering ONLY the transparent wavelength range – still get thickness and refractive index.



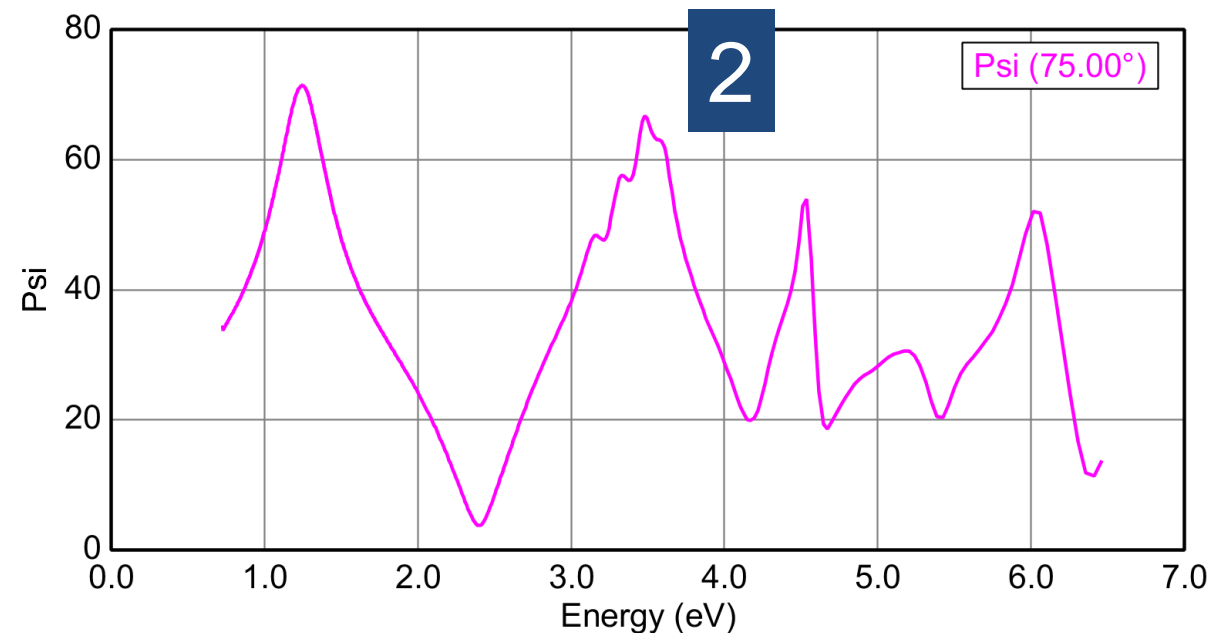


Identifying the Absorbing Region

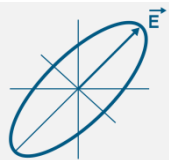
1. Absorbing region affects “amplitude” of thickness oscillations.
2. Absorptions have different frequency than thickness oscillations.



Variable Angle Spectroscopic Ellipsometric (VASE) Data

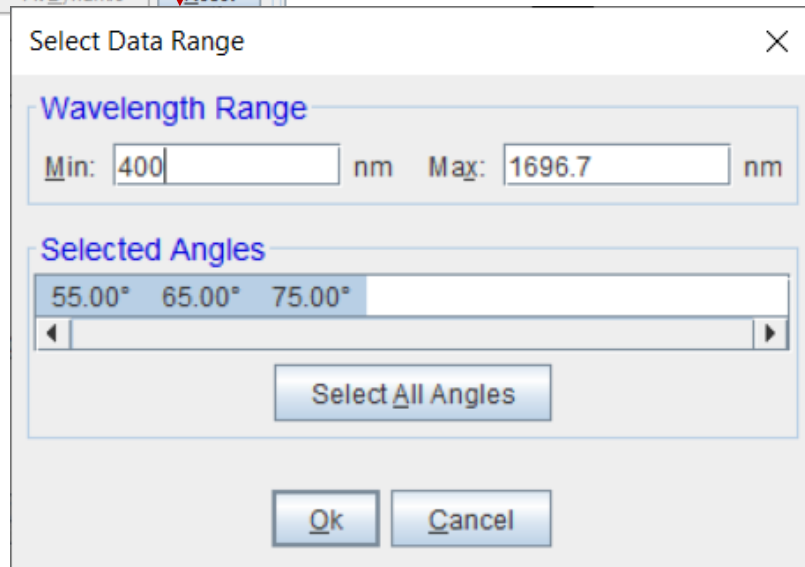
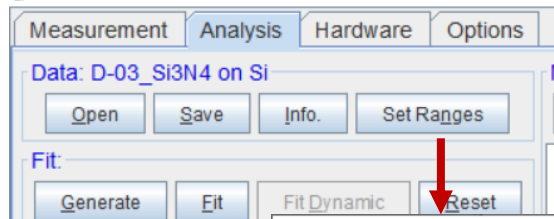


CTRL-ALT-W
switches between
Wavelength and Energy



How to Range-Select Wavelengths

CompleteEASE

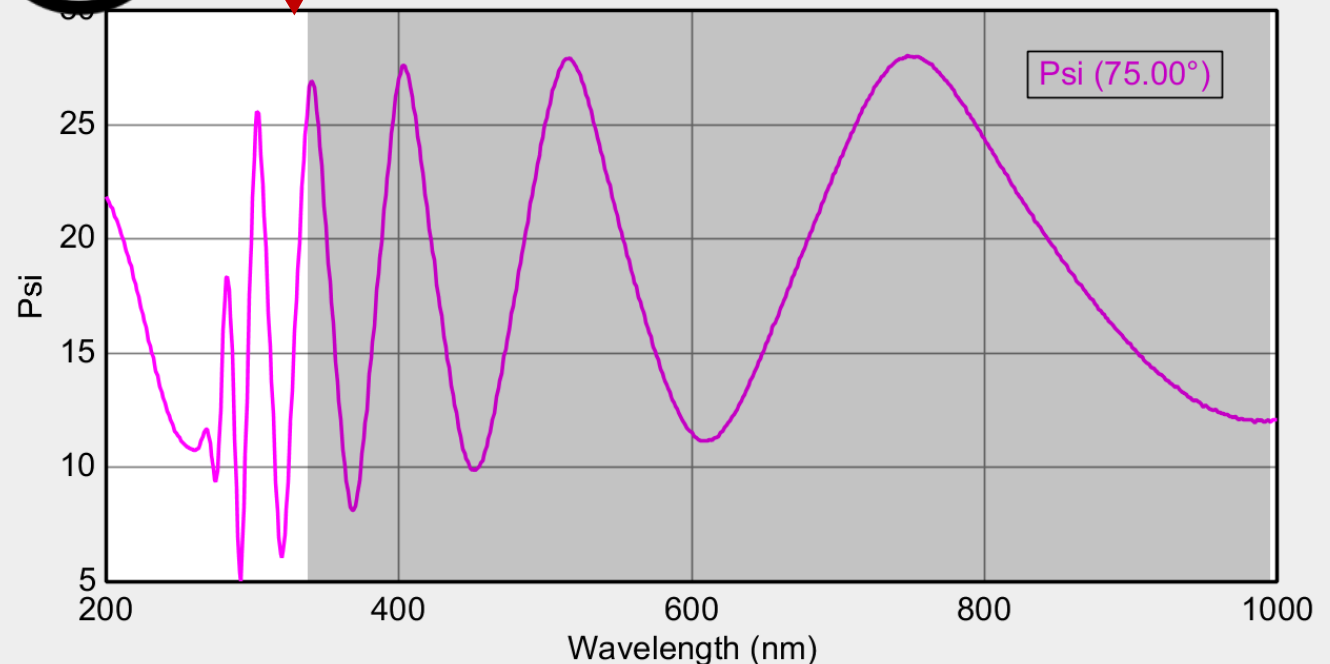


OR



Drag Mouse
across Graph

Variable Angle Spectroscopic Ellipsometric (VASE) Data



**Double-click on
Graph to Select All
Wavelengths**

[2-06] YbF_3 on Ge

- Find index and thickness for YbF_3 in transparent region
 - Where is the film transparent?
 - Can you use built-in model?



What happens if you use the wrong substrate in the model?

- Compare MSE for best fit with [Si_jaw.mat](#) and [Ge.mat](#) as the substrate material



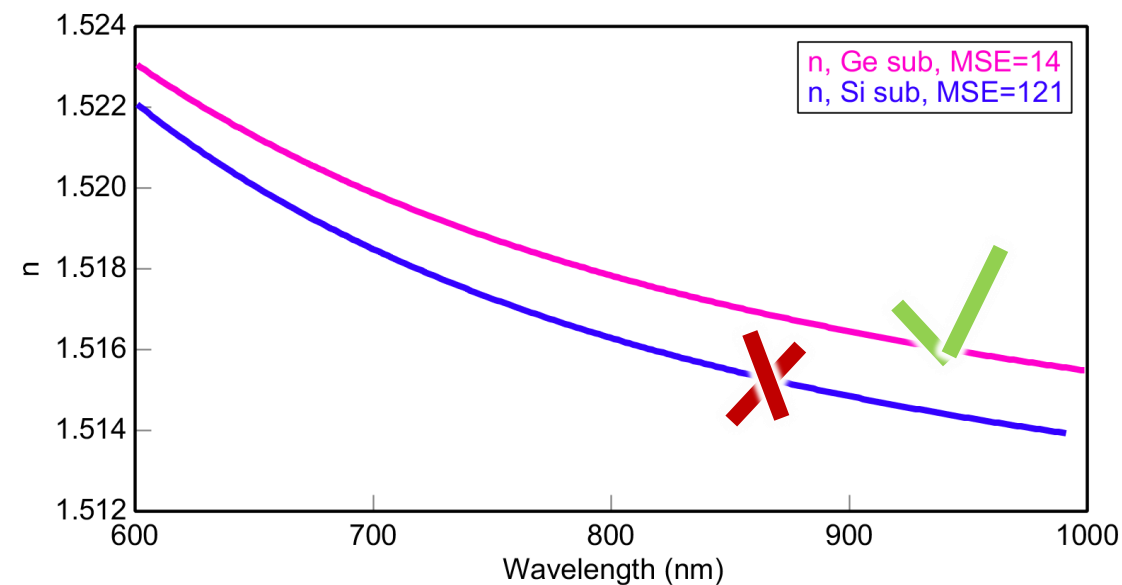
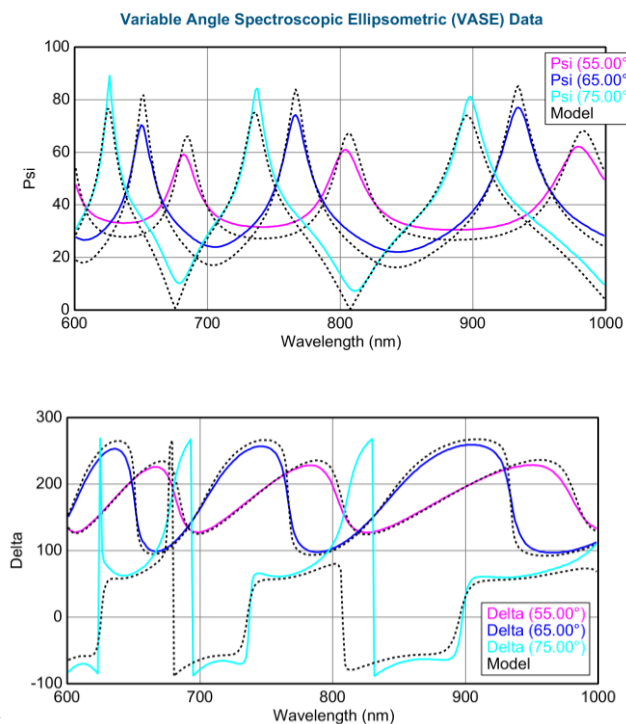
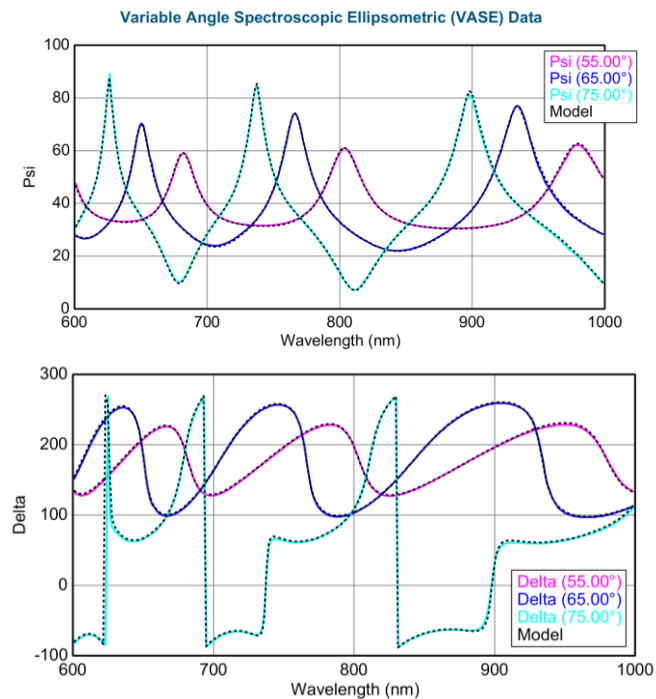
2-06 YbF₃ on Ge: Results



Ge sub,
MSE=14



Si sub,
MSE=121





Restricting Data Range in Model

Layer Commands: [Add](#) [Delete](#) [Save](#)

Include Surface Roughness = [ON](#) Roughness = [14.30 nm](#) (fit)

+ Layer # 1 = [Cauchy Film](#) Thickness # 1 = [1730.80 nm](#) (fit)

Substrate = [Ge](#)

+ MODEL Options

- FIT Options

Perform Thickness Pre-Fit = [OFF](#)

Use Global Fit = [OFF](#)

Fit Weight = [N.C.O](#)

Limit Wvl. for Fit = [ON](#) Range = [600.0 nm - 1000.0 nm](#)

Limit Angles for Fit = [OFF](#)

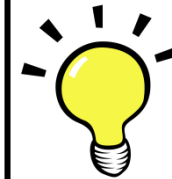
Max. Acceptable MSE = [100.000](#)

+ Include Derived Parameters = [ON](#)

+ OTHER Options

[Configure Options](#)

[Turn Off All Fit Parameters](#)



Useful when automating a model for repeat use.



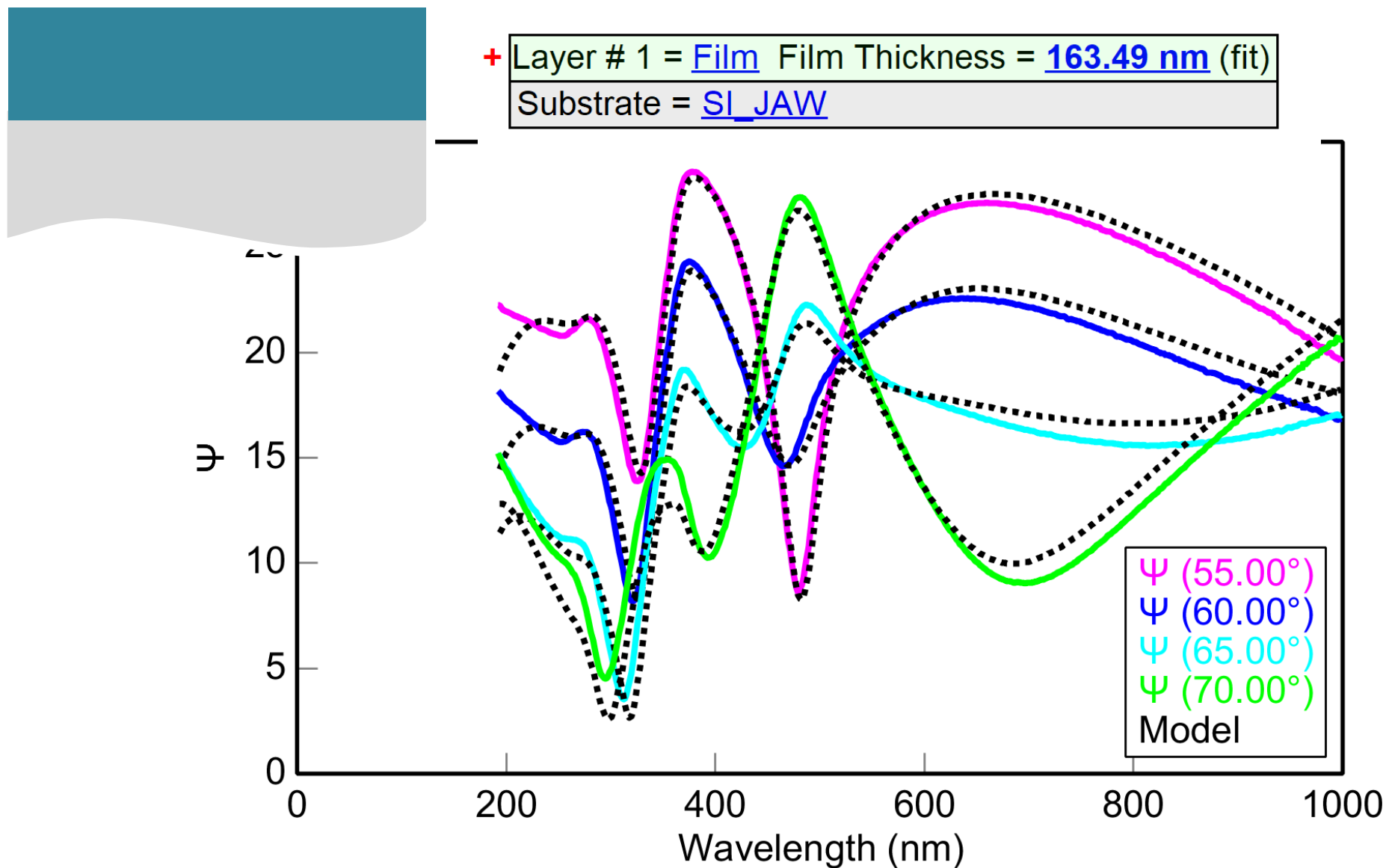
Recap: Transparent Thin Films



- We use **Cauchy** layer to determine the index of refraction $n(\lambda)$.
- Cauchy is **only** valid in transparent region
- Successful fitting requires good initial estimate for thickness and index.
- Use **built-in model** to automate.
 - Identify the transparent region before using the built-in model
- For **ultrathin** films ($< 10\text{-}30\text{ nm}$), determine thickness only!
- Save **model** for later use.



What's next when ideal model is not adequate?





2B: Typical Thin Film Complexities

Fit Thickness &
Cauchy Parameters



Add to improve MSE:

Roughness?
Index Grading?
Anisotropy?
Non-idealities?
Absorption?

Roughness often improves fit for higher index and absorbing films. Tends to “tip” Delta curves.

Grading is common with many metal-dielectrics.

Anisotropy is common with polymers.

Non-uniformity affect the data more as film gets thicker (bandwidth has similar effect)

Absorption reduces oscillation amplitudes



Non-Ideal Thin Films in CompleteEASE

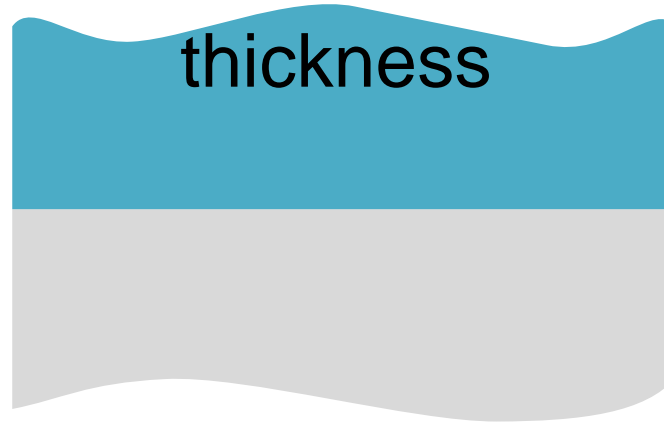
Rough surface



Roughness = **1.37 nm** (fit)

+ Layer # 1 = Cauchy Film Thickness # 1 = **152.57 nm** (fit)
Substrate = SI_JAW

Non-uniform thickness



Layer Commands: Add Delete Save

Include Surface Roughness = OFF

+ Layer # 1 = Cauchy Film Thickness # 1 = **152.57 nm** (fit)
Substrate = SI_JAW

- MODEL Options

Angle Offset = 0.00

Include Substrate Backside Correction = OFF

Model Calculation = Include Thickness Non-uniformity

% Thickness Non-uniformity = 10.00

of Pts = 9

+ FIT Options

Options

Show Options

Fit All Fit Parameters

Index Grading



Include Surface Roughness = OFF

+ Layer # 1 = Cauchy Film Thickness # 1 = **152.57 nm** (fit)
Substrate = SI_JAW

+ MODEL Options

+ FIT Options

+ OTHER Options

Configure Options

Turn Off All

Graph Layer Optical Constants

Graph Layer Absorption Coefficient

Rename Layer and Fit Parameters

Save Layer Optical Constants

Parameterize Layer

View Layer Comment

Convert To EMA

Convert To Transparent B-Spline

Convert To Anisotropic

Grade Layer

Start Supercell

- Graded Layer Thickness # 1 = **152.57 nm** (fit)

Grade Type = Simple # of Slices = 5

% Inhomogeneity = 0.00 (fit)

+ Material = Cauchy Film

Substrate = SI_JAW



**Roughness and Non-uniformity
differ on lateral length-scales**



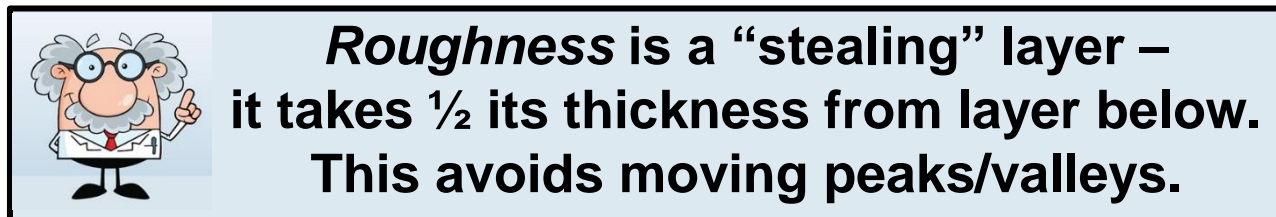
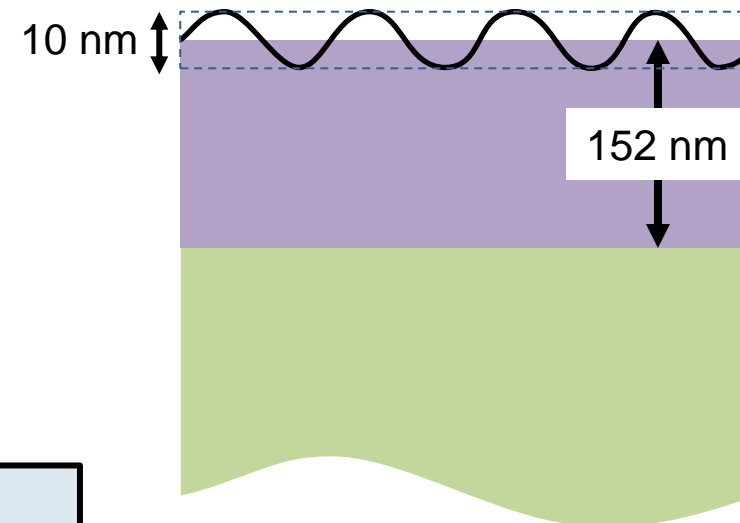
Surface Roughness

- Describes ultra-thin layers ($< 10\text{nm}$) on a surface.
 - Roughness, oxidation, adsorbed organic contaminates...
- Modeled by mixing index of top layer with void (50% - 50%)

Roughness = 10.00 nm (fit)

+ Layer # 1 = Cauchy Film Thickness # 1 = 152.34 nm (fit)
Substrate = SI_JAW

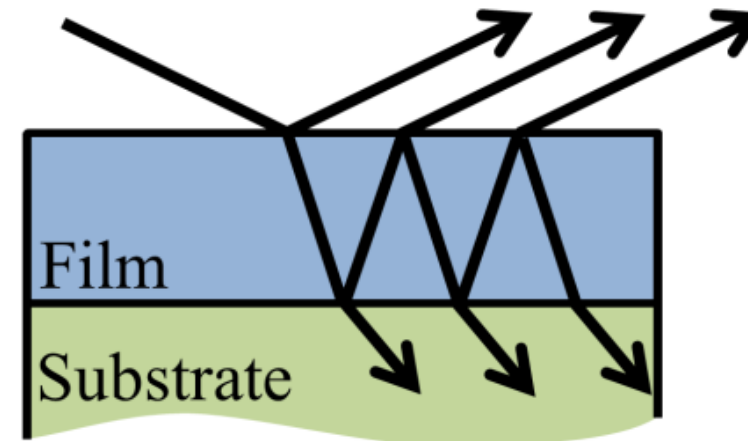
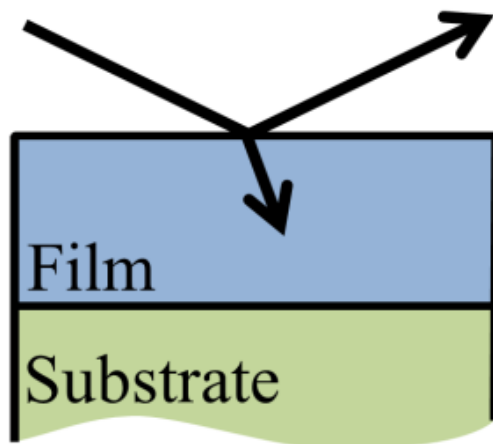
Total thickness = Film thickness + $\frac{1}{2}$ roughness

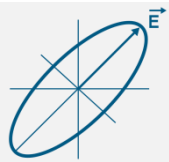




Surface Roughness

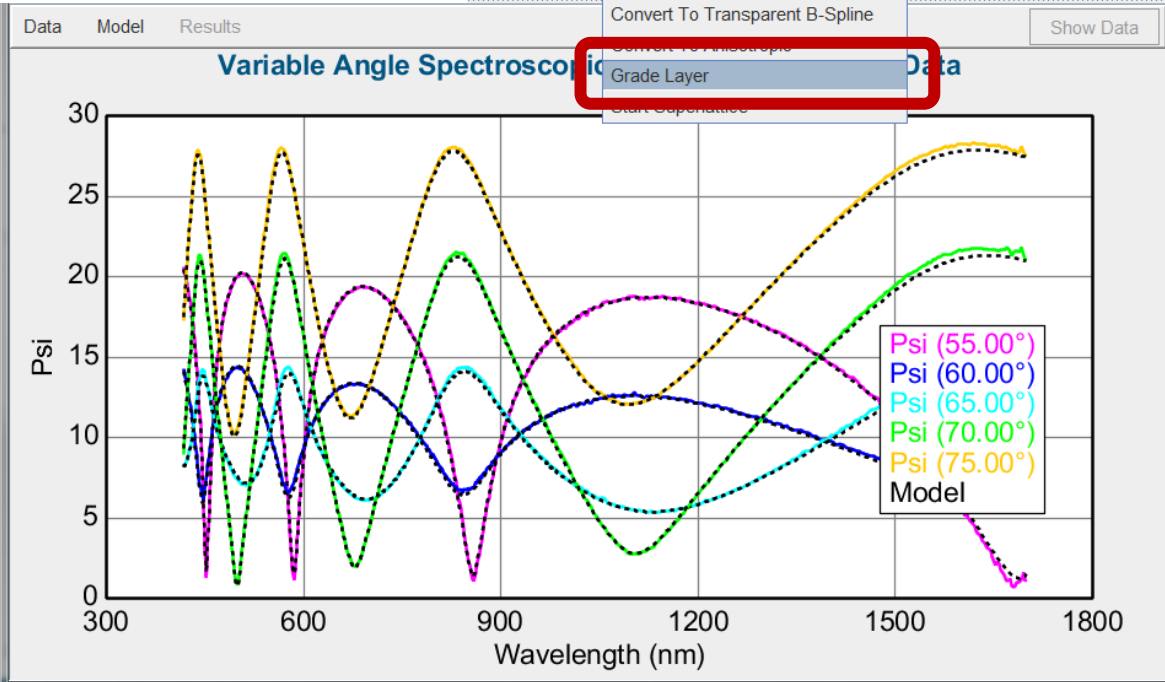
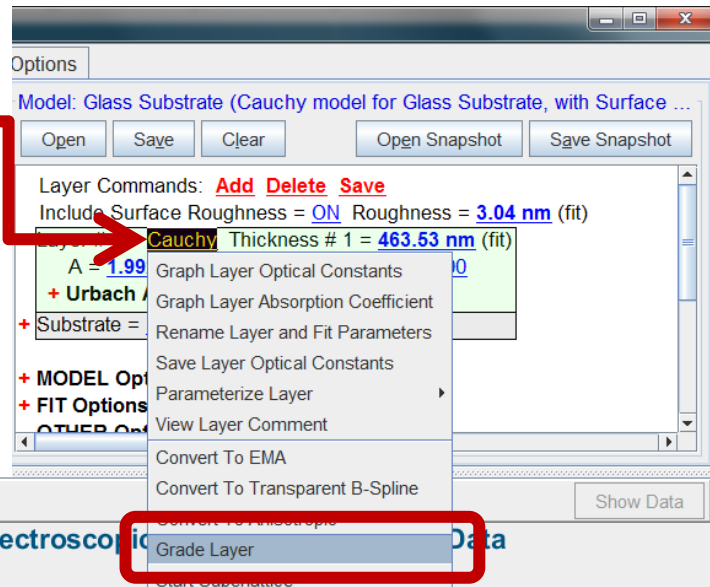
- Best sensitivity to surface roughness when:
 - Top layer has large index
 - More contrast for surface that is mixed with void ($n=1$)
 - Top layer is absorbing
 - No light penetrates the film, so all detected light is from surface!



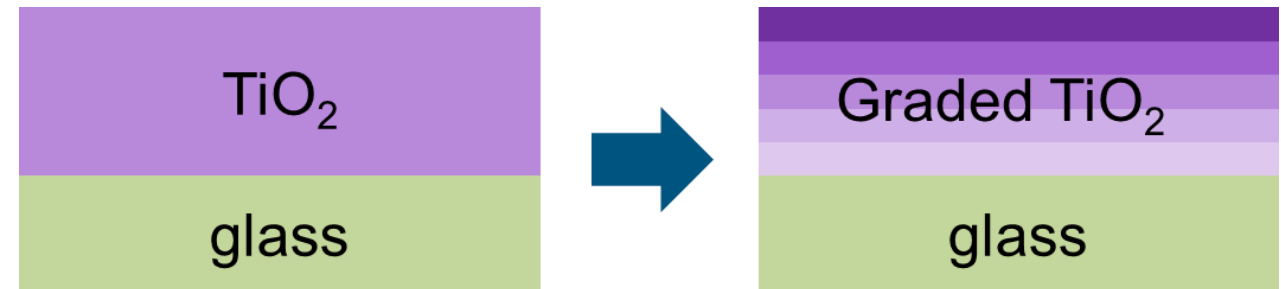


Index Grading

Right-click
layer name



Divides film into 'slices' with varying index.



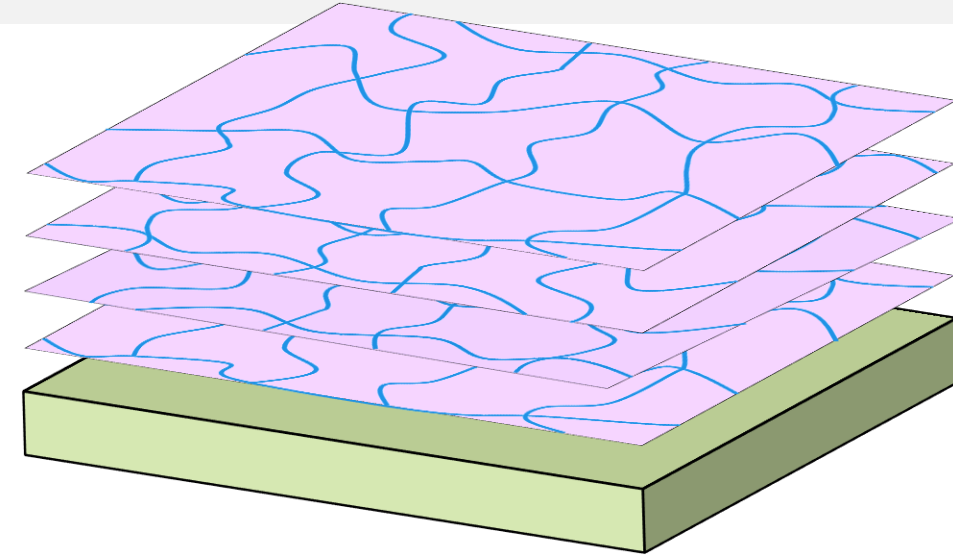
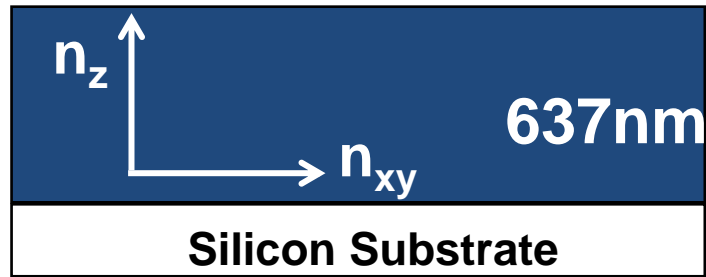
Roughness = 3.04 nm (fit)

- Graded Layer Thickness # 1 = 463.53 nm (fit)
 - Grade Type = Simple # of Slices = 5
 - % Inhomogeneity = 10.00 (fit)
- Material = Cauchy
 - A = 1.992 (fit) B = 0.02617 (fit) C = 0.0000
 - + **Urbach Absorption Parameters**
- + Substrate = Cauchy Substrate

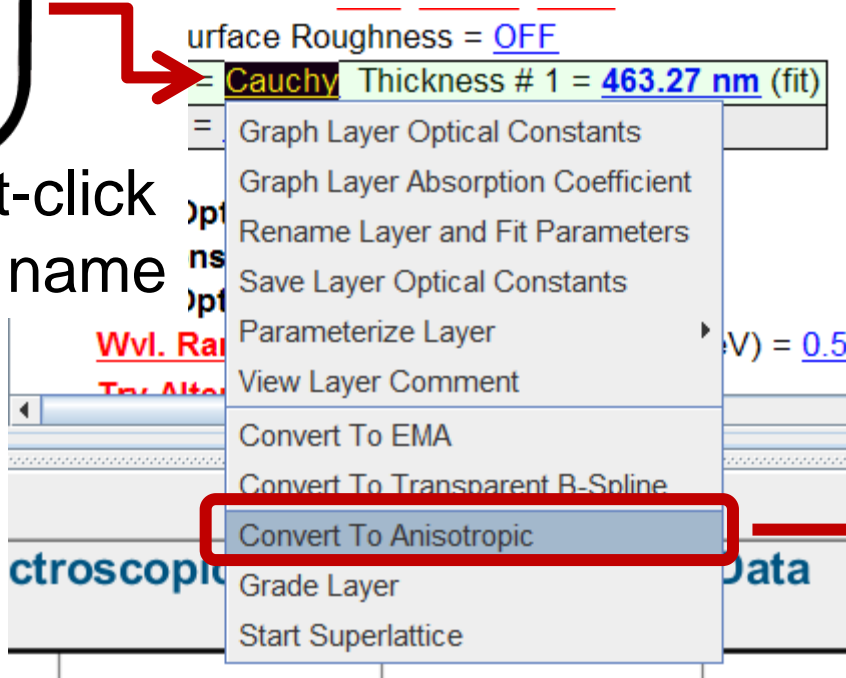


Anisotropy

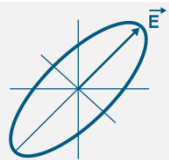
- Index varies with direction.



Right-click
layer name



- Layer # 1 = Biaxial Thickness # 1 = 463.27 nm (fit)
Type = Uniaxial
Optical Constants: Difference Mode = OFF
+ Ex = Cauchy
+ Ez = Cauchy
Euler Angles: Phi = 0.00 Theta = 0.00
- + Substrate = Cauchy Substrate



Shortcut: Try Alternate Models

Layer Commands: [Add](#) [Delete](#) [Save](#)

Include Surface Roughness = [OFF](#)

- Layer # 1 = [Cauchy Film](#) Thickness # 1 = [129.79 nm](#) (fit)

A = [1.879](#) (fit) B = [0.01903](#) (fit) C = [-0.00129](#) (fit)

+ Urbach Absorption Parameters

Substrate = [SI_JAW](#)

+ MODEL Options

+ FIT Options

- OTHER Options

[Try Alternate Models](#) MSE Improvement Threshold = [25](#) %

[Fit Parameter Error Estimation](#)

Add Opt. Const. to Report = [OFF](#)

[Configure Options](#)

[Turn Off All Fit Parameters](#)

Analysis Results

[Copy Table to Clipboard](#)

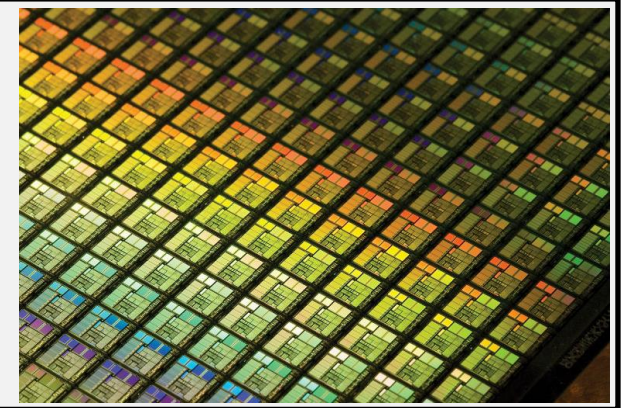
Parameter	Ideal	Roughness	Grating	Roughness & Grating	Anisotropy
MSE	25.415	25.259	17.201	14.079	24.940
Roughness	N/A	-1.72 ± 0.426 nm	N/A	6.35 ± 0.260 nm	N/A
A	1.887 ± 0.00088467	1.882 ± 0.001564	1.865 ± 0.00081890	1.874 ± 0.00091512	1.882 ± 0.001022
B	0.01278 ± 0.00058122	0.01724 ± 0.001271	0.02775 ± 0.00054623	0.01970 ± 0.00066902	0.01436 ± 0.00059163
C	-0.00037363 ± 5.6772E-05	-0.00078979 ± 0.00011954	-0.00100 ± 4.3315E-05	3.6114E-05 ± 6.9339E-05	-0.00054004 ± 5.8270E-05
% Inhomogeneity	N/A	N/A	24.08 ± 0.498	34.59 ± 0.620	N/A
Thickness # 1	129.62 ± 0.058 nm	129.39 ± 0.081 nm	125.43 ± 0.088 nm	124.51 ± 0.081 nm	130.10 ± 0.078 nm
n of Cauchy Film @ 632.8 nm	1.91677	1.92015	1.92855	1.92387	N/A

[<<](#) [Apply Chosen Model](#) [>>](#)

[Show Graphs](#)

[2-07] SiO_xN_y on Si

- Use Automated Model to find Cauchy for SiO_xN_y



Estimate
Index & Thickness

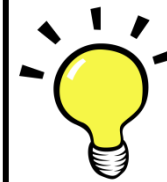


Fit Thickness &
Cauchy Parameters

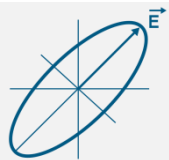


Add roughness,
does it improve MSE?

Si with Transparent Film.mod



YOU will have to choose the
transparent wavelength range
for all examples



2-07 SiOxNy on Si: Results



SiOxNy on Si

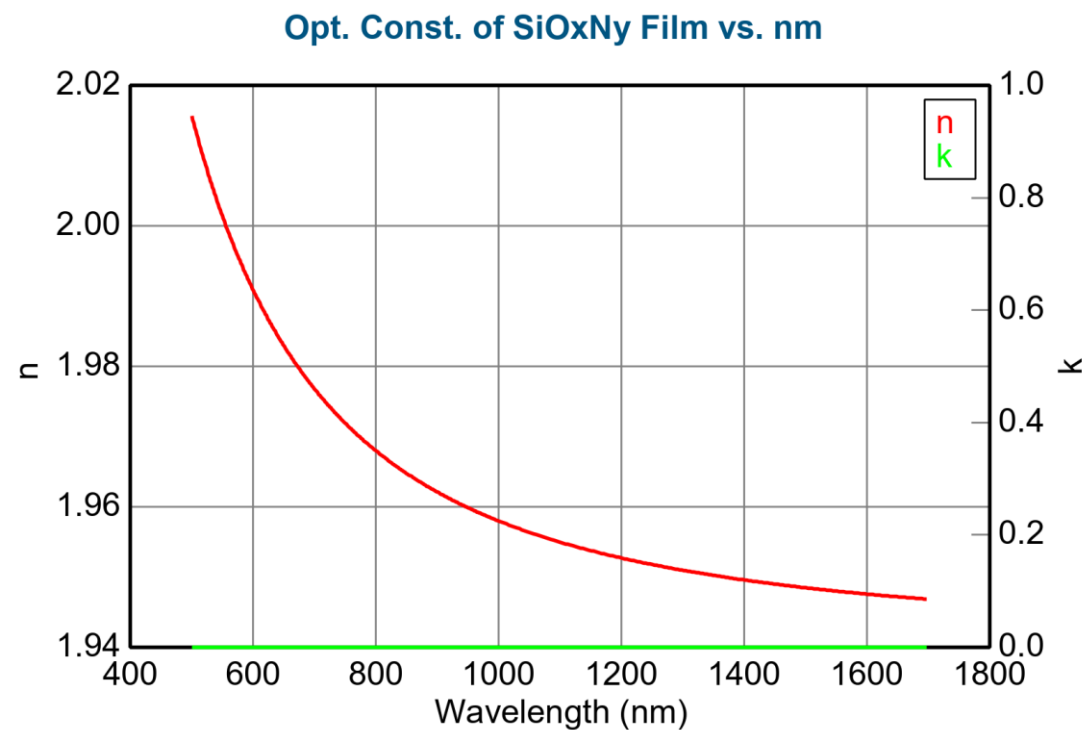
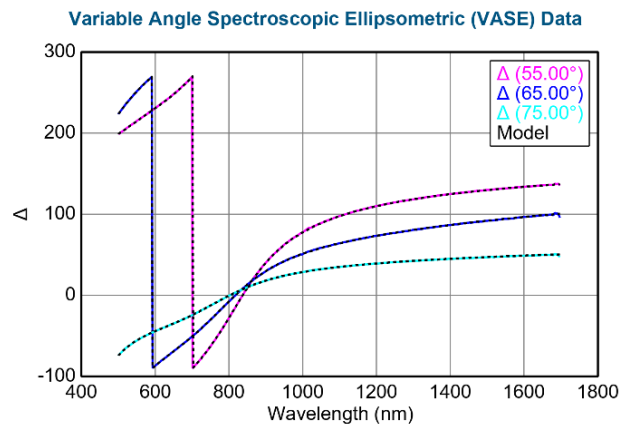
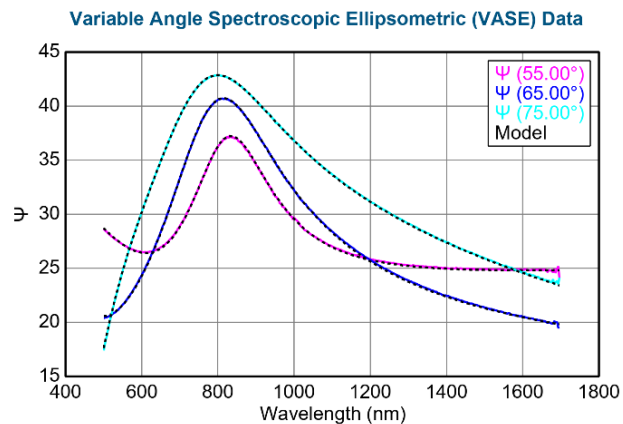
Fit Results

MSE = 2.391
Roughness = 6.67 ± 0.046 nm
Thickness # 1 = 118.11 ± 0.008 nm
 $A = 1.941 \pm 0.00027878$
 $B = 0.01623 \pm 0.00026828$
 $C = 0.00060462 \pm 6.1831E-05$
n of Cauchy Film @ 632.8 nm = 1.98546

Optical Model

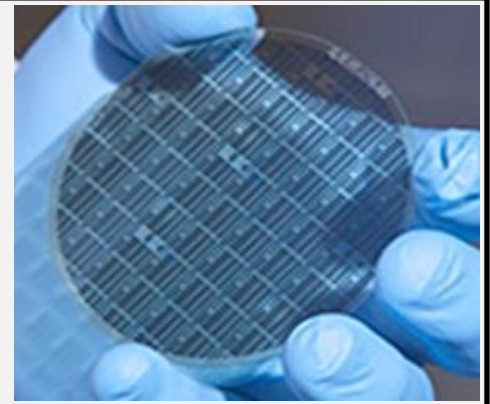
Roughness = 6.67 nm (fit)
+ Layer # 1 = Cauchy Film Thickness # 1 = 118.11 nm (fit)
Substrate = SI_JAW

Experimental and Model Generated Data Fits



[2-08] SiC on Si

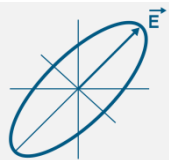
- Find best model for SiC on Si



**Fit Thickness &
Cauchy Parameters**



Add to improve MSE:
Roughness?
Index Grading?
Anisotropy?
Thickness Non-uniformity?



2-08 SiC on Si: Results



SiC on Si

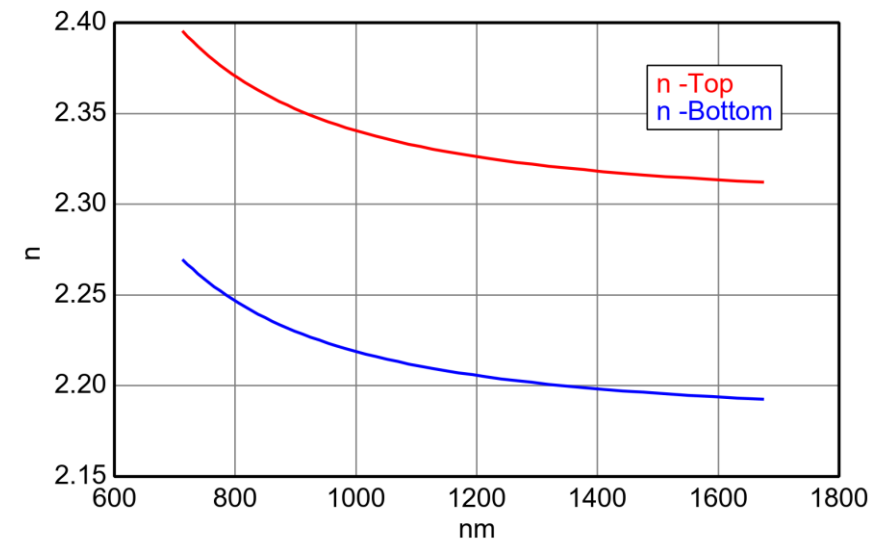
Fit Results

MSE = 3.471
Roughness = 1.29 ± 0.093 nm
 $A = 2.241 \pm 0.00080736$
 $B = 0.03236 \pm 0.001048$
 $C = 0.00747 \pm 0.00041129$
% Inhomogeneity = 13.20 ± 0.176
Thickness # 1 = 766.45 ± 0.222 nm
n of Cauchy Film @ 632.8 nm = 2.36805

Optical Model

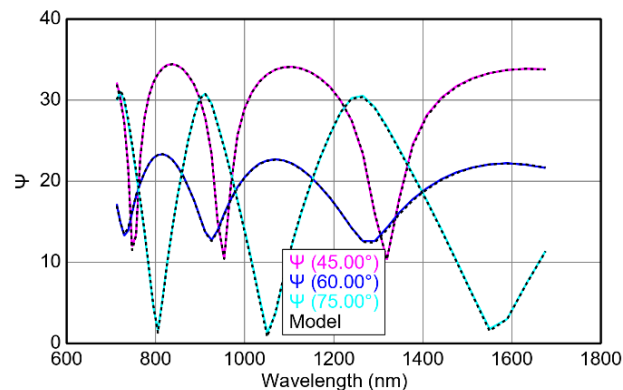
Roughness = **1.29 nm** (fit)
- **Graded Layer** Thickness # 1 = **766.45 nm** (fit)
Grade Type = **Simple** # of Slices = **5**
% Inhomogeneity = **13.20** (fit)
+ Material = **Cauchy Film**
Substrate = **SI_JAW**

Opt. Const. of Graded SiC Film vs. nm

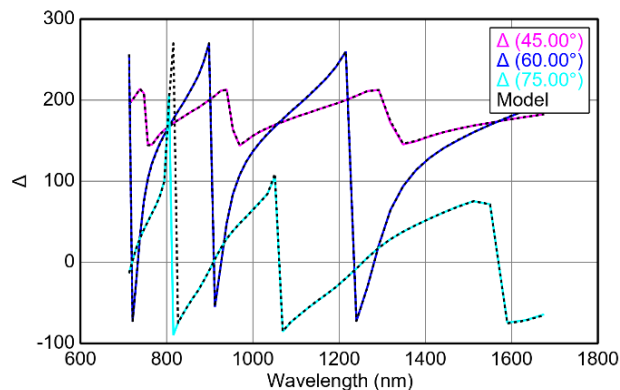


Experimental and Model Generated Data Fits

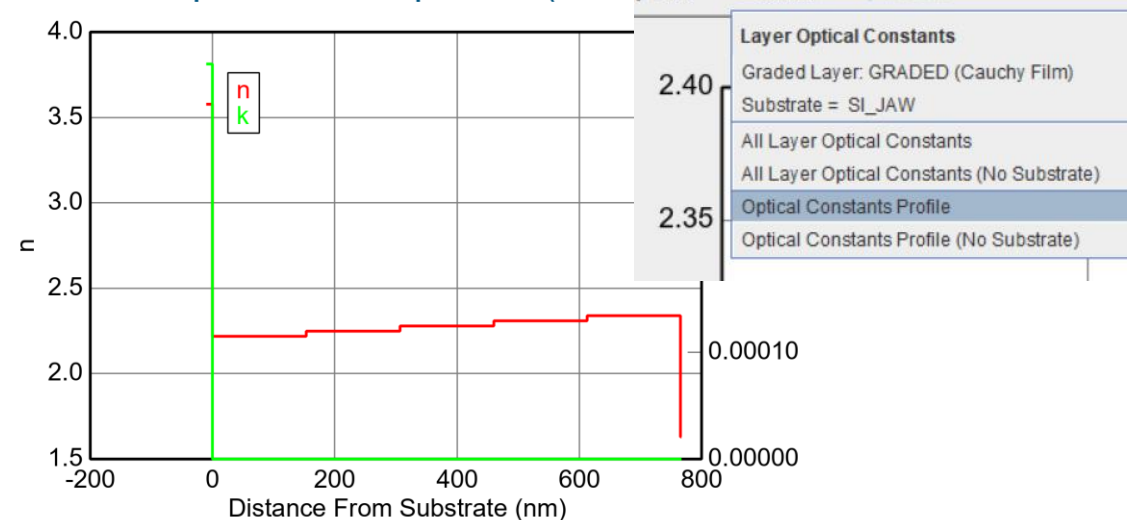
Variable Angle Spectroscopic Ellipsometric (VASE) Data



Variable Angle Spectroscopic Ellipsometric (VASE) Data



Optical Constant Depth Profile (1000.0)



[2-09] Polymer on Si

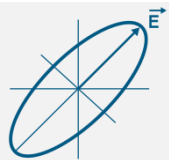
- Find a model that matches this data.



**Fit Thickness &
Cauchy Parameters**



Add to improve MSE:
Roughness?
Index Grading?
Anisotropy?
Thickness Non-uniformity?



2-09 Polymer on Si: Results



Polymer on Si

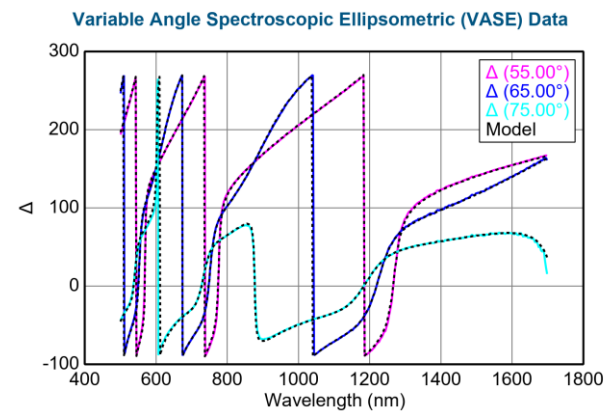
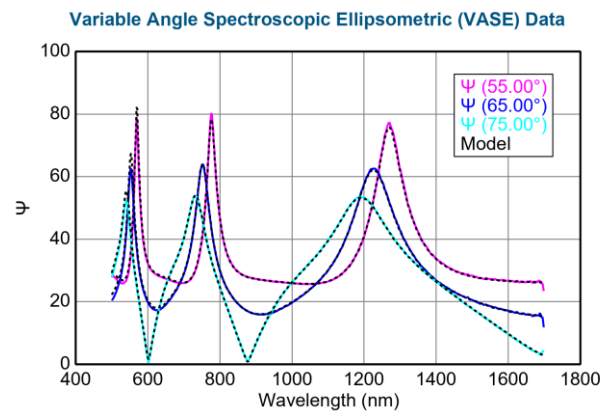
Fit Results

MSE = 17.186
Thickness # 1 = 640.70 ± 0.211 nm
 $A = 1.682 \pm 0.00045756$
 $B = 0.02330 \pm 0.00027551$
 $C = 0.00039654 \pm 6.4547E-05$
 $dZ_A = -0.095334 \pm 0.00071389$
 $dZ_B = 0.089431 \pm 0.0039384$
 n_o of Biaxial @ 632.8 nm = 1.74271
 n_e of Biaxial @ 632.8 nm = 1.62608

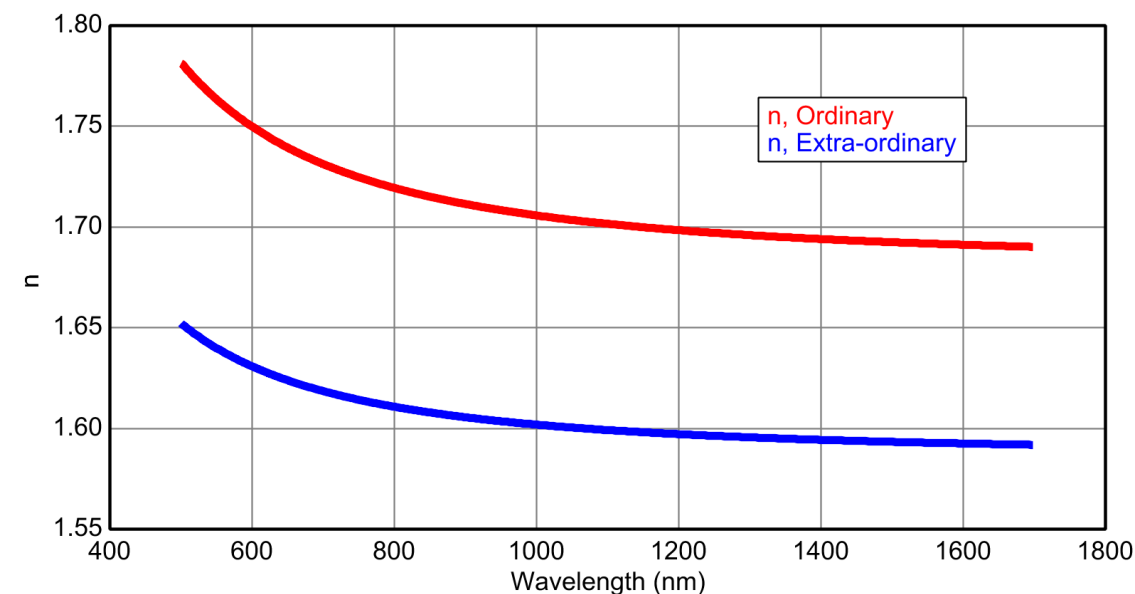
Optical Model

Layer # 1 = Biaxial Thickness # 1 = 640.70 nm (fit)
Type = Uniaxial
Optical Constants: Difference Mode = QN
Ex = Cauchy Film
Index Differences:
 $dZ_A = -0.095334$ (fit) $dZ_B = 0.089431$ (fit) $dZ_C = 0.00000$ $dZ_D = 0.00000$ $dZ_IR = 0.00000$
Euler Angles: Phi = 0.00 Theta = 0.00
Substrate = Si_JAW

Experimental and Model Generated Data Fits

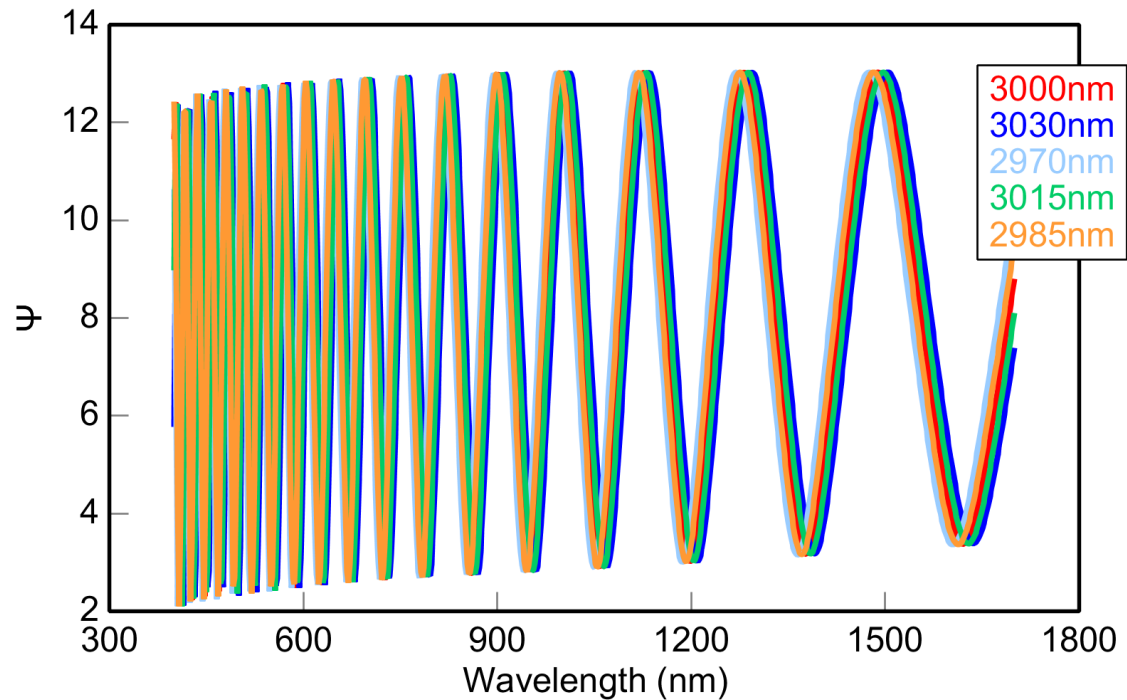


Opt. Const. of Biaxial vs. nm

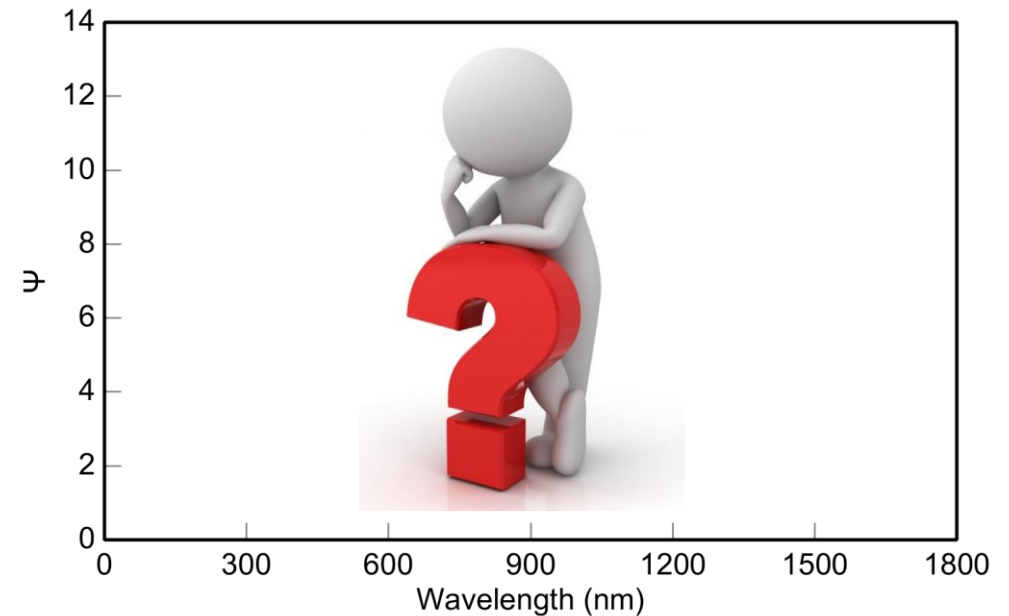




Thickness effect on SE Data

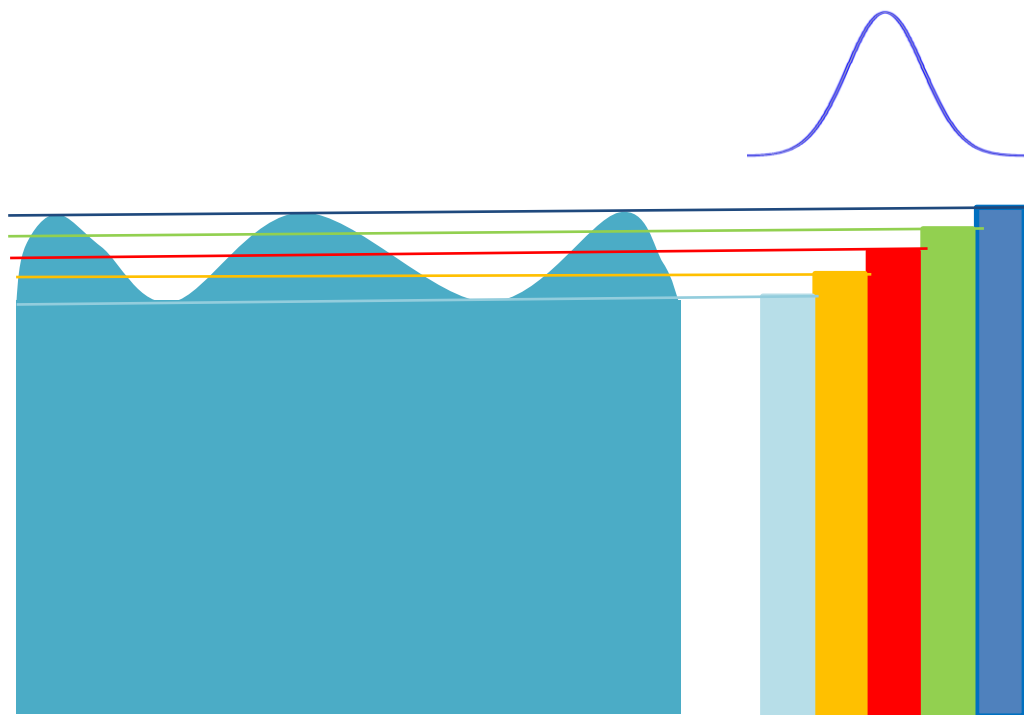


Spectroscopic Ellipsometric (SE) Data

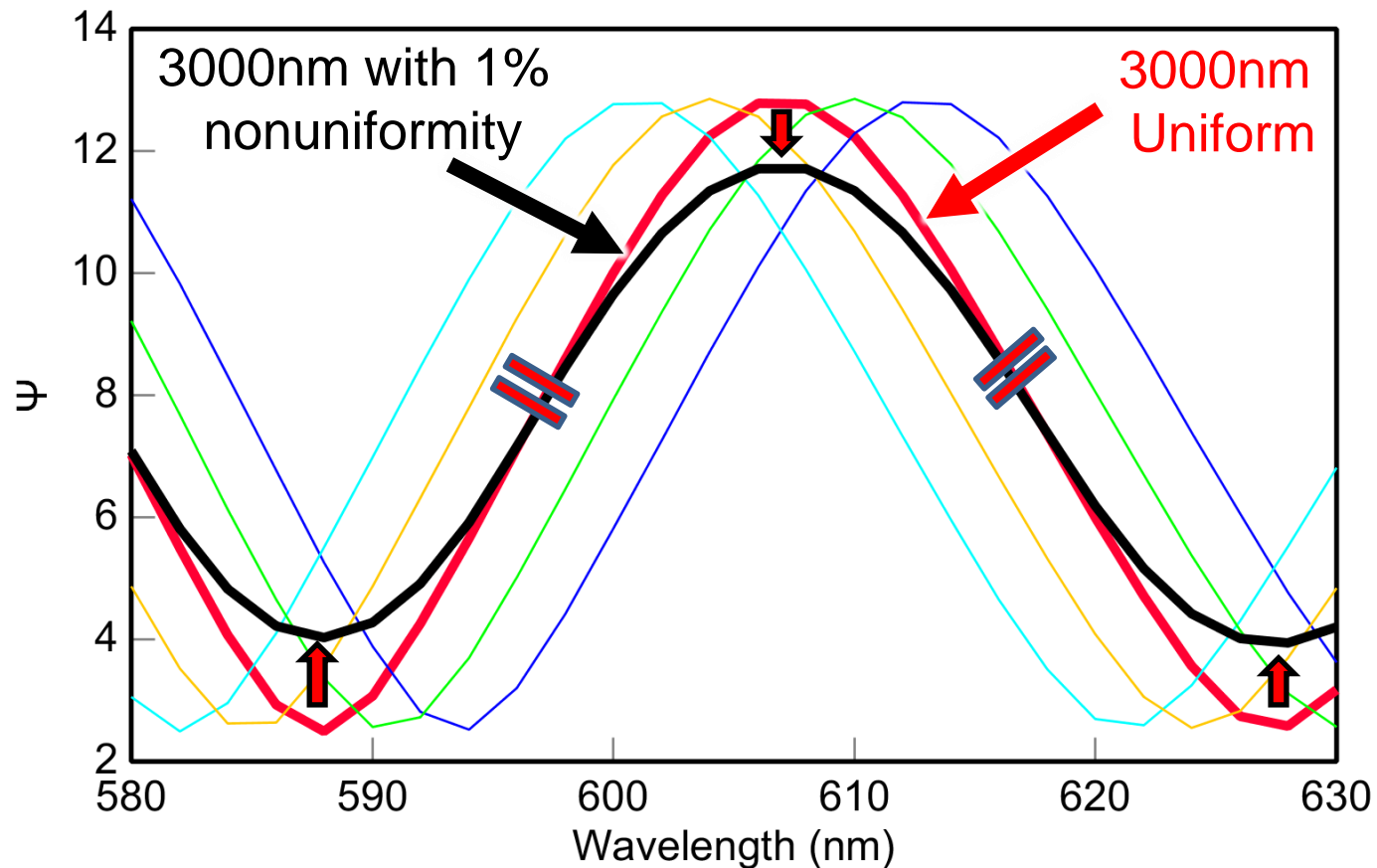




Non-Uniformity Effect on Raw Data



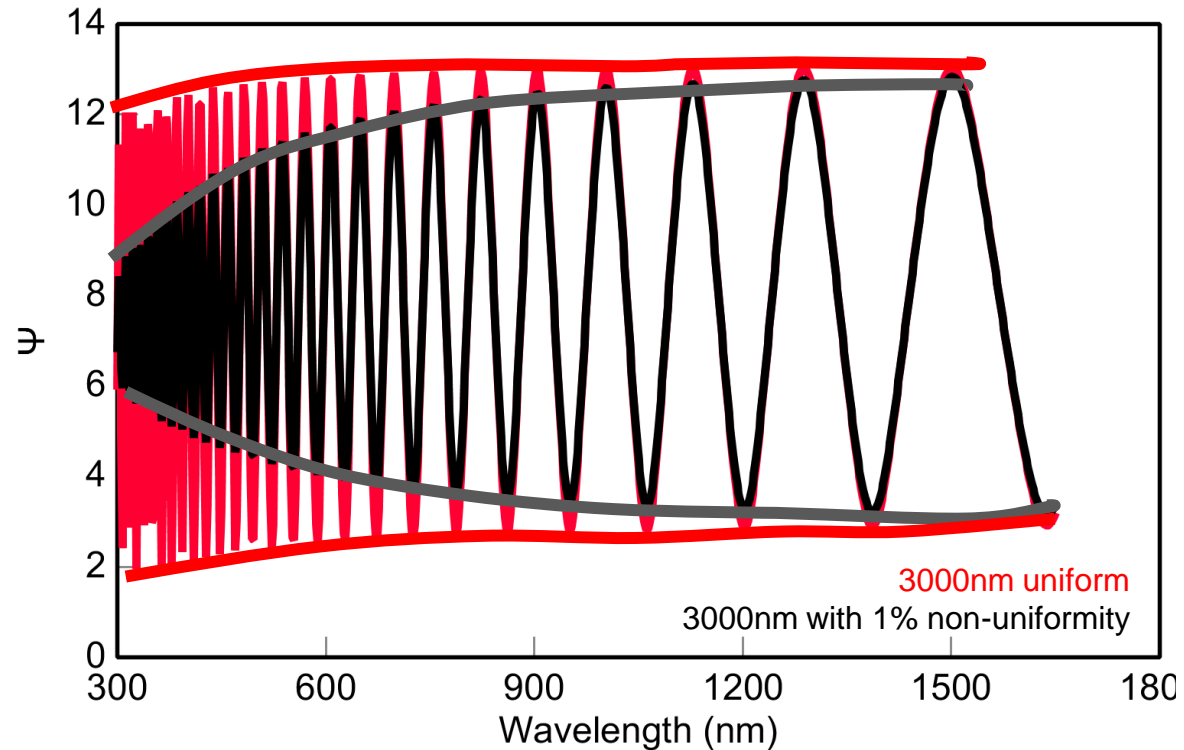
Spectroscopic Ellipsometric (SE) Data



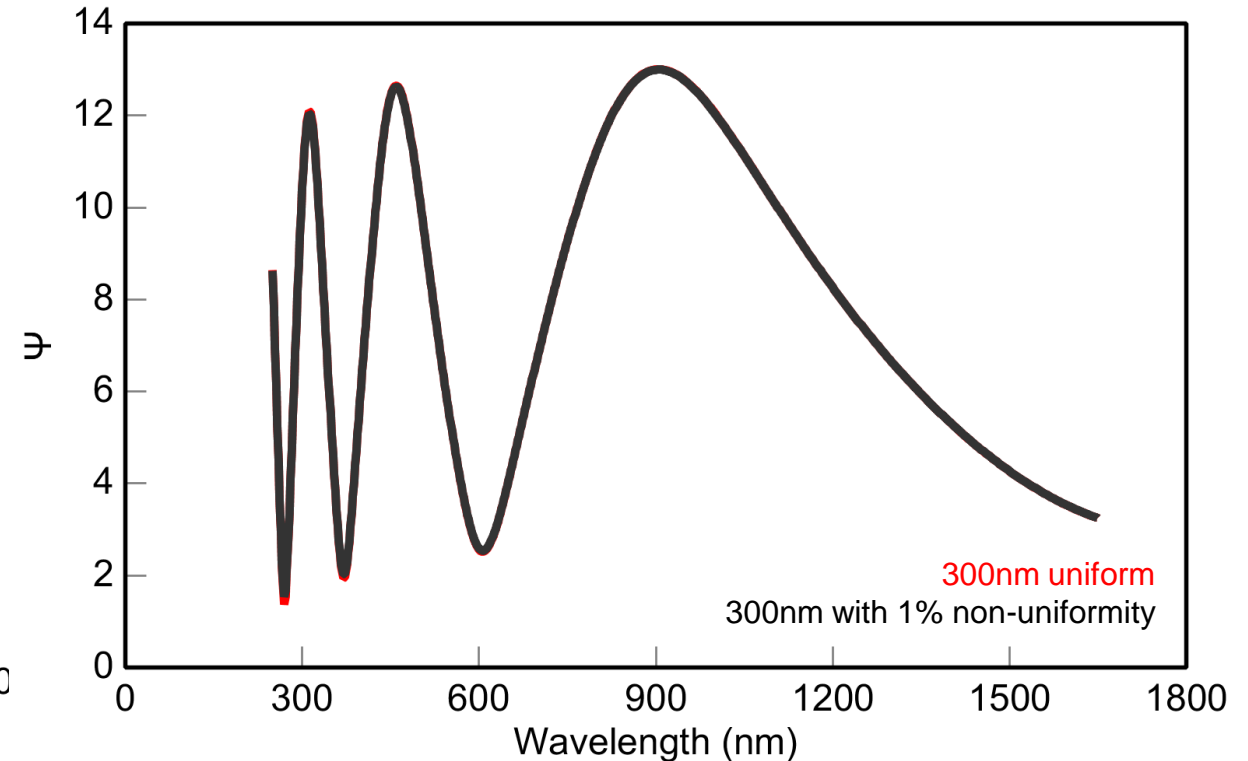


Non-Uniformity Effect

Spectroscopic Ellipsometric (SE) Data



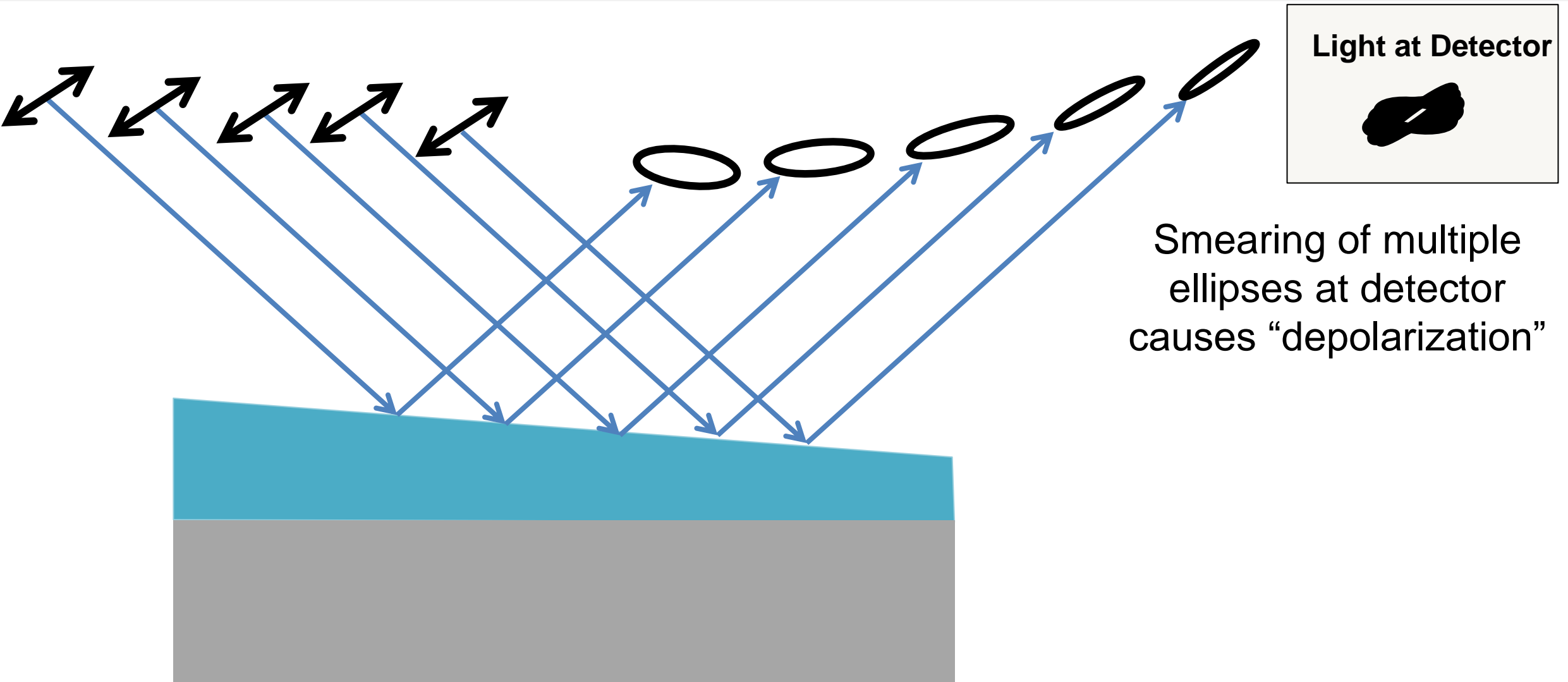
Spectroscopic Ellipsometric (SE) Data



- Nonuniformity produces differences at peaks and valleys comparing to uniform films
- The differences are more pronounced towards short wavelength
- Better sensitivity to nonuniformity in thicker films.

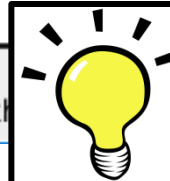
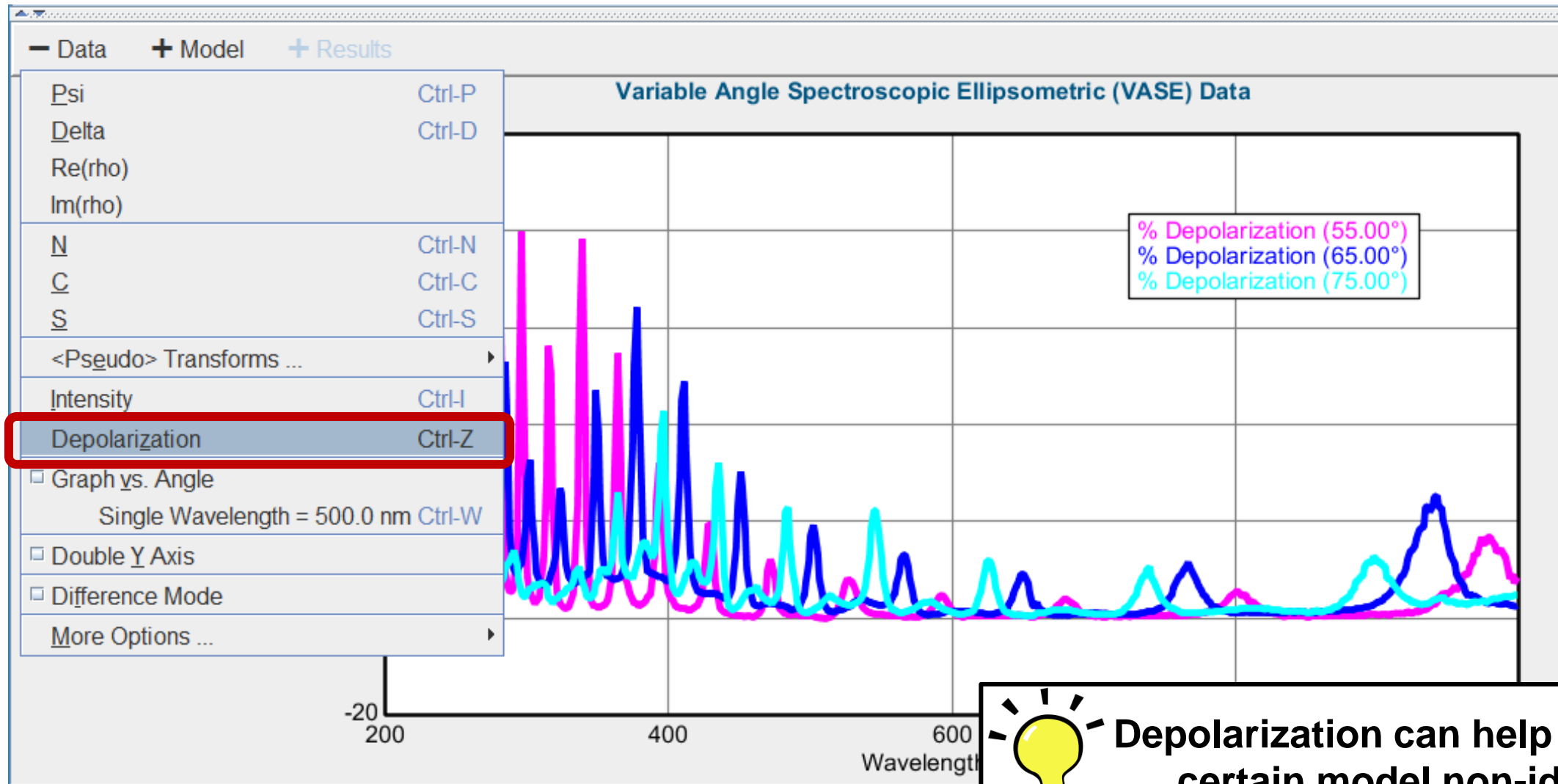


Thickness Non-Uniformity on Polarization States





Depolarization



Depolarization can help us identify certain model non-idealities



Causes of Depolarization

Instrument related:

- Bandwidth
- Angular spread

Sample related:

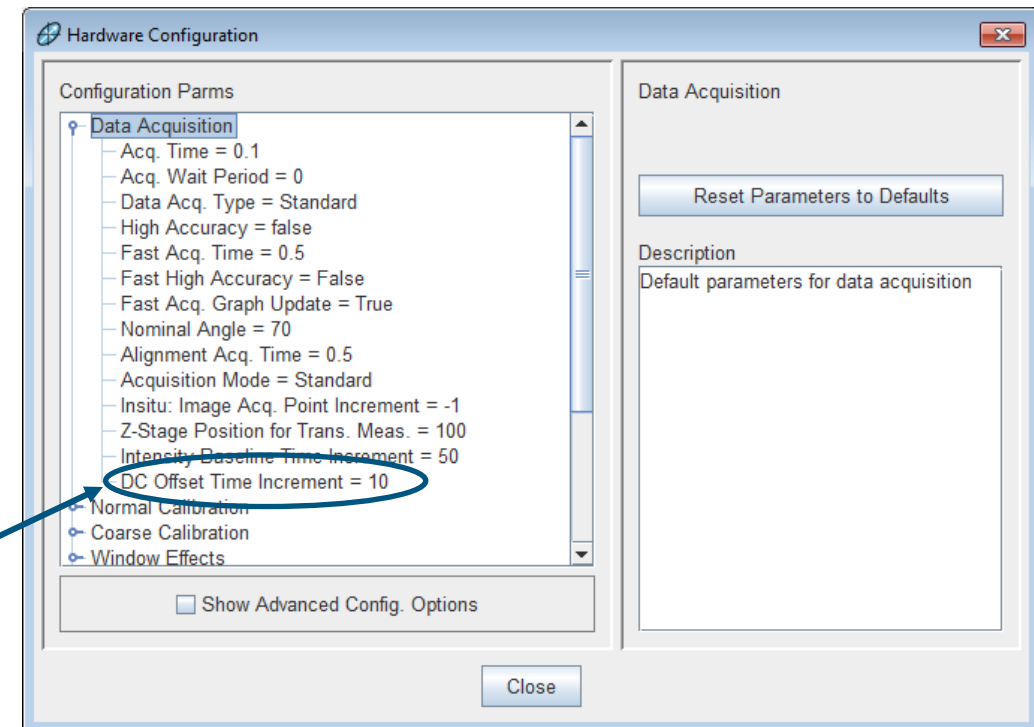
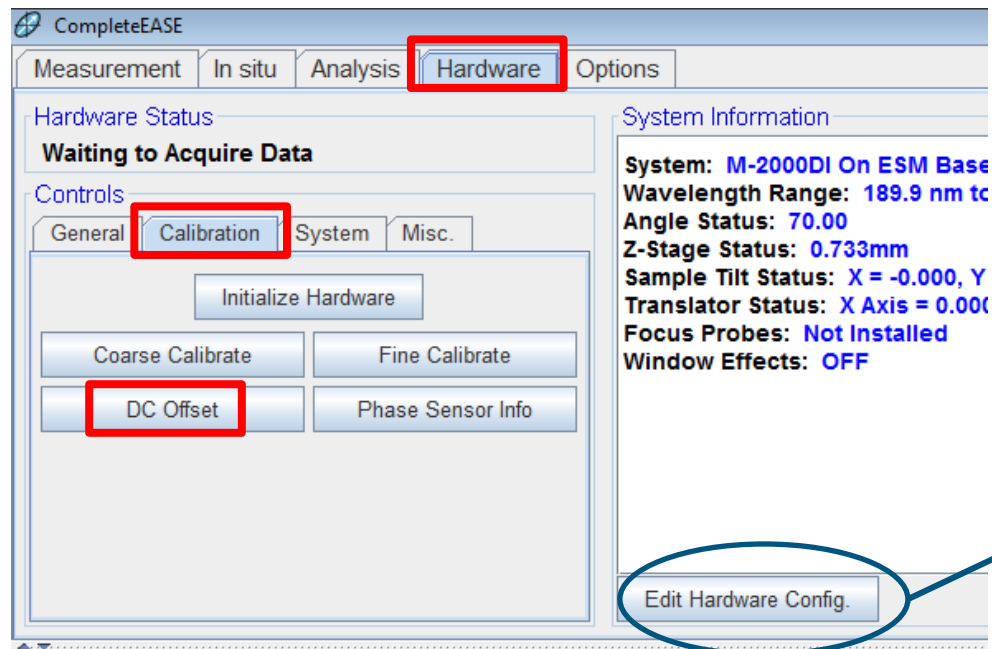
- Backside reflections
- Thickness non-uniformity

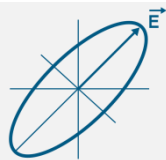
- These sample related features do NOT cause depolarization
 - Roughness
 - Grading
 - Anisotropy
 - Absorption



Acquiring Good Depolarization Data

- DC Offset calibration necessary to obtain good Depolarization data
- Can set time increment in “Edit Hardware Config.” menu
 - Negative increments turn off DC offset calibration
 - Set to “0” to perform DC offset calibration before every measurement





Modeling non-idealities that cause depolarization

Layer Commands: **Add Delete Save**

Include Surface Roughness = **OFF**

+ Layer # 1 = **Cauchy Film** Thickness # 1 = **9708.94 nm** (fit)
Substrate = **SI_JAW**

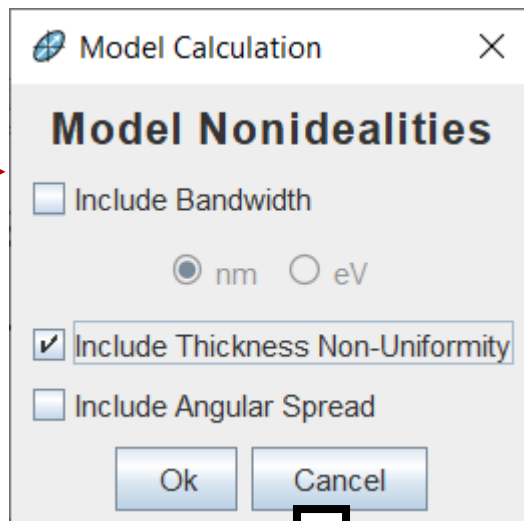
- MODEL Options

Angle Offset = **0.00**

Include Substrate Backside Correction = **OFF**

Model Calculation = **Ideal**

1) select



2) select desired Model calculation type

+ Layer # 1 = **Cauchy Film** Thickness # 1 = **9687.26 nm** (fit)
Substrate = **SI_JAW**

- MODEL Options

Angle Offset = **0.00**

Include Substrate Backside Correction = **OFF**

Model Calculation = **Include Thickness Non-uniformity**

% Thickness Non-uniformity = **0.96** (fit)

of Pts = **9**

3) Fit



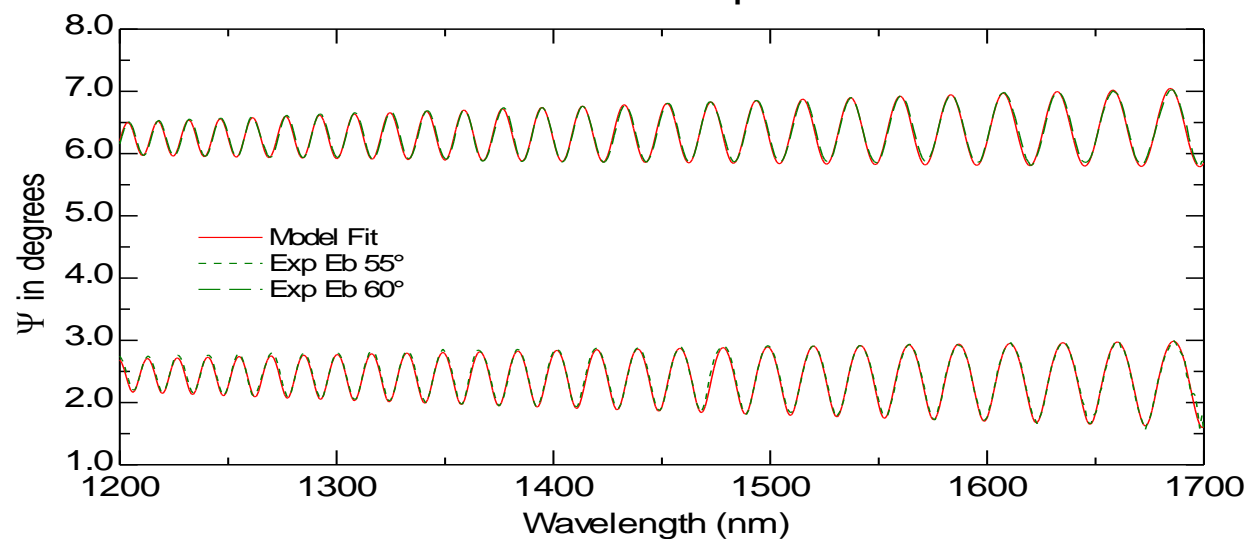
Thick Films

- Become trickier:

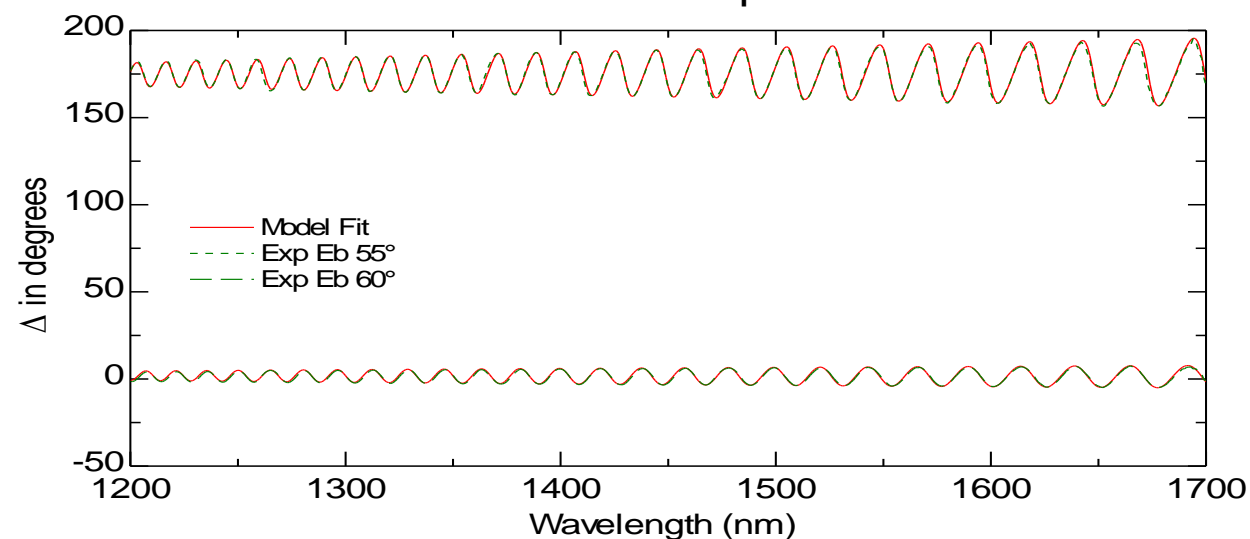
- Need (i) fine wavelength resolution, (ii) uniform film, and (iii) longer wavelengths to resolve oscillations.

Roughness	5 nm
Epoxy Film	42.16 μm
Glass	2.28 mm

Generated and Experimental

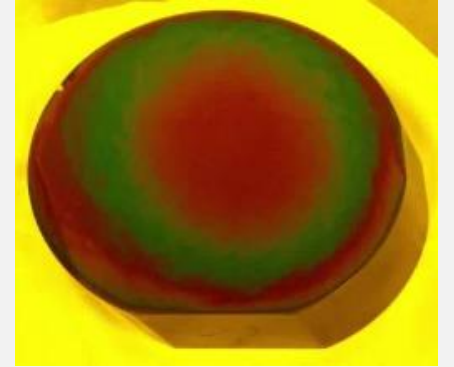


Generated and Experimental



[2-10] Ultra thick Photoresist on Si

- Find a model that matches this data.



**Fit Thickness &
Cauchy Parameters**



Add to improve MSE:
Roughness?
Index Grading?
Anisotropy?
Thickness Non-uniformity?



2-10 Ultra Thick PR on Si: Results



Ultra thick PR on Si

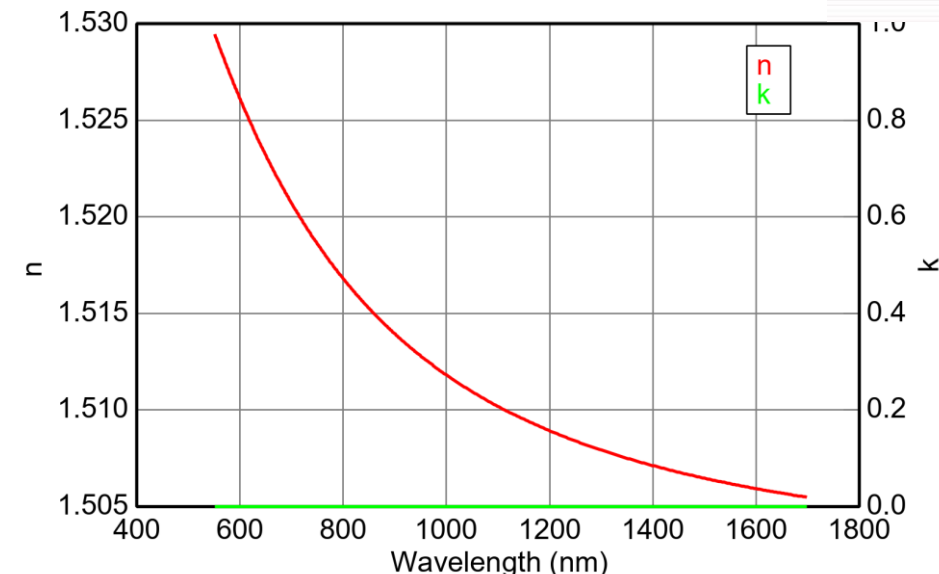
Fit Results

MSE = 58.084
 Thickness # 1 = 9687.09 ± 3.421 nm
 $A = 1.502 \pm 0.00035882$
 $B = 0.01059 \pm 7.8812E-05$
 $C = -0.00067494 \pm 2.1864E-05$
 % Thickness Non-uniformity = 0.96 ± 0.00767
 n of Cauchy Film @ 632.8 nm = 1.52414

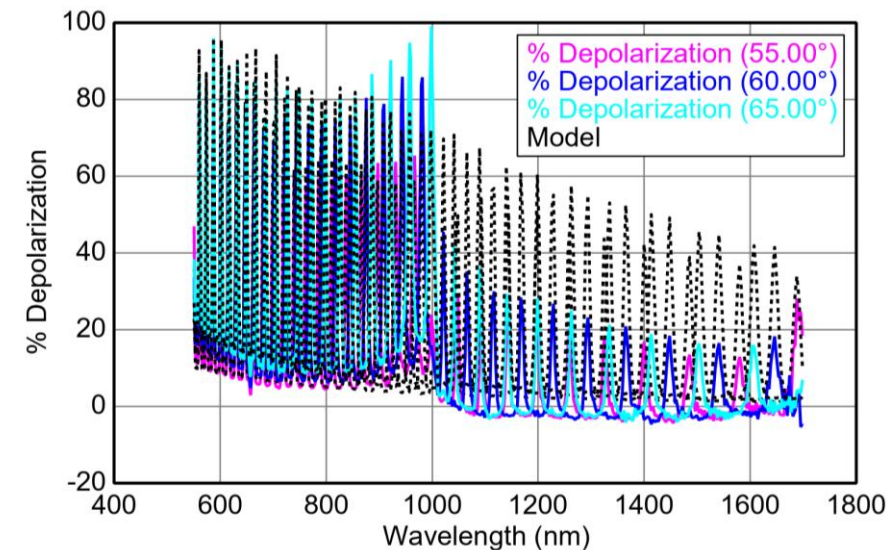
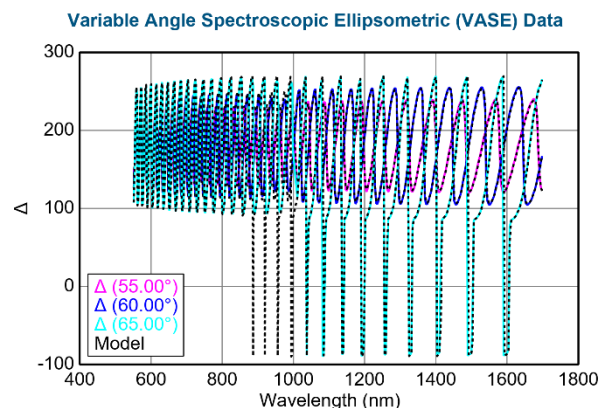
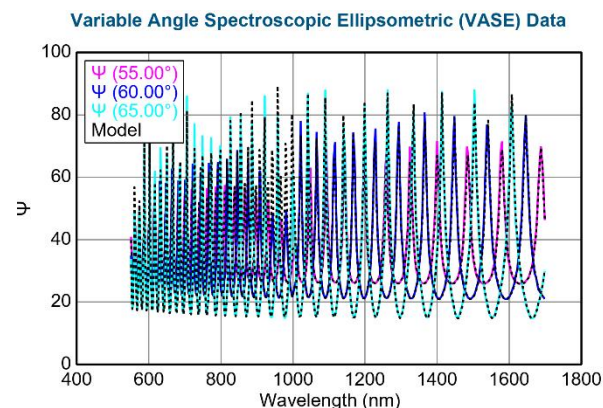
Optical Model

- Layer # 1 = [Cauchy Film](#) Thickness # 1 = [9687.09 nm](#) (fit)
 $A = 1.502$ (fit) $B = 0.01059$ (fit) $C = -0.00067494$ (fit)
 + Urbach Absorption Parameters
 Substrate = [SL_JAW](#)

Opt. Const. of PR Film vs. nm



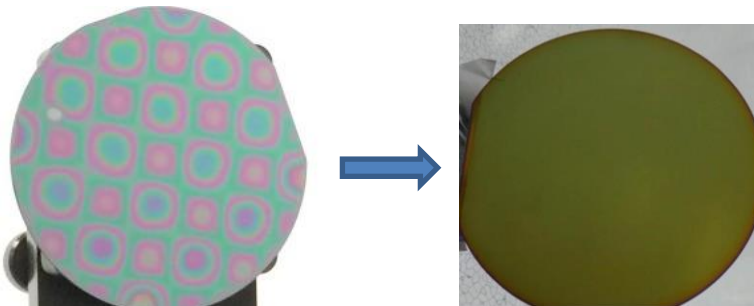
Experimental and Model Generated Data Fits



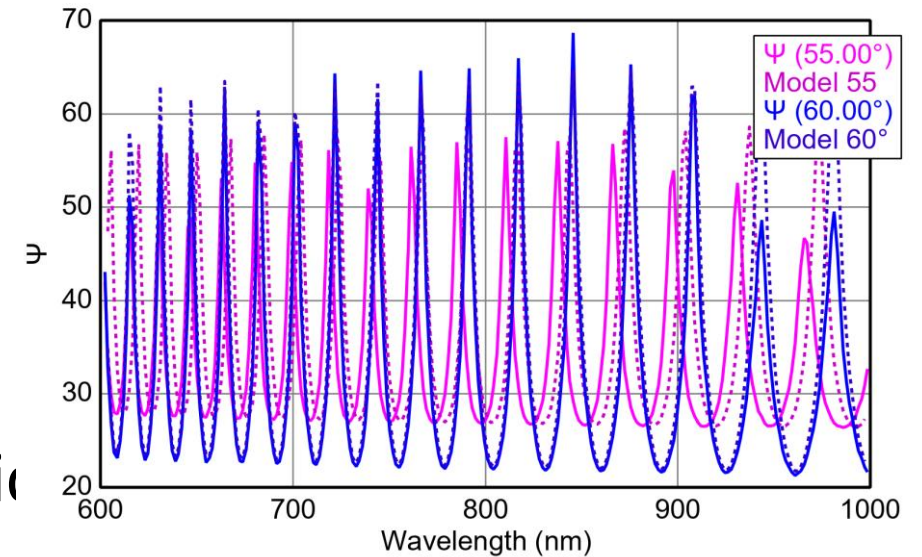


Tips on Thick Films

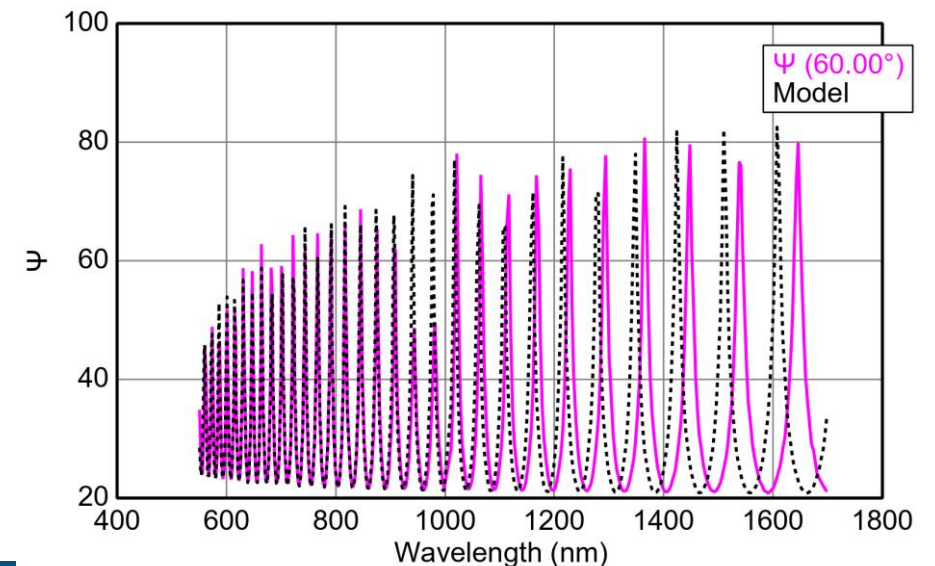
- Make the film as uniform as possible
- Measure at Multiple angles of incidence
- Measure into longer wavelength range
- Reduce the measurement area
- Modify process conditions to reduce film thickness



Not matching multiple angles



Not matching long wavelengths

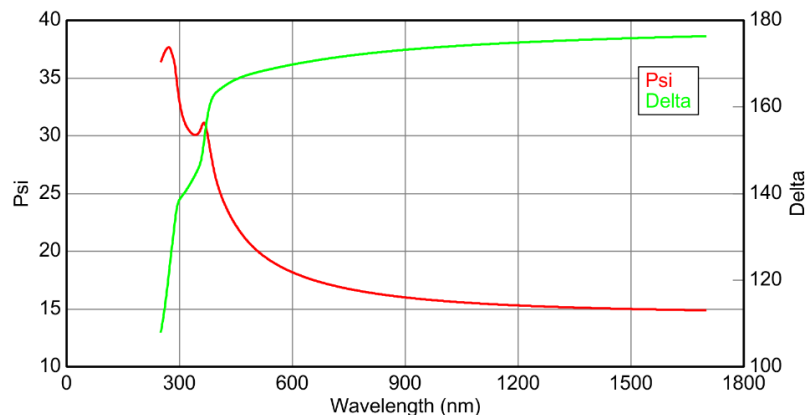




Thickness Ranges

Ultra-thin films

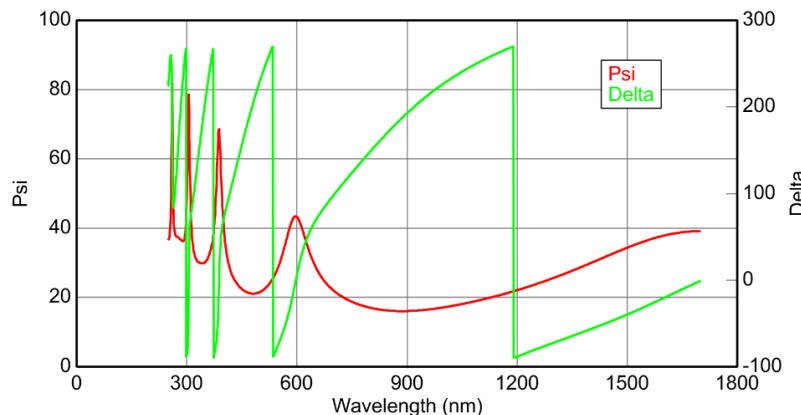
Spectroscopic Ellipsometric (SE) Data



- 10 to 30nm or less
- No interference peaks
- Sensitive to thickness
- Not sensitive to refractive index (use fixed RI)

Thin films

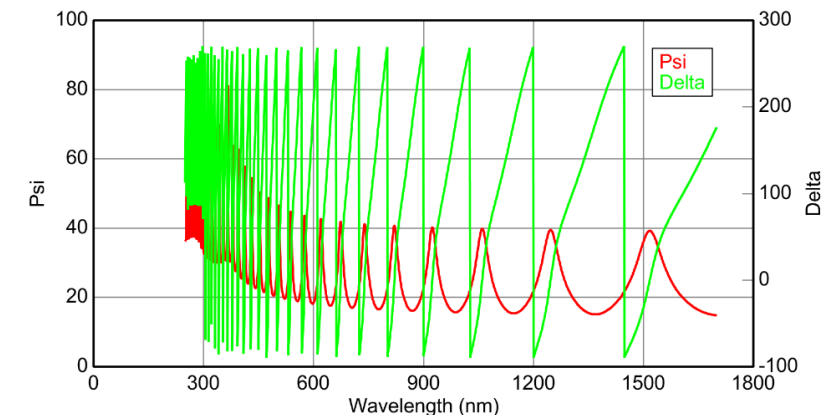
Spectroscopic Ellipsometric (SE) Data



- Tens of nms up to a couple of microns
- A few interference peaks and valleys
- Sensitive to both thickness and index

Thick films

Spectroscopic Ellipsometric (SE) Data



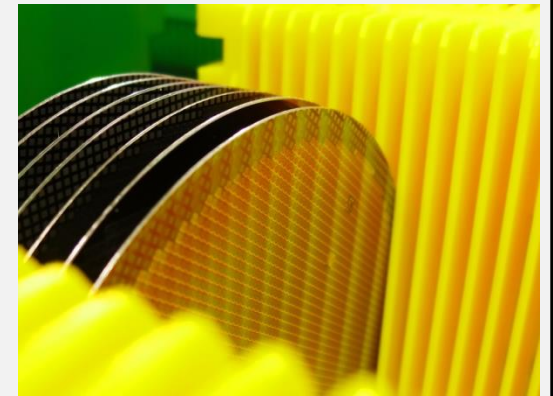
- Hundreds of nms to a few microns
- Many interference peaks and valleys
- Sensitive to thickness non-uniformity
- Long wavelength range and multiple AOIs are recommended



Practice Set

[2-11] TiO_x on Si

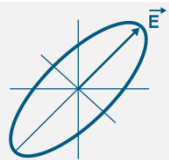
- **Find a model that best matches data.**



**Fit Thickness &
Cauchy Parameters**



Add to improve MSE:
Roughness?
Index Grading?
Anisotropy?



2-11 TiOx on Si: Results



TiOx on Si

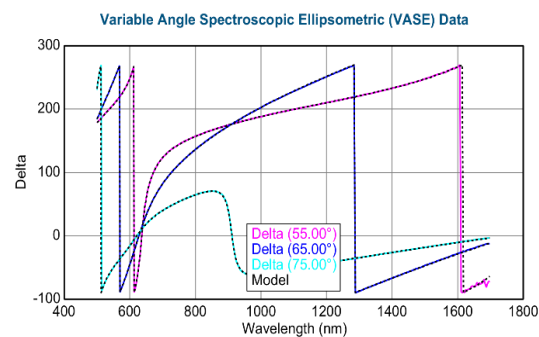
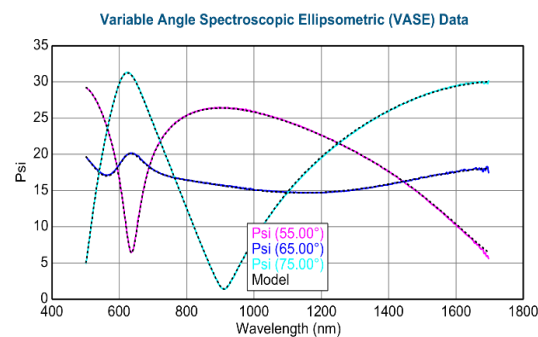
Fit Results

MSE = 2.720
Roughness = 3.66 ± 0.021 nm
Thickness # 1 = 216.70 ± 0.020 nm
 $A = 2.245 \pm 0.00021244$
 $B = 0.04193 \pm 0.00028478$
 $C = 0.00190 \pm 6.8897E-05$
% Inhomogeneity = -2.81 ± 0.0380
n of Cauchy Film @ 632.8 nm = 2.36106

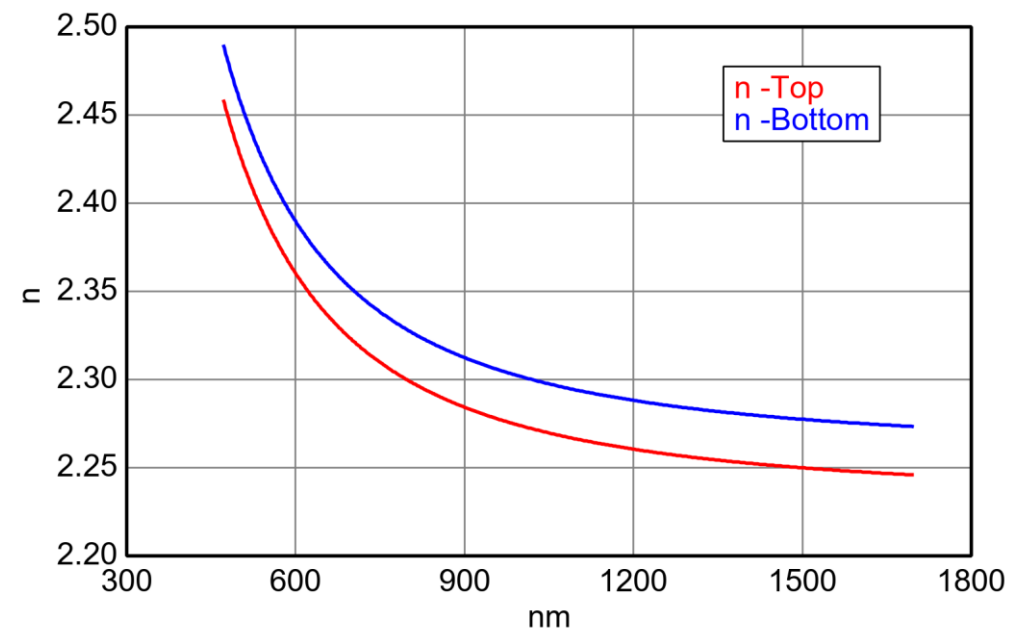
Optical Model

Roughness = **3.66 nm** (fit)
- Layer # 1 = **Graded Layer** Thickness # 1 = **216.70 nm** (fit)
Grade Type = **Simple** # of Slices = **5**
% Inhomogeneity = **-2.81** (fit)
+ Material = **Cauchy Film**
Substrate = **SI_JAW**

Experimental and Model Generated Data Fits

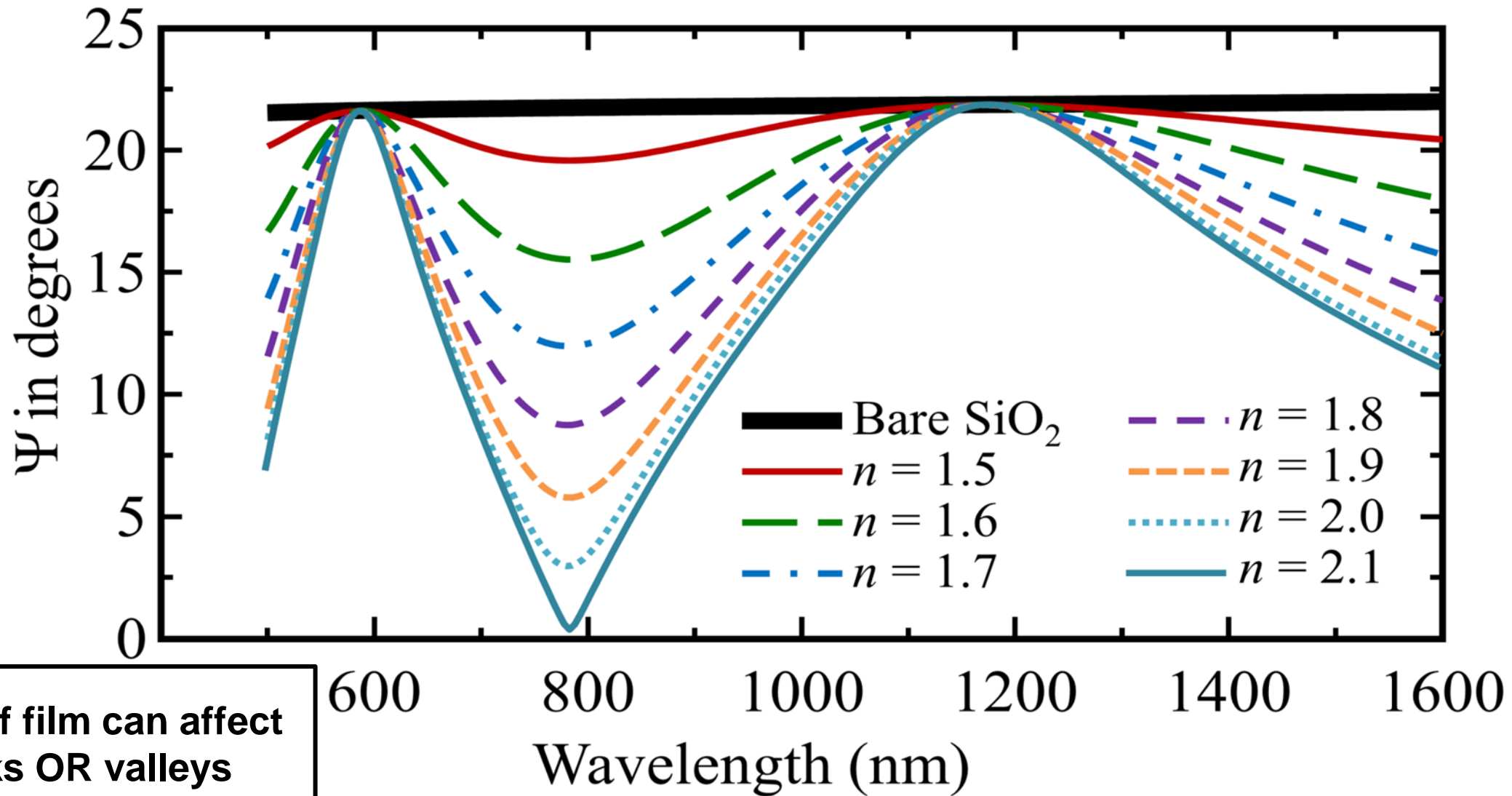


Opt. Const. of Graded TiOx vs. nm





Data Features - Thin Films on Glass

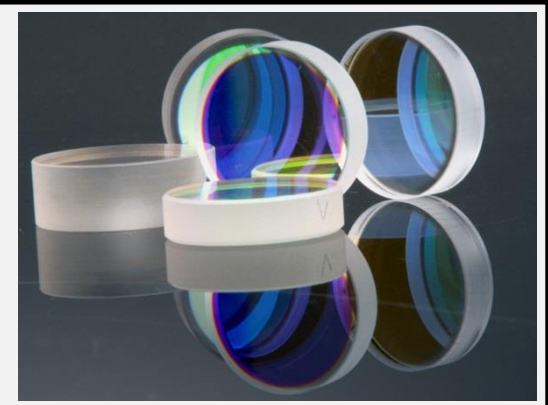


Index of film can affect
peaks OR valleys

[2-12] Oxide on Fused Silica

- **Determine index and thickness of oxide.**

- Fused silica is “2-12_Fused Silica_Genosc.mat”



**Estimate
Index & Thickness**



**Fit Thickness &
Cauchy Parameters**



**What else to improve
MSE?**

Si with Transparent Film.mod
Change substrate

What happens when wrong material file, such as 7059 Glass.mat is used as substrate?



2-12_Oxide on Fused Silica: Results



Sample: 2-12_Oxide on Fused Silica

Fit Results

MSE = 10.792

Thickness # 1 = 480.14 ± 0.132 nm

A = 1.625 ± 0.00030898

B = $0.00527 \pm 7.3463\text{E-}05$

C = $0.00013987 \pm 3.2436\text{E-}06$

% Thickness Non-uniformity = 7.28 ± 0.0630

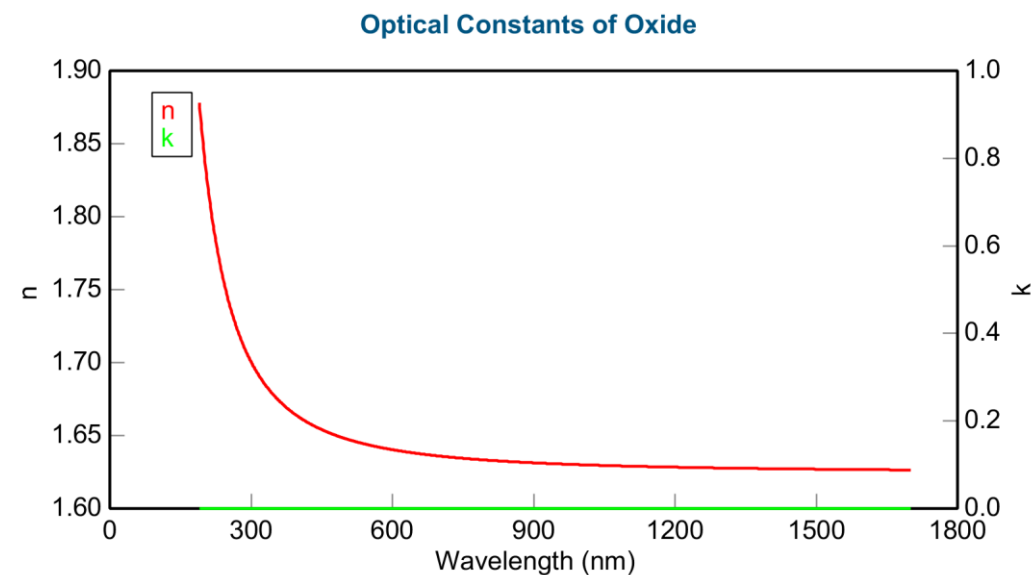
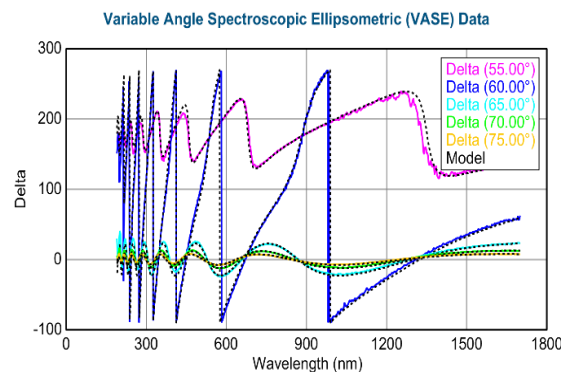
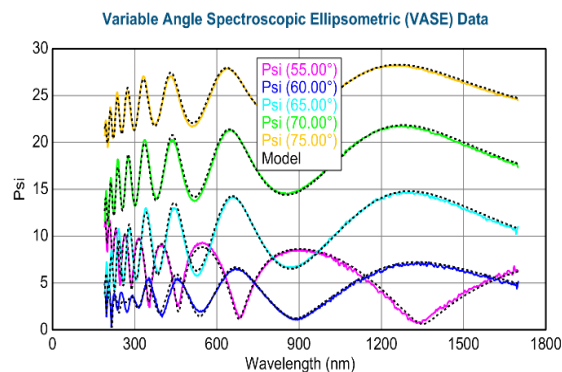
n of Cauchy Film @ 632.8 nm = 1.63863

Optical Model

+ Layer # 1 = [Cauchy Film](#) Thickness # 1 = **480.14 nm** (fit)

+ Substrate = [2-12_Fused Silica_Genosc](#)

Experimental and Model Generated Data Fits



$[2-13]$ SiN_x on Si

- Find a model that matches this data.



**Fit Thickness &
Cauchy Parameters**



Add to improve MSE:
Roughness?
Index Grading?
Anisotropy?
Thickness Non-uniformity?



2-13 SiN_x on Si: Results



Sample: 2-13 SiN_x on Si

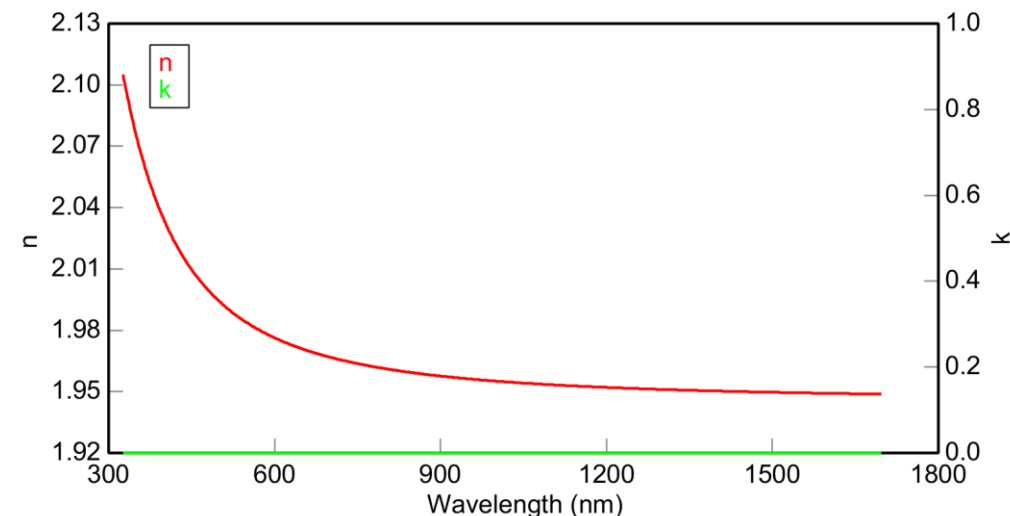
Fit Results

MSE = 8.964
Thickness # 1 = 104.61 ± 0.018 nm
 $A = 1.946 \pm 0.00053876$
 $B = 0.00853 \pm 0.00033049$
 $C = 0.00089549 \pm 3.6230E-05$
Back Reflections = 0.558 ± 0.003123
n of Cauchy Film @ 632.8 nm = 1.97260

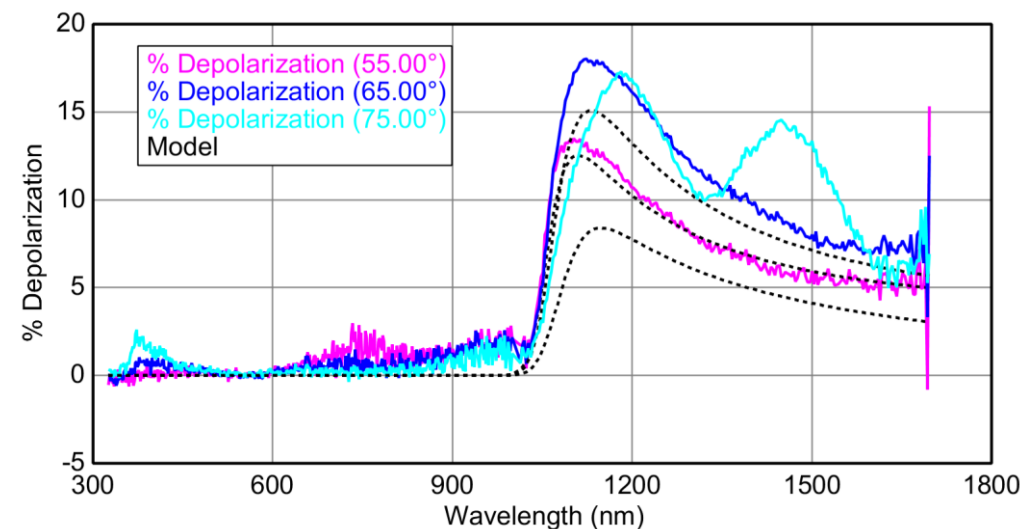
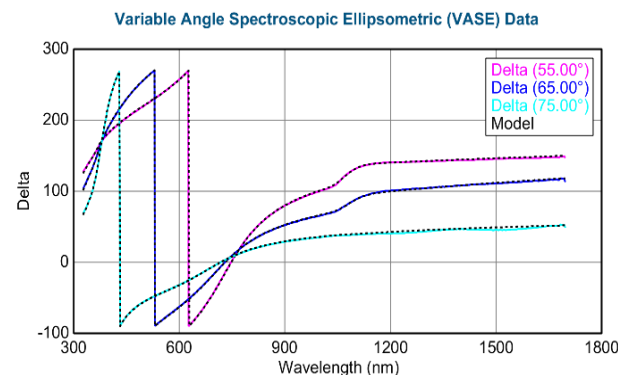
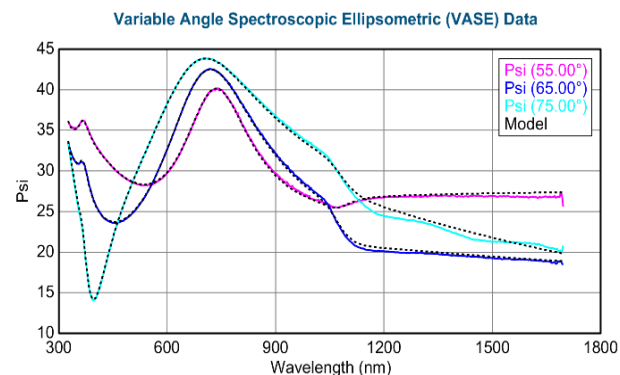
Optical Model

+ Layer # 1 = [Cauchy Film](#) Thickness # 1 = **104.61 nm** (fit)
Substrate = [SI_JAW](#) Substrate Thickness = **0.7500 mm**

Optical Constants of SiN_x

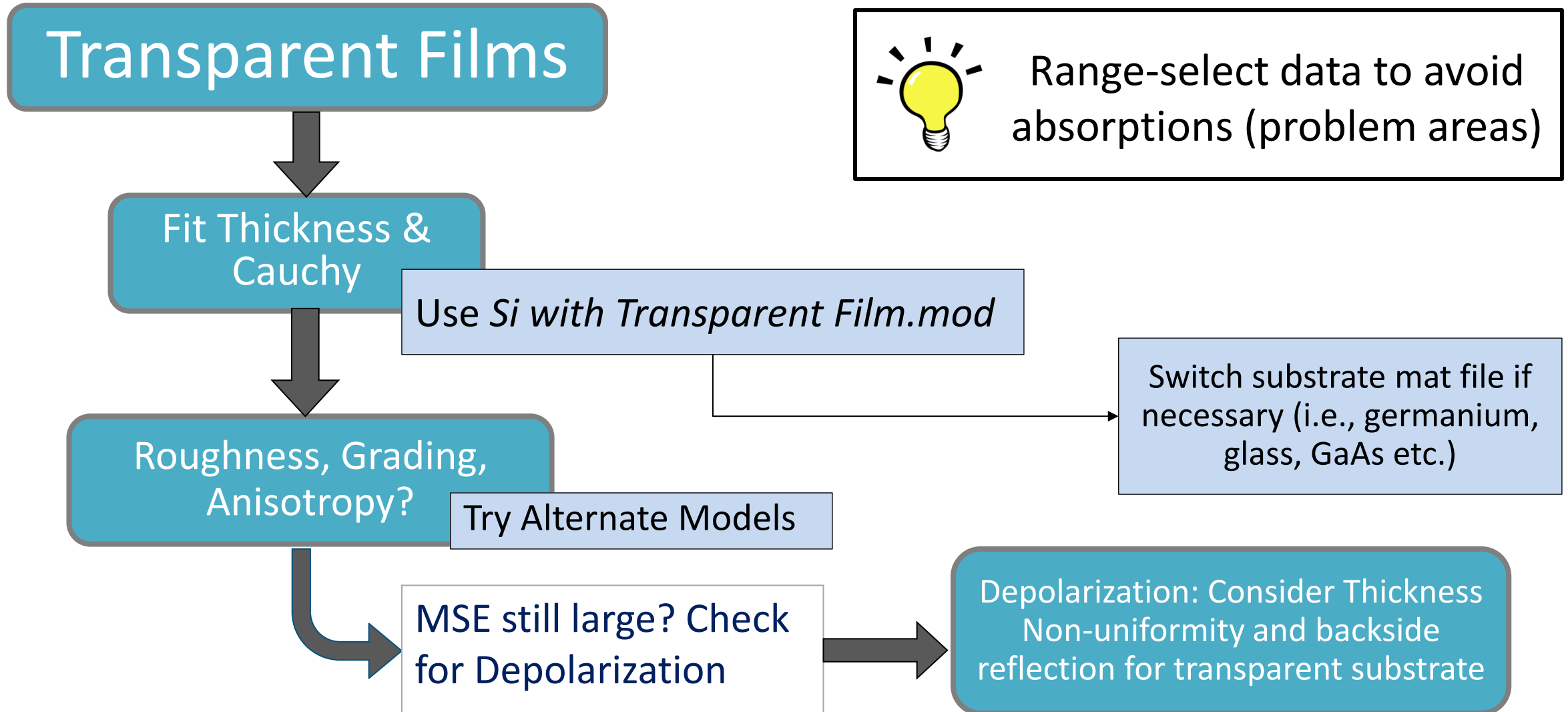


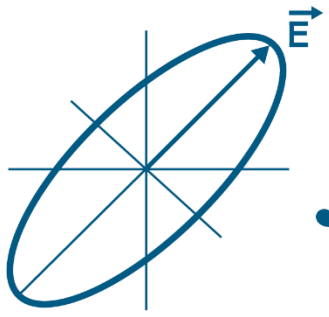
Experimental and Model Generated Data Fits





Summary Transparent films





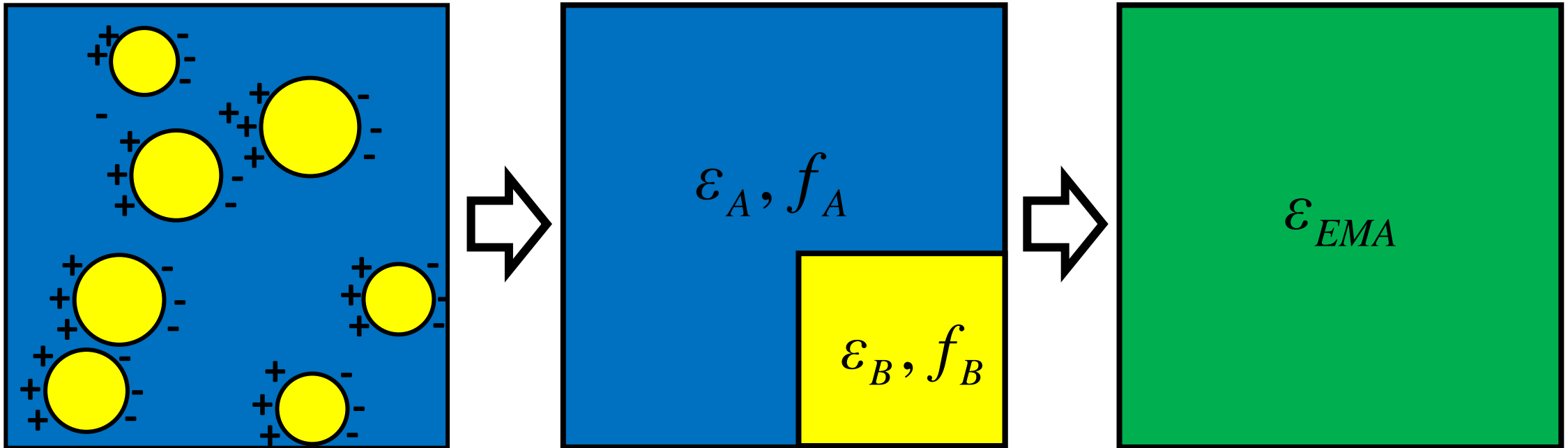
J.A. Woollam

EXTRA SLIDES



Effective Medium Approximation (EMA)

- Composites of more than 1 material are often described by EMA
- EMA considers volume fractions and possible charge screening:



$$f_a \frac{\epsilon_a - \epsilon_{EMA}}{\epsilon_a + 2\epsilon_{EMA}} + (1 - f_a) \frac{\epsilon_b - \epsilon_{EMA}}{\epsilon_b + 2\epsilon_{EMA}} = 0$$



Using EMA in CompleteEASE

- Roughness:
50%-50% void and layer below
- EMA.mat: Use to mix multiple 2-3 mats
 - Coupled.mat helps “tie” to other layers
- Graded Layer: Can increase/decrease index of a material by mixing with void.

Roughness = [10.00 nm](#)

-	Graded Layer	Thickness # 3 = 100.00 nm Grade Type = Standard # of Slices = 5 Bottom % = 0.00 Top % = 10.00 Exponent = 1.0000 Symmetric Profile = ON Draw Profile EMA Mode = Bruggeman Depolarization = 0.333 + Material = Cauchy Film 2nd Material = Void
-	Layer # 2 = EMA	Thickness # 2 = 100.00 nm # of Constituents = 2 - Material 1 = Coupled Coupled to Layer # 1 (a-Si) Material 2 = Void EMA % (Mat 2) = 20.0 depolarization = 0.333 Analysis Mode = Bruggeman
	Layer # 1 = a-Si	Thickness # 1 = 50.00 nm
	Substrate = Si_JAW	



TRY ALTERNATE MODELS

