

J.A. Woollam

# ADVANCED TOPICS & REVIEW

## SESSION 6

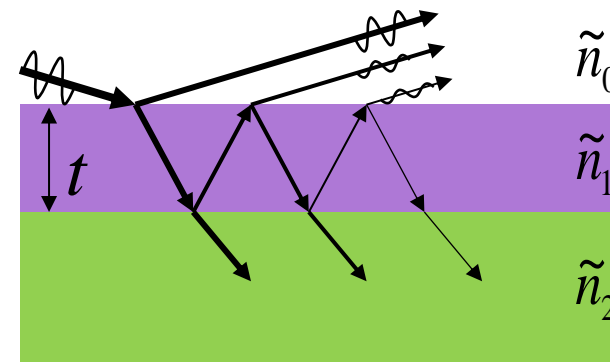
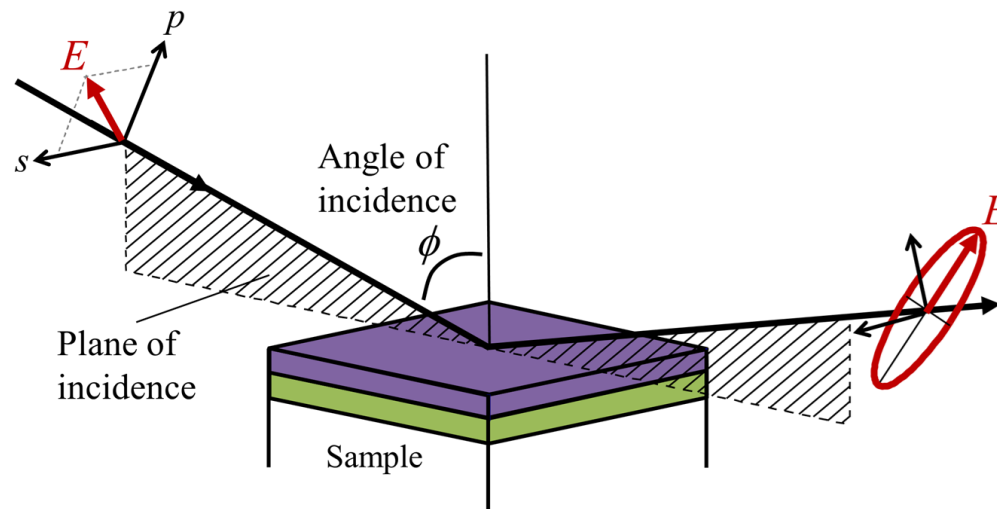
Jianing Sun

Yale University  
March 2025



# COURSE OUTLINE

- Session 1: Introduction to Ellipsometry
- Session 2: Transparent Materials
- Session 3: Materials with Absorption (B-Spline)
- Session 4: Materials with Absorption (Gen-Osc)
- Session 5: Thin Absorbing Films & Multi-Sample Analysis
- **Session 6: Advanced Topics and Review**





# SESSION 6 OUTLINE

- Advanced Topics:
  - #1: Fit Log and Batch Analysis
  - #2: Mapping Data
  - #3: In-Situ Dynamic Data
- REVIEW

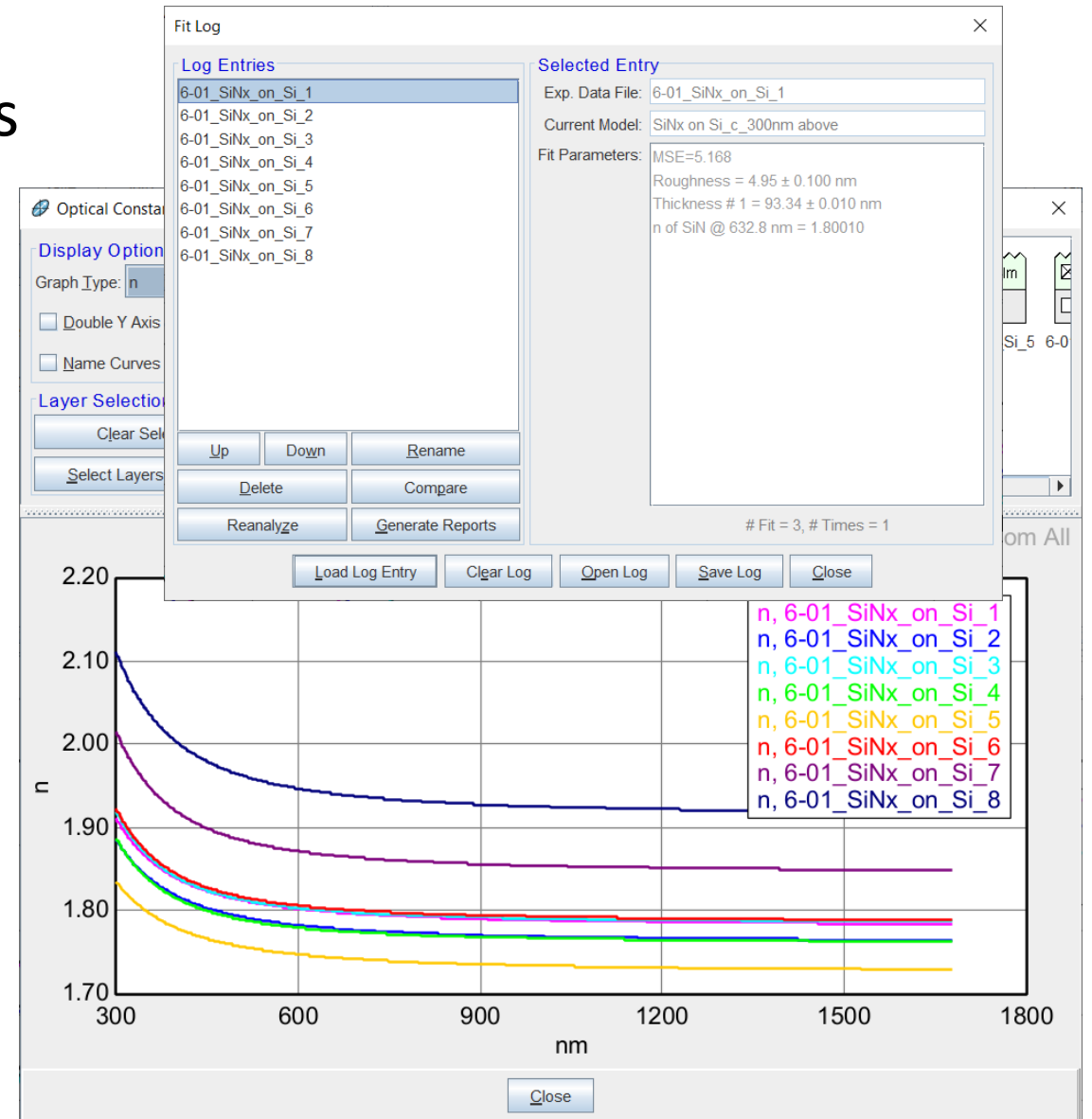


# Topic #1: Batch Analysis

- Automate analysis of multiple data-sets
- Suitable for analyzing and comparing similar samples



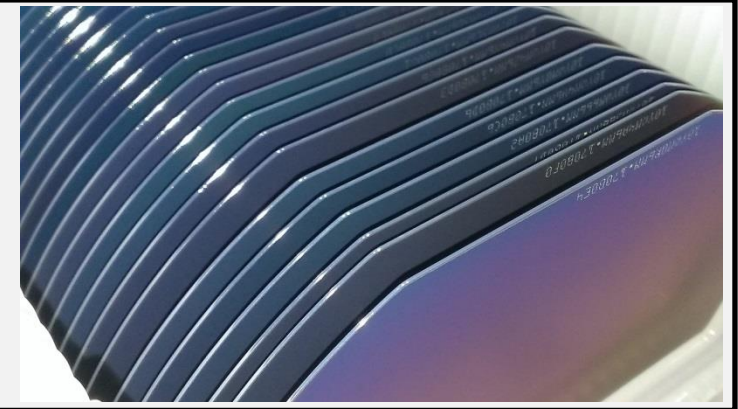
- Set up flexible model.
- Analyze multiple data sets
- Report and compare results





# [6-01] SiNx on Si (Batch Analysis)

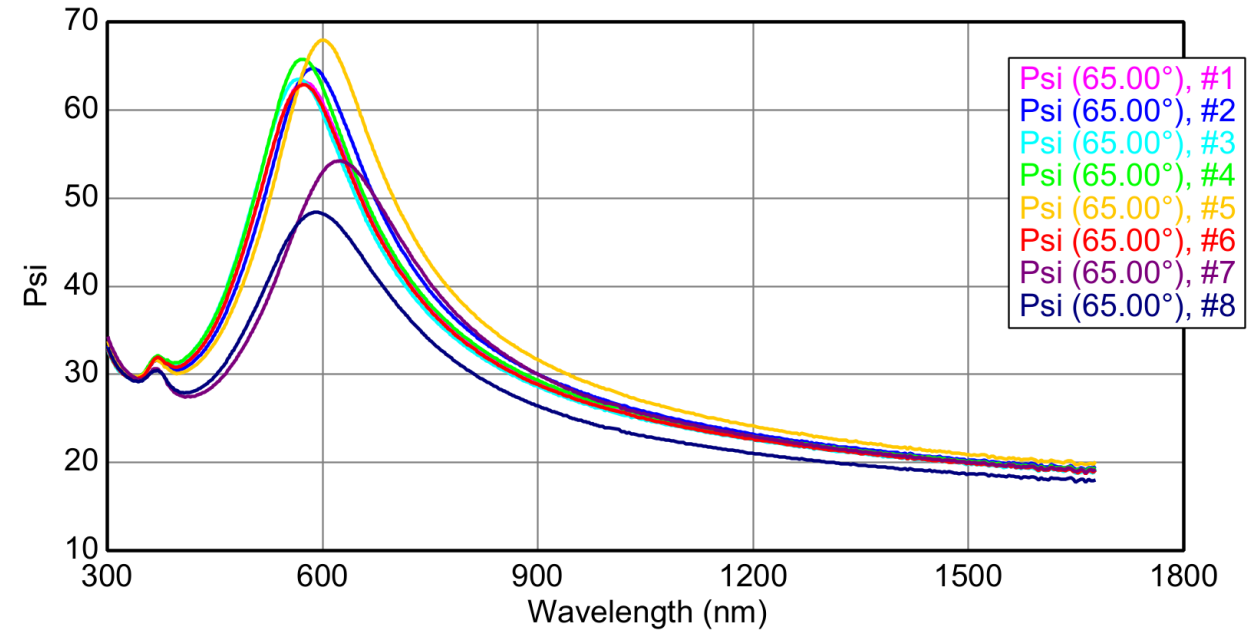
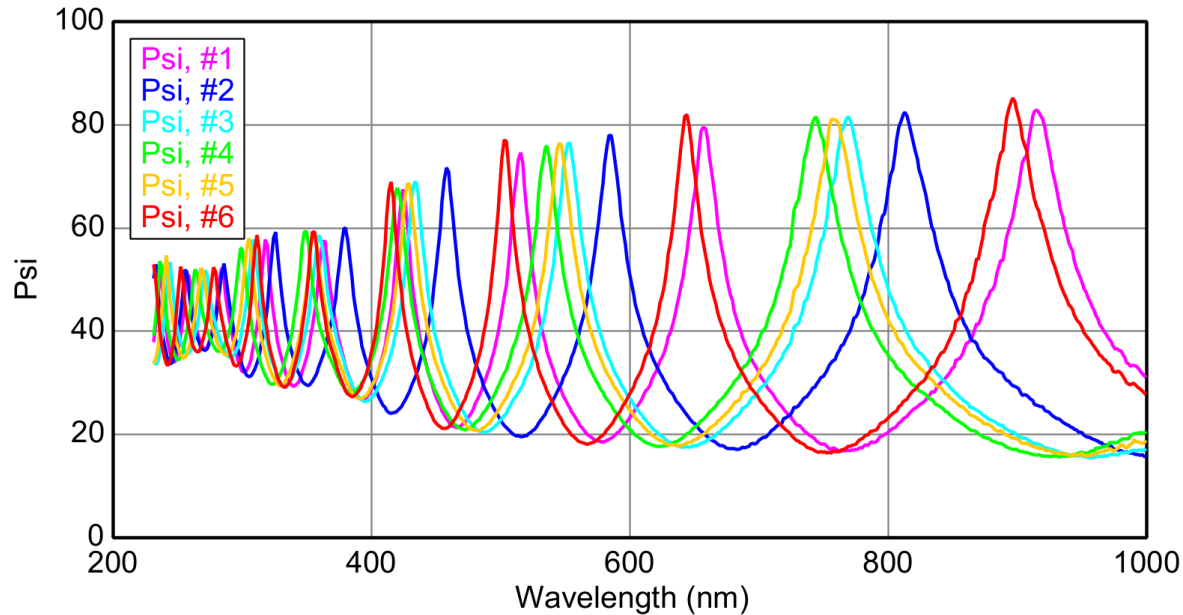
- **Build model & analyze all 8 data sets for thickness and index at 633 nm.**



- Compare table of thicknesses and index at 633 nm.
- Compare index spectra for all wafers.



# PREVIEW OF RAW DATA

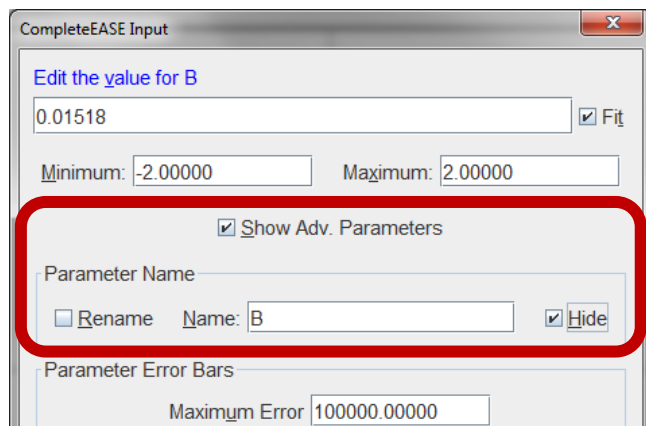


- Observe data spread and variations to guide model setting strategy
  - Thickness and/or refractive index?



# PREPARING MODEL FOR AUTOMATION

- Make sure it fits all data.
  - Thickness Pre-fit
  - Global Fit
  - Limit Wavelength range / Angles for fit
- Customize what to report.
  - Rename / Hide Fit Parameters
  - Add Derived Parameters
- Save the model



Roughness = [4.95 nm](#) (fit)

- Layer # 1 = [Cauchy Film](#) Thickness # 1 = [93.34 nm](#) (fit)  
A = [1.782](#) (fit) B = [0.00576](#) (fit) C = [0.00053061](#) (fit)  
+ Urbach Absorption Parameters  
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. = [1.500](#) Max. = [2.500](#) # Guesses = [10](#)

### + Customize Global Fit

Fit Weight = [N C S](#)

Limit Wvl. for Fit = [ON](#) Range = [300.0 nm - 1700.0 nm](#)

Limit Angles for Fit = [OFF](#)

Max. Acceptable MSE = [100.000](#)



**Set Max. Acceptable MSE  
to warn when fit fails**

- Include Derived Parameters = [ON](#)

### Add Derived Parameter

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

# of Decimal Places = [5](#)

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

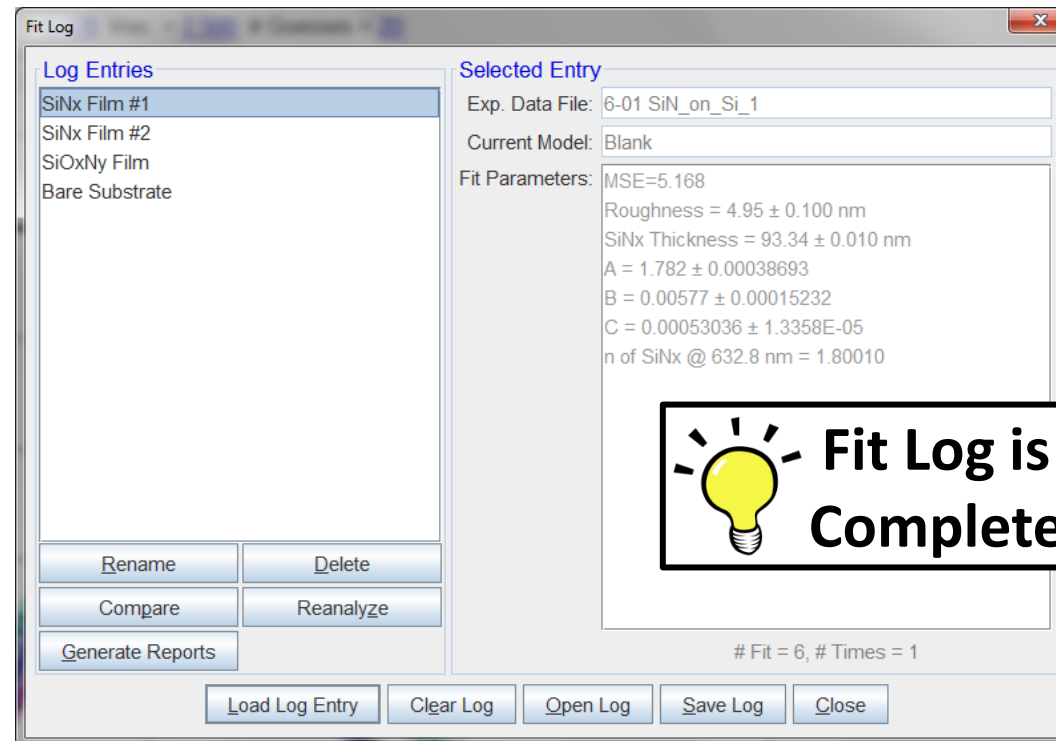
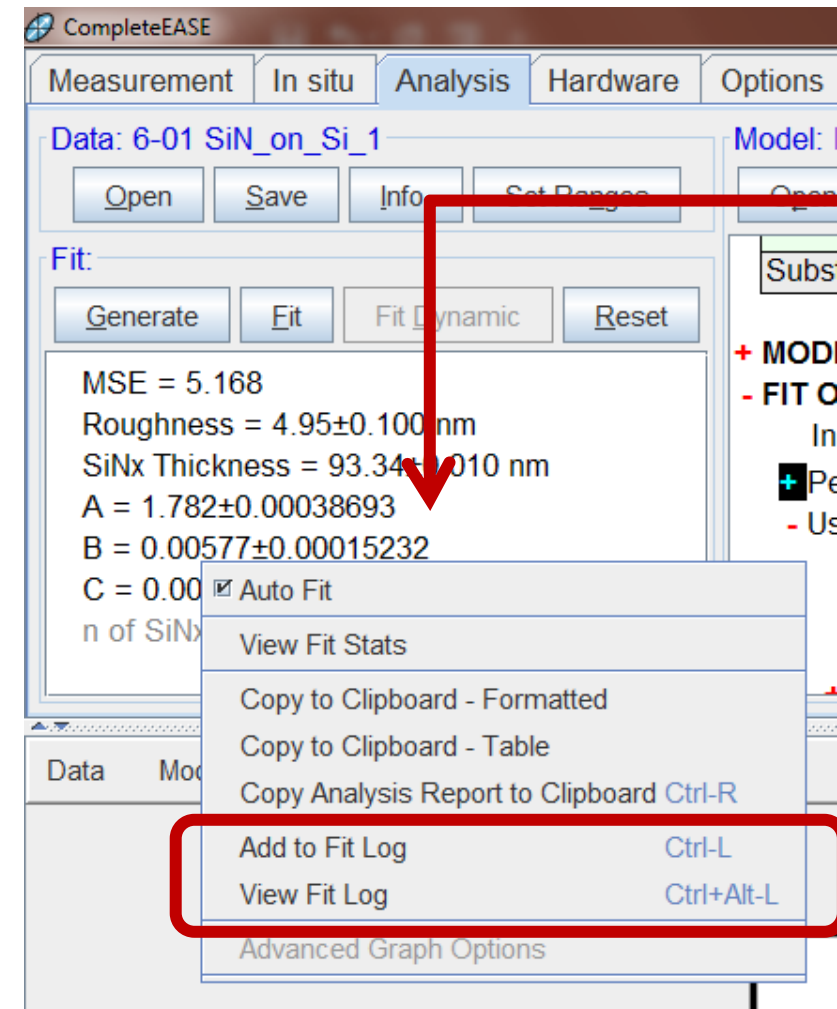



# FIT LOG



Right-click in fit panel:

- Add to Fit Log (Ctrl-L)
- View Fit Log (Ctrl+Alt-L)



 **Fit Log is cleared when CompleteEASE is closed**



# BATCH ANALYSIS (FROM FIT LOG)

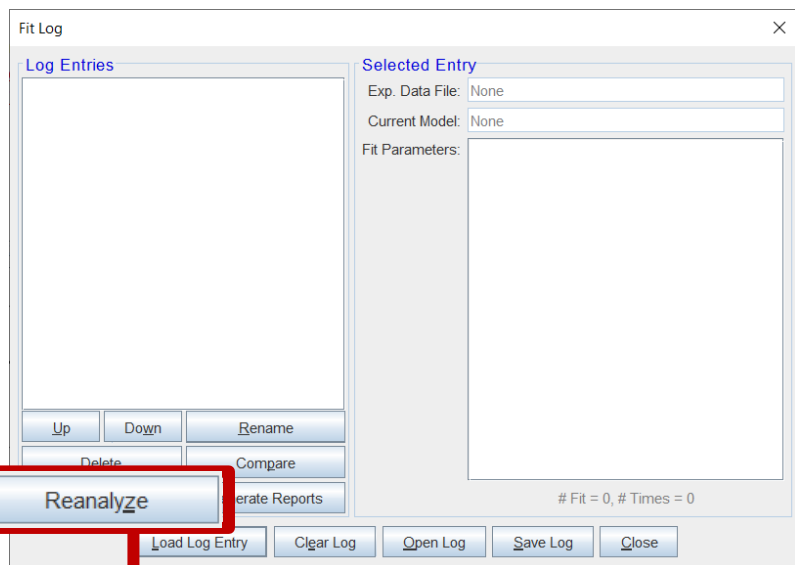
1

Select 'Reanalyze' from Fit Log

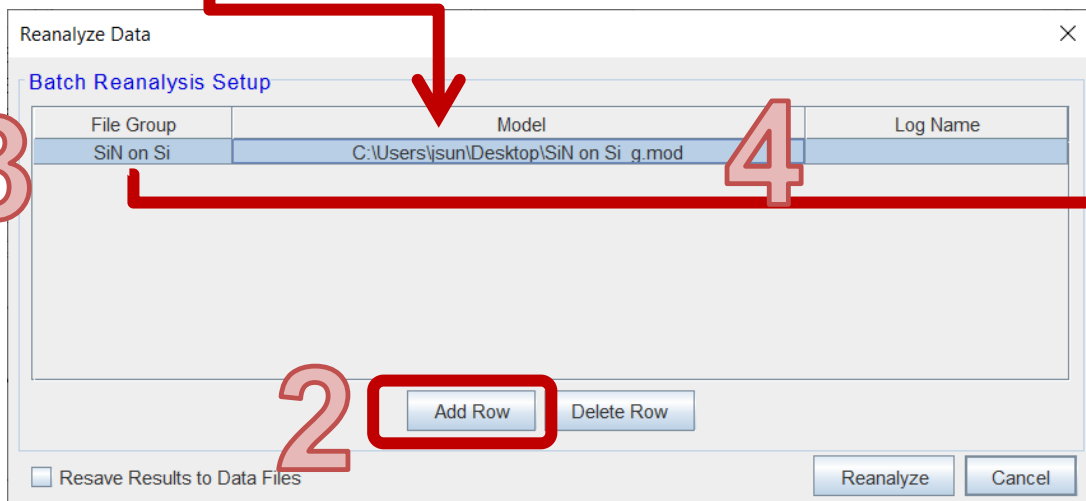
2-4

Add Row and populate with data sets & corresponding model.

1



3



4

2

Files:


Name	Date	Size
1-Thermal Oxide on Si.SE	5/11/15 1...	25 KB
2-Transparent Film on Si.SE	5/11/15 1:...	25 KB
3_Transparent Film on Glass.SE	5/30/17 4:...	77 KB
4-SiN_on_Si_1.SE	8/24/10 1...	35 KB
4-SiN_on_Si_2.SE	8/24/10 1...	35 KB
4-SiN_on_Si_3.SE	8/24/10 1...	35 KB
4-SiN_on_Si_4.SE	8/24/10 1...	35 KB
4-SiN_on_Si_5.SE	8/24/10 1...	35 KB
4-SiN_on_Si_6.SE	8/24/10 1...	35 KB
4-SiN_on_Si_7.SE	8/24/10 1...	35 KB
4-SiN_on_Si_8.SE	8/24/10 1...	35 KB
5_Rough-Graded_SiC_on_Si.SE	8/20/10 5:...	5 KB
6_Opaque Metal.SE	7/2/15 4:5...	28 KB
6_Thickness Uniformity Map.SE	7/12/16 1...	1315 KB
7_Dye on glass.SE	5/6/09 5:2...	91 KB
8_a-Si on Glass.SE	9/14/09 5:...	30 KB
9_Photoresist on Si.SE	7/2/15 5:2...	69 KB
Demo-Transparent Film on Si.SE	5/30/17 3:...	25 KB

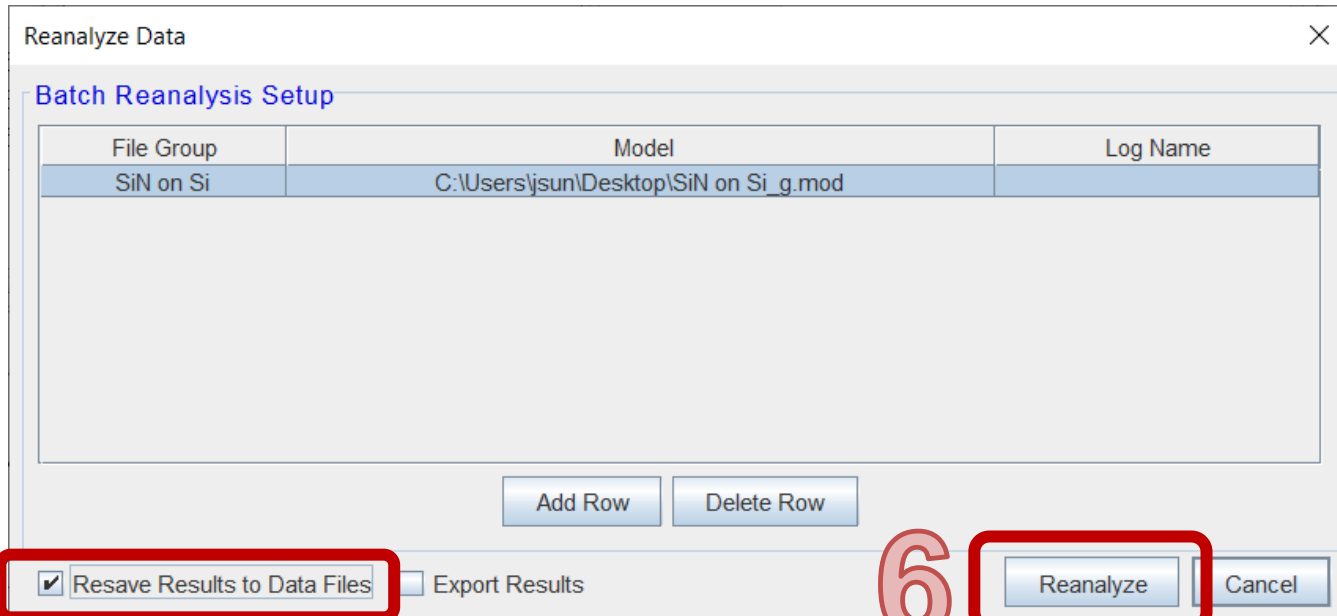


# BATCH ANALYSIS (FROM FIT LOG)

## 5 - optional

“Resave Results to Data Files” will add fit results to data files

- It will overwrite previous fit results saved with the raw data
- Be sure to rename files if overwritten is not desirable 



File Group	Model	Log Name
SiN on Si	C:\Users\jsun\Desktop\SiN on Si_g.mod	

5 ☒ Resave Results to Data Files ☐ Export Results

6

6 “Reanalyze”: fit all data sets to the corresponding model and add results to the Fit Log.



# 6-01 SiNx ON Si "BATCH": RESULTS



Roughness = **3.95 nm** (fit)

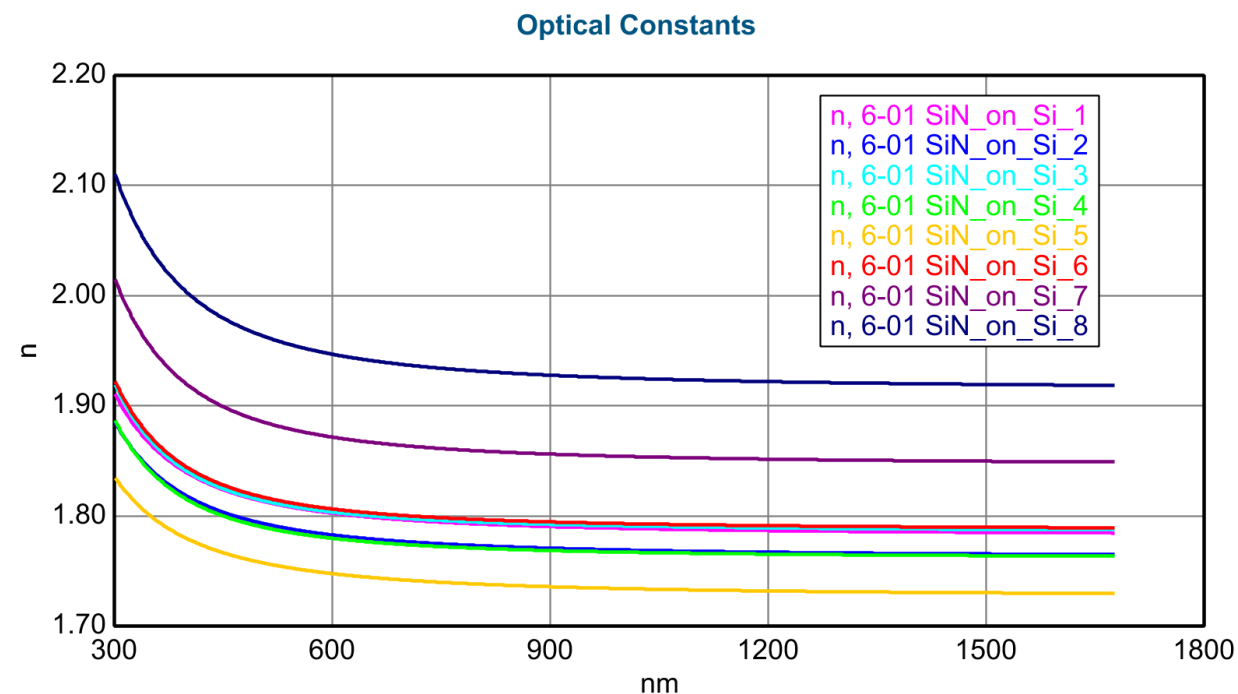
- Layer # 1 = **SiNx** SiNx Thickness = **87.64 nm** (fit)  
A = **1.915** (fit) B = **0.00932** (fit) C = **0.00075636** (fit)  
+ Urbach Absorption Parameters  
Substrate = **Si\_JAW**

Comparison

Entry Comparison Table

	MSE	SiNx Thickness (nm)	Roughness (nm)	n of SiNx @ 632.8 nm
6-01 SiN on Si 1	5.168	93.34	4.95	1.80010
6-01 SiN on Si 2	5.168	96.50	4.60	1.78035
6-01 SiN on Si 3	7.147	92.09	5.46	1.80121
6-01 SiN on Si 4	6.566	94.44	4.96	1.77741
6-01 SiN on Si 5	3.886	101.45	4.43	1.74532
6-01 SiN on Si 6	6.822	92.96	5.10	1.80391
6-01 SiN on Si 7	7.059	96.95	4.72	1.86848
6-01 SiN on Si 8	6.196	87.64	3.95	1.94308
Average	6.00124	94.421	4.771	1.81498
Std. Dev.	1.15414	4.049	0.456	0.06241

☐ Reverse Columns/Rows ☒ Add Statistics





# COMPARING RESULTS (IN FIT LOG)

**Fit Log**

**Log Entries**

- 6-01\_SiNx\_on\_Si\_2
- 6-01\_SiNx\_on\_Si\_3
- 6-01\_SiNx\_on\_Si\_4
- 6-01\_SiNx\_on\_Si\_5
- 6-01\_SiNx\_on\_Si\_6
- 6-01\_SiNx\_on\_Si\_7
- 6-01\_SiNx\_on\_Si\_8
- 6-01\_SiNx\_on\_Si\_1
- 6-01\_SiNx\_on\_Si\_2
- 6-01\_SiNx\_on\_Si\_3
- 6-01\_SiNx\_on\_Si\_4
- 6-01\_SiNx\_on\_Si\_5
- 6-01\_SiNx\_on\_Si\_6
- 6-01\_SiNx\_on\_Si\_7
- 6-01\_SiNx\_on\_Si\_8

**Selected Entry**

Exp. Data File: 6-01\_SiNx\_on\_Si\_1

Current Model: SiNx on Si\_g

Fit Parameters:

- MSE=7.538
- Roughness =  $5.36 \pm 0.053$  nm
- Thickness # 1 =  $93.33 \pm 0.014$  nm
- Einf =  $1.044 \pm 0.0223$
- UV Pole Amp. =  $202.2692 \pm 8.68522$
- Amp1 =  $43.658 \pm 95.2108$
- Br1 =  $1.980 \pm 0.0972$
- Eo1 =  $7.049 \pm 0.0237$
- Eg1 =  $2.819 \pm 0.1155$
- Ep1 =  $15.000 \pm 17.6921$
- n of SiN @ 632.8 nm = 1.80007

# Fit = 10, # Times = 1

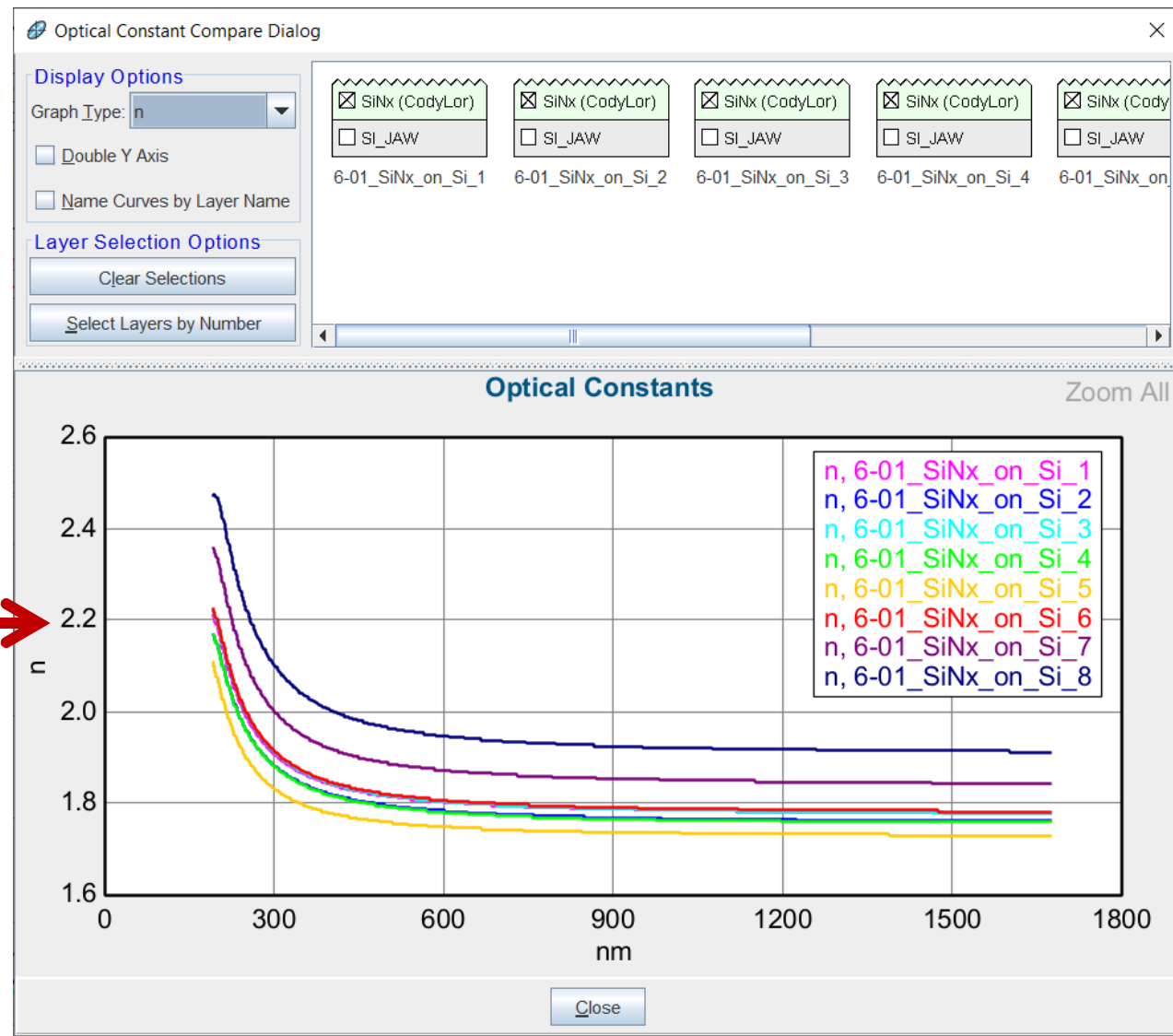
Buttons: Up, Down, Delete, Compare, Reanalyze, Generate Reports, Load Log Entry, Clear Log, Open Log, Save Log, Close

**Comparison**

**Entry Comparison Table**

	MSE	Roughness...	Thickness #...	Einf	UV Pole A...	Am
6-01_SiNx_on_Si_1	7.538	5.36	93.33	1.044	202.2692	43.658
6-01_SiNx_on_Si_2	8.400	5.45	96.47	1.096	194.3761	38.137
6-01_SiNx_on_Si_3	9.913	5.82	92.08	0.950	211.8514	43.898
6-01_SiNx_on_Si_4	9.989	5.77	94.43	1.064	193.7914	38.385
6-01_SiNx_on_Si_5	7.864	5.84	101.45	1.470	122.5450	53.720
6-01_SiNx_on_Si_6	9.485	5.69	92.96	0.977	210.4765	43.926
6-01_SiNx_on_Si_7	9.290	5.25	97.01	0.869	224.7179	67.157
6-01_SiNx_on_Si_8	7.140	4.26	87.69	0.476	292.7044	76.342
Average	8.70235	5.431	94.429	0.99337	206.59149	50.6528
Std. Dev.	1.11288	0.522	4.043	0.27536	46.57147	14.0846

Buttons: Reverse Columns/Rows, Add Statistics, Copy to Clipboard, Close, Compare Optical Constants



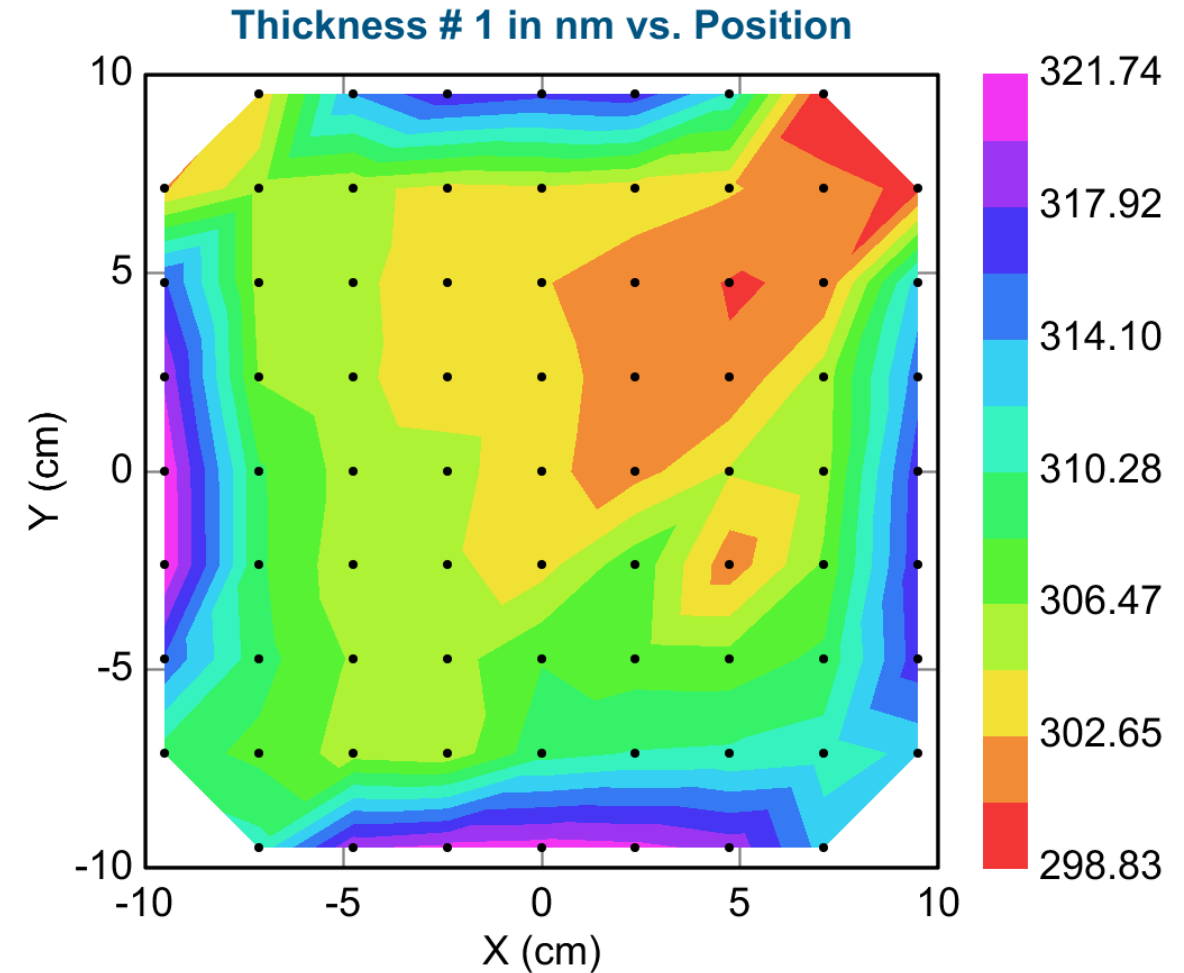


# Topic #2: Mapping Data

- Analyze data from multiple sites across sample to study thin film uniformity.



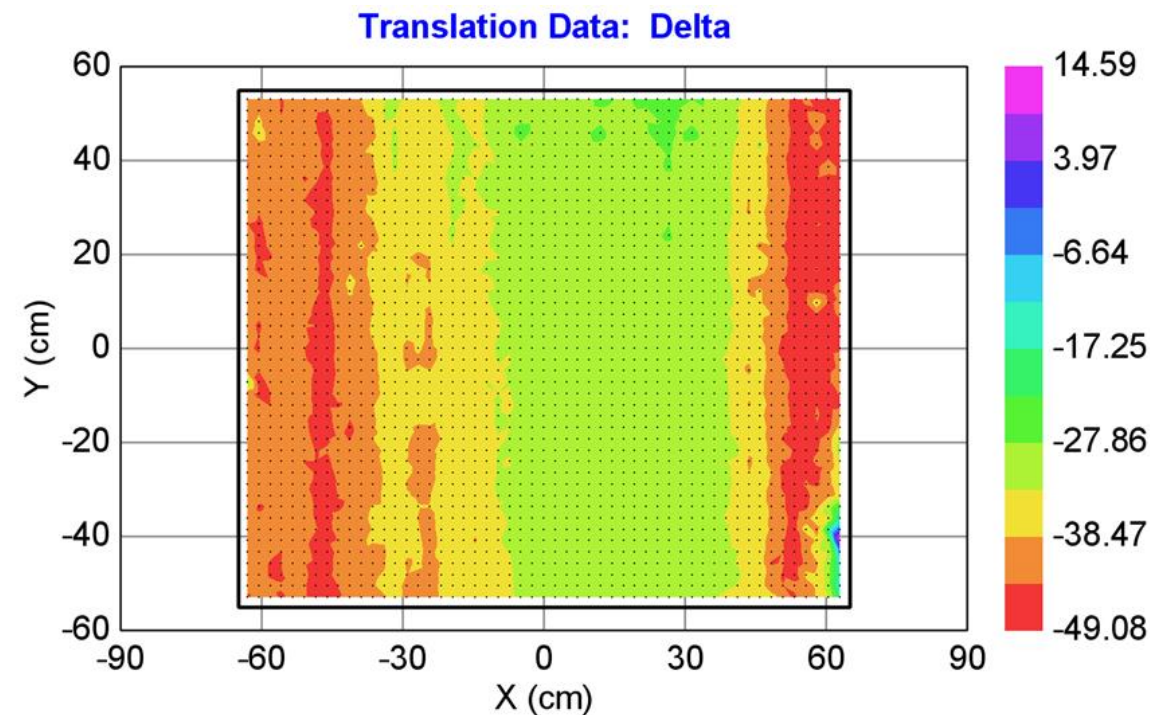
- Set up flexible model.
- Fit all points from map.
- View results.





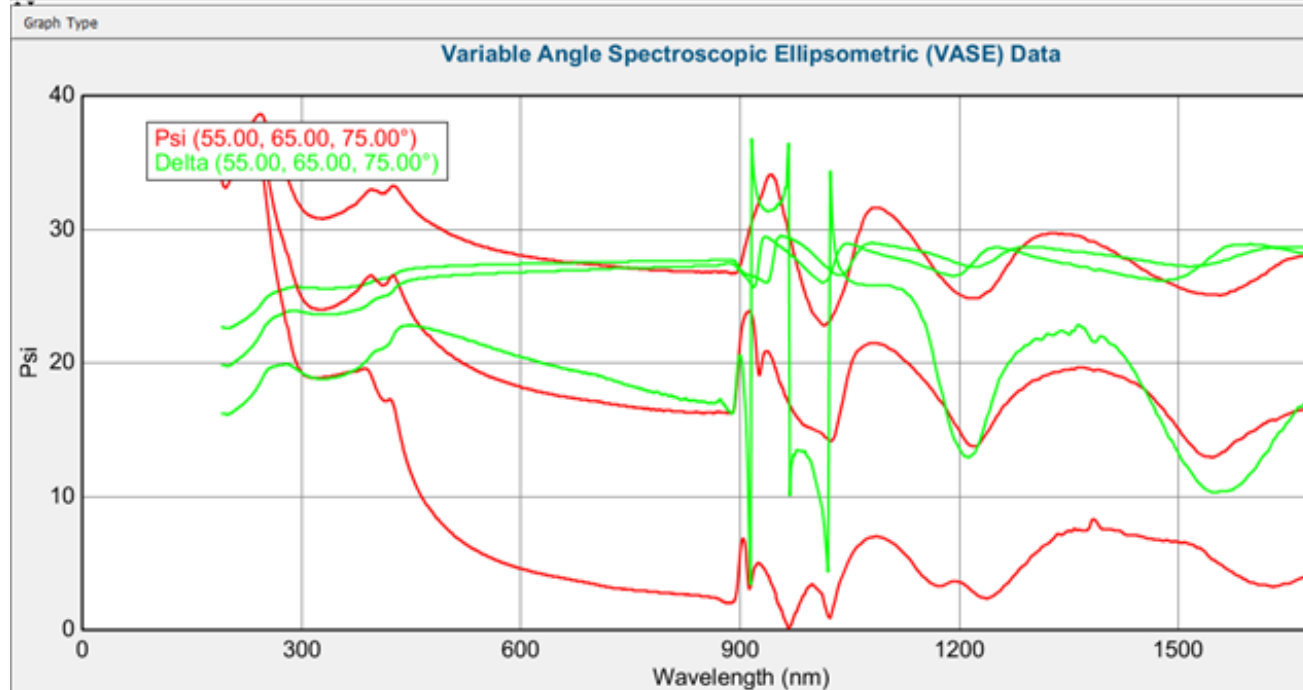
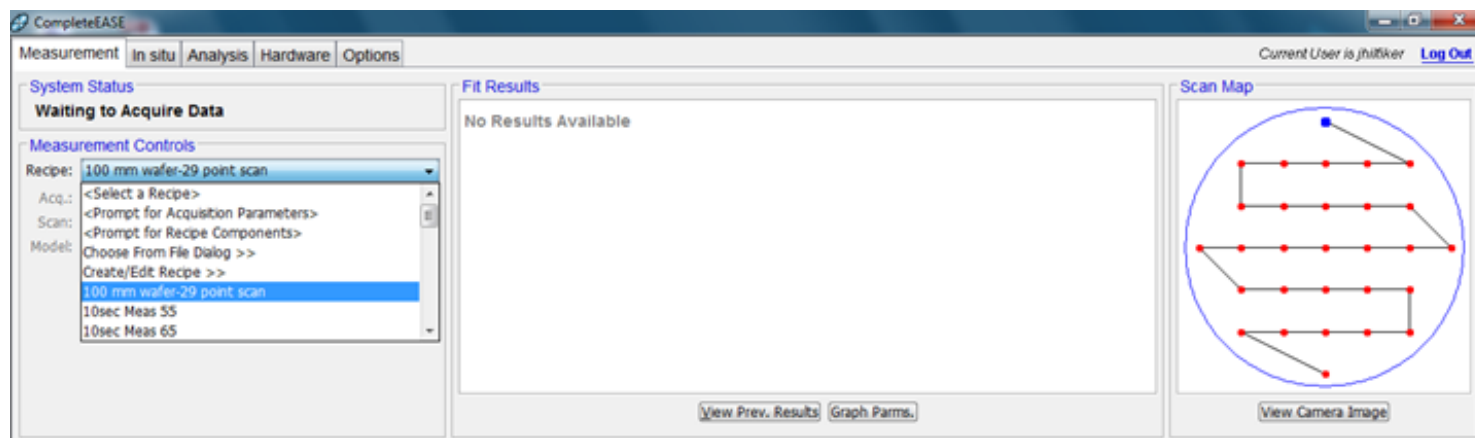
# MAPPING DATA

- Analysis Procedure:
  1. Develop model from single point data
  2. Test/Optimize at multiple points.
  3. Fit All Points.
  4. View Results.





# RECIPES IN COMPLETEEASE



Create/Edit Recipe

**Recipe**

Acq. Params: 3 seconds Edit/Create

Scan Pattern: 20 pts Edit/Create

Model: Si with Transparent Film

**Additional Parameters**

Folder for saving acquired data: Choose

☐ Save Results Only - No Raw Data

☐ Export measurement results

Load Existing Recipe Save Recipe Close



# RECIPE COMPONENTS

## Acquisition Parameters

How to collect the data

Acquisition Parameters Setup

**Data Acquisition Parameters**

Data Type: Standard

Acq. Time: 3 ☒ High Accuracy Mode

**Scan Options**

Angle Scan: 70.00 To 70.00 By 5.00

☐ Measure In Transmission Mode

**Alignment Options**

Sample Tilt Alignment: Automatic

Sample Height Alignment: Automatic-Quick

Sample Thickness: 0.55 mm

☒ Align At First Angle Alignment Angle: 70.00

**Other Options**

☐ Do Not Return To Sample Load Position

☐ Do Not Reposition Translator

## Scan Pattern

Where to collect data

Scan Pattern Editor: (not saved)

**Substrate Dimensions**

Circle  Dia. (cm): 10.00000 ☒ Draw Wafer Notch

**Point List (cm)**

1:	-1.00000	4.33013
2:	0.00000	4.33013
3:	1.00000	4.33013
4:	2.50000	3.46410
5:	1.50000	3.46410
6:	0.50000	3.46410
7:	-0.50000	3.46410
8:	-1.50000	3.46410
9:	-2.50000	3.46410
10:	-3.00000	2.59808
11:	-2.00000	2.59808
12:	-1.00000	2.59808
13:	0.00000	2.59808
14:	1.00000	2.59808
15:	2.00000	2.59808
16:	3.00000	2.59808

☐ Translate in R-Theta If Possible

**Point Commands:**

**Alignment Position**

X: 0.00000 Y: 0.00000

**Transmission Intensity Baseline**

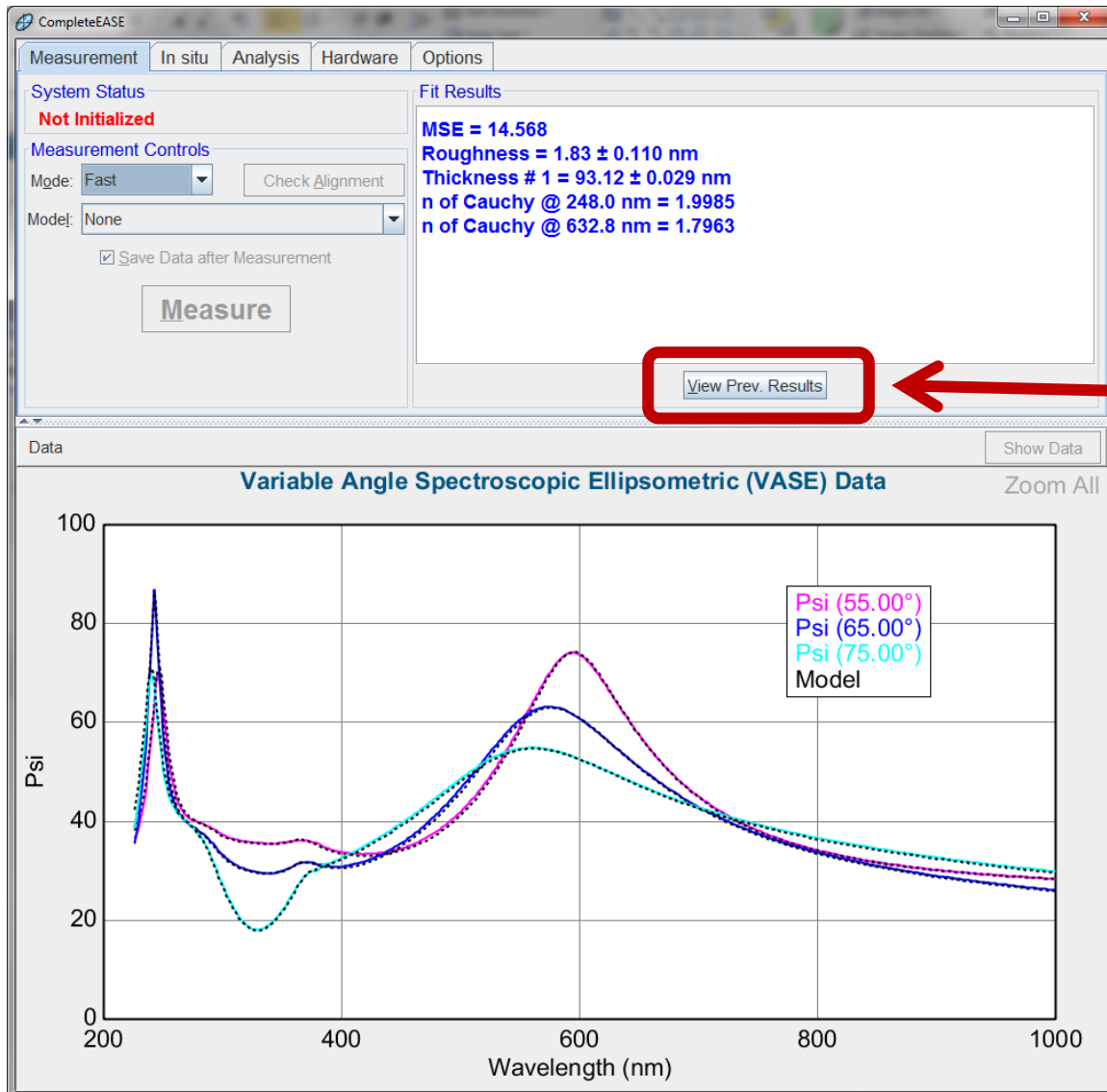
☐ Use Point For Transmission Baseline X: 0.00000 Y: 0.00000

**Pattern Offset**

X: 0.00000 Y: 0.00000 Theta (°): 180 ☐ Use Initial Position



# VIEWING PREVIOUS RESULTS



Show results saved by in data files

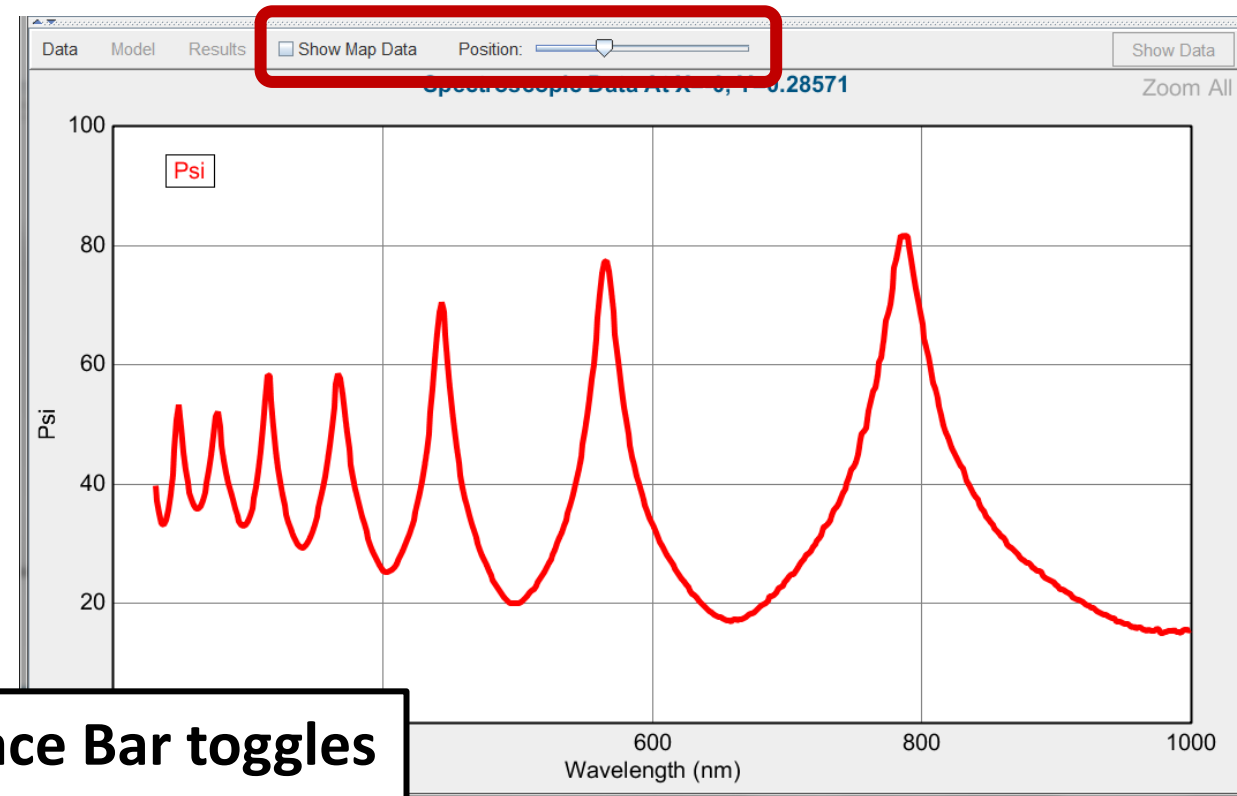
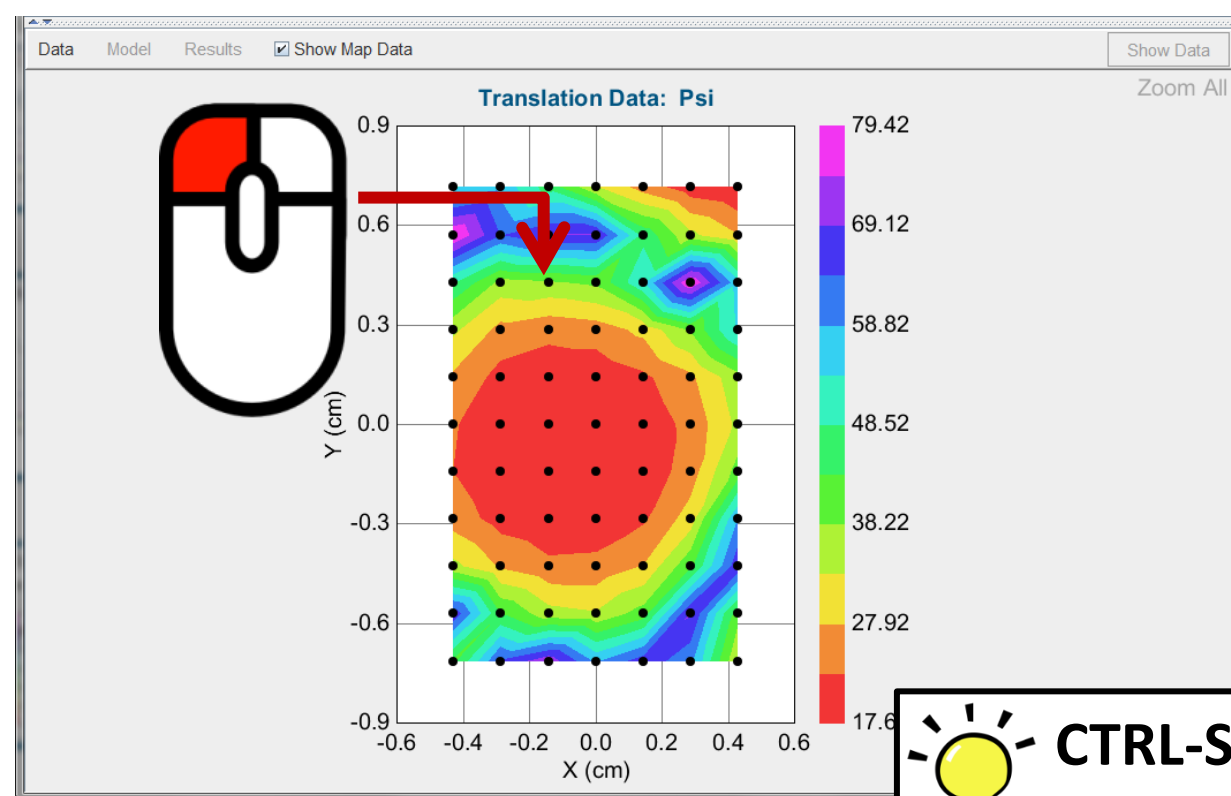


Data files (.SE) also contain modeling results when optical model presents in recipe



# SELECTING SINGLE DATA POINT

- Left-click any point to view spectroscopic data.
- Move through points with slider.
- Check-box returns to Map view.

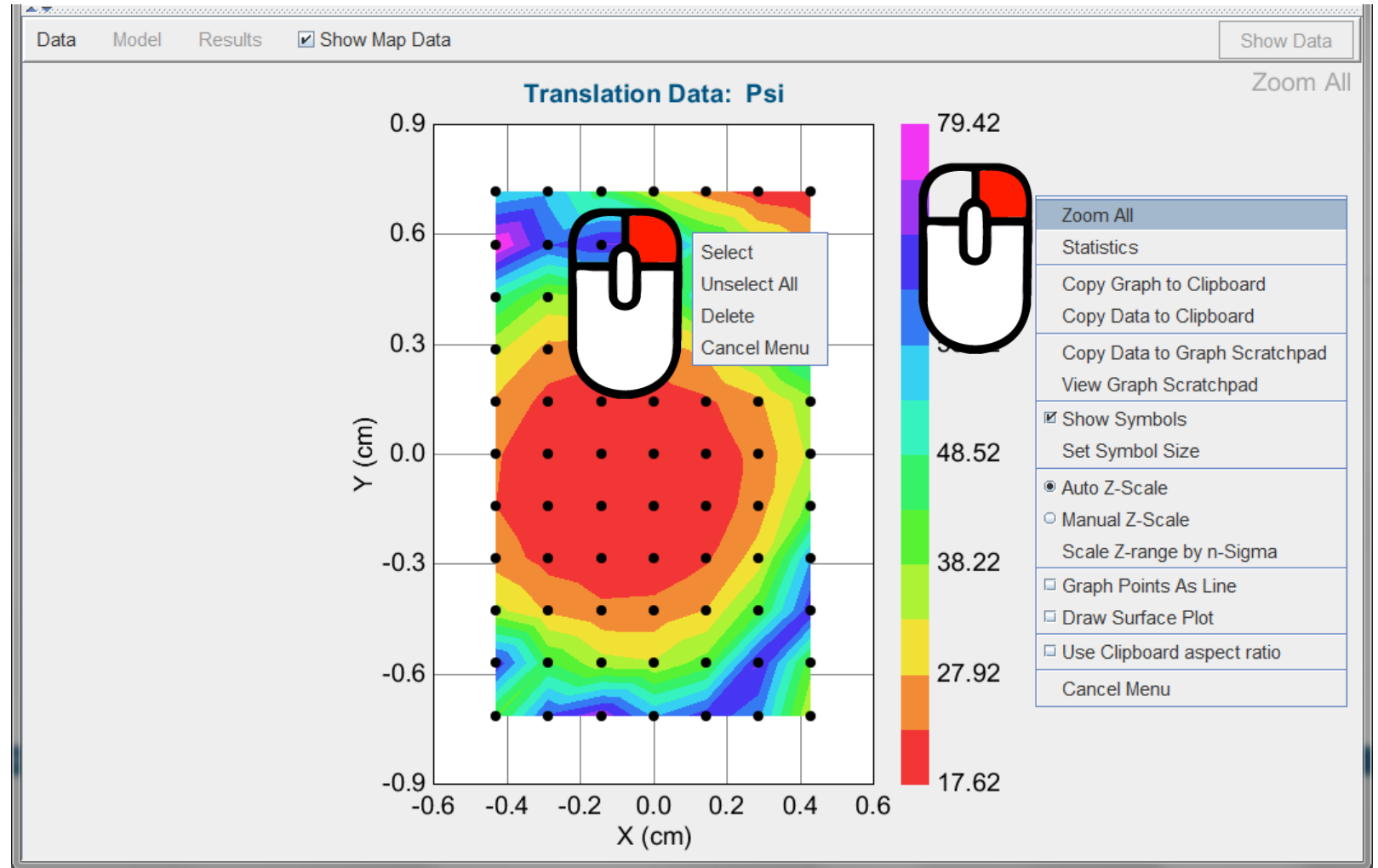


**CTRL-Space Bar toggles  
from Map to Spectra**



# WORKING WITH MAPPING DATA

- Right-click menu on individual point is different from right-click menu outside the graph.

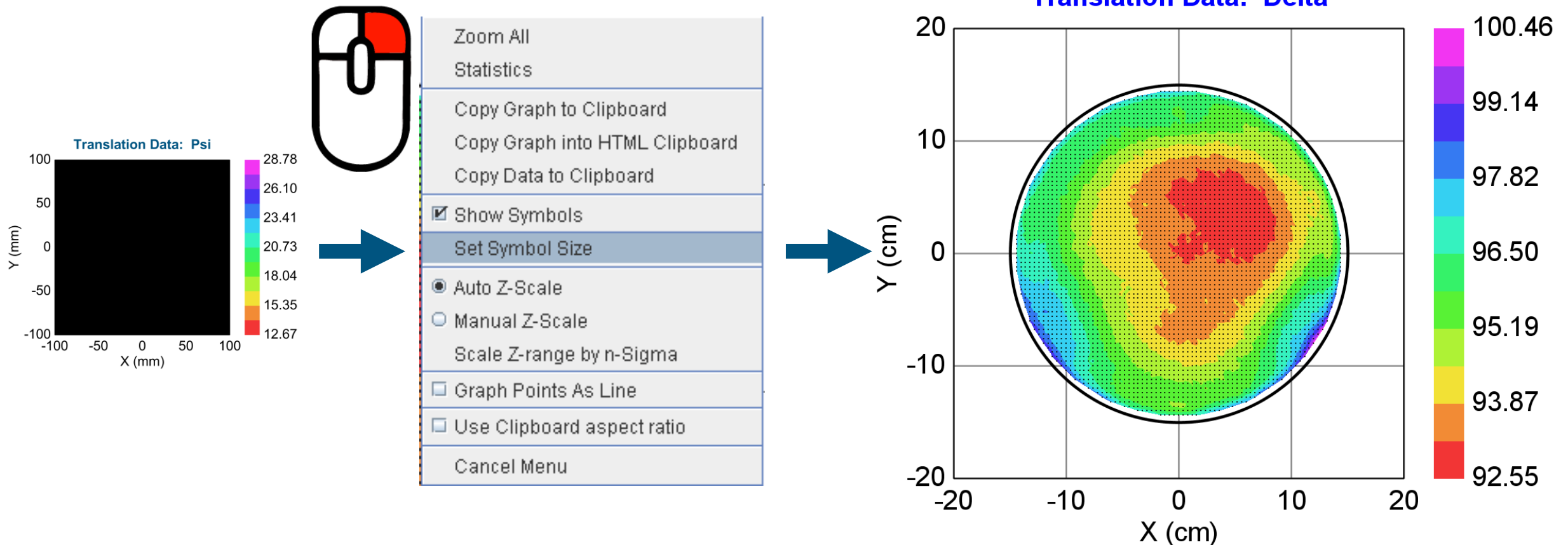






# CHANGING THE SYMBOL SIZE

- Change point symbol size on graph with right-click menu outside of the measurement points.

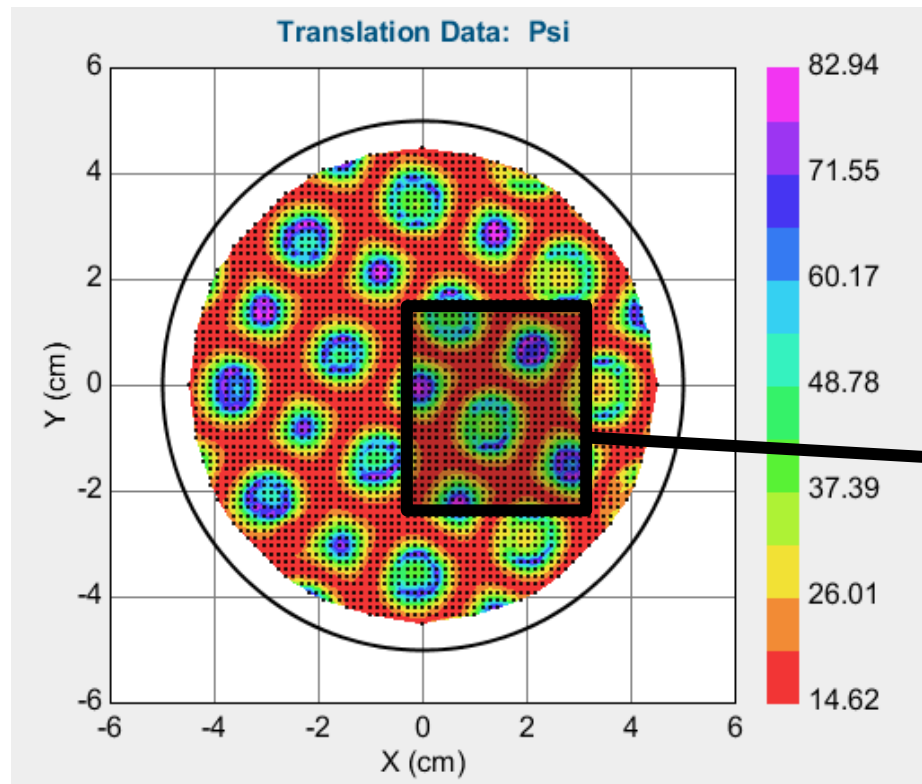




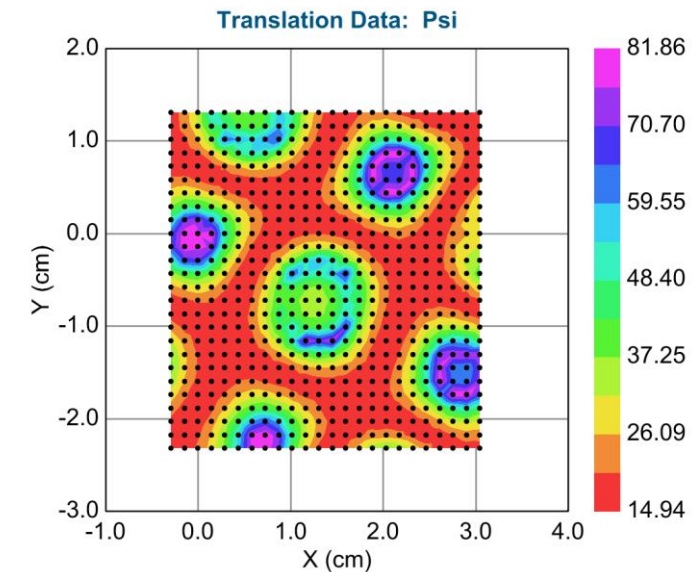


# ZOOMING/SAVING WITH GRAPHS

- DRAG across graph to Zoom into a smaller range
  - This does not select points, but only zooms the graph.



Right-Click on Data 'Save' to  
"Save Subset",  
which is the smaller map

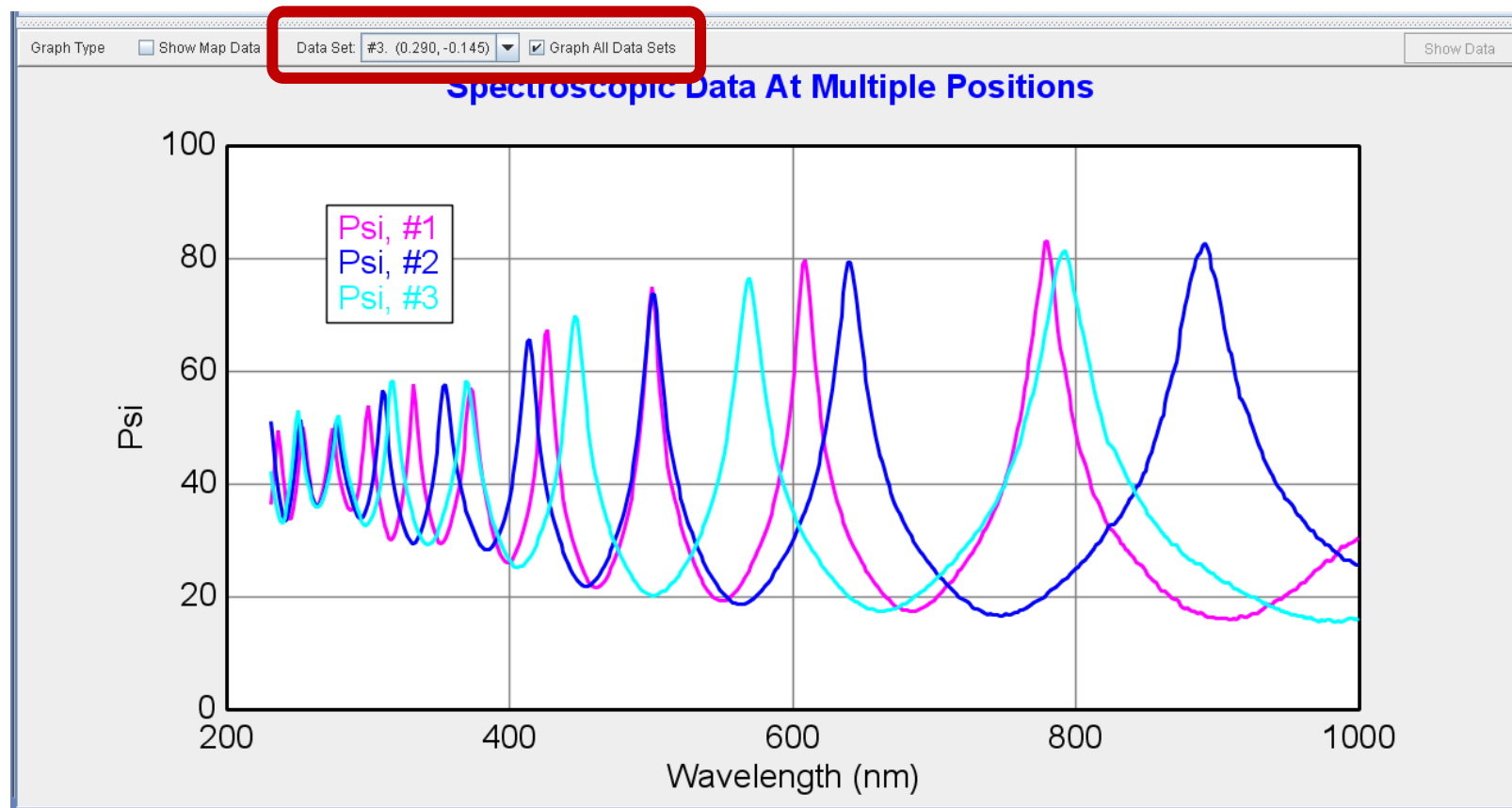
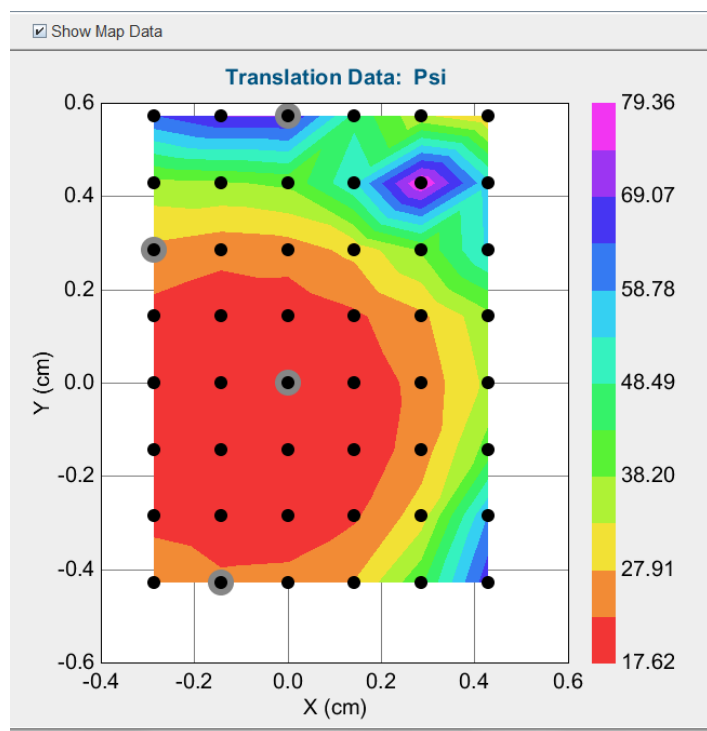


- Use CTRL+DRAG across graph to select multiple points



# COMPARE DATA AT MULTI-POINTS

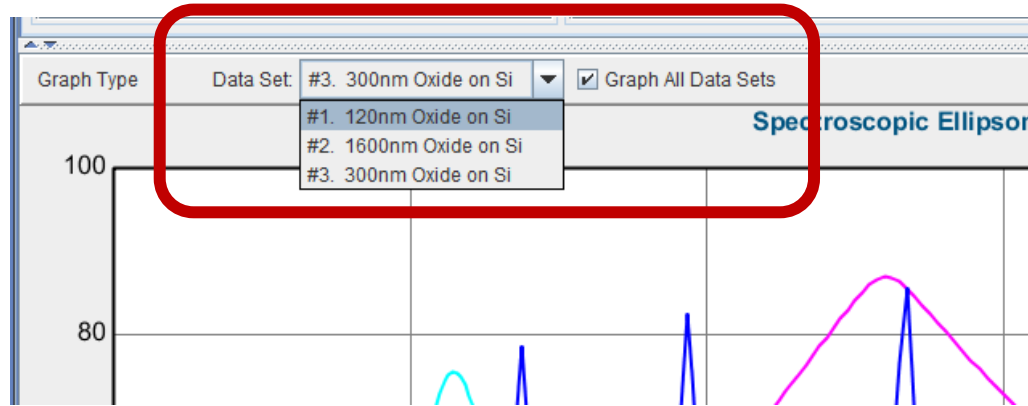
- CTRL+Click or right-click > “select” on multiple points to setup *Multi-Data Set Mode*
  - select “Graph All Data Sets”



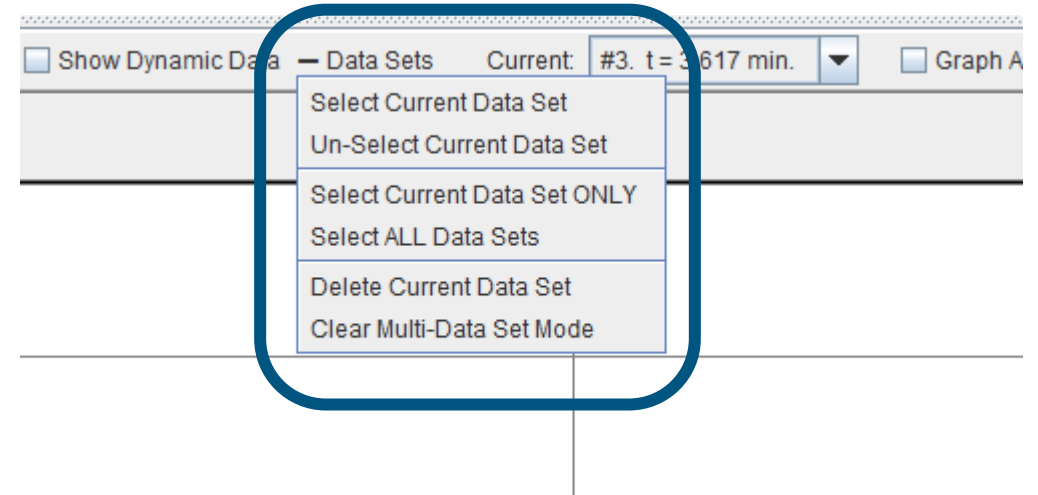


# MULTI-DATA SETS

## ■ Graphing and Handling

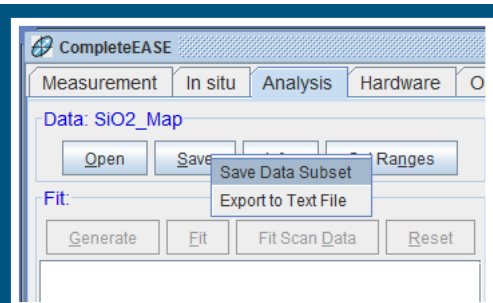


## Drop Down Menu for Data Sets

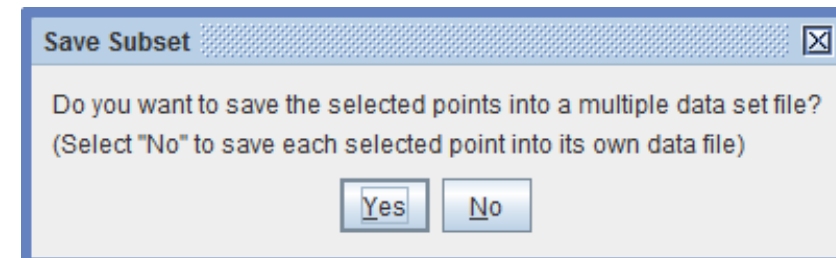


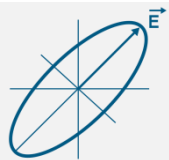
## ■ Saving

Right-click over Data  
'Save' button and  
press "Save Data  
Subset"



## Save Data Subset as Individual or Multi-Data Set file





# SETTING UP MULTI-SAMPLE ANALYSIS

- Need to tell CompleteEASE which parameters to vary between multiple data sets

## Configure Options

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

Include Surface Roughness = [OFF](#)

Substrate = [none](#)

Angle Offset = [0.000](#)

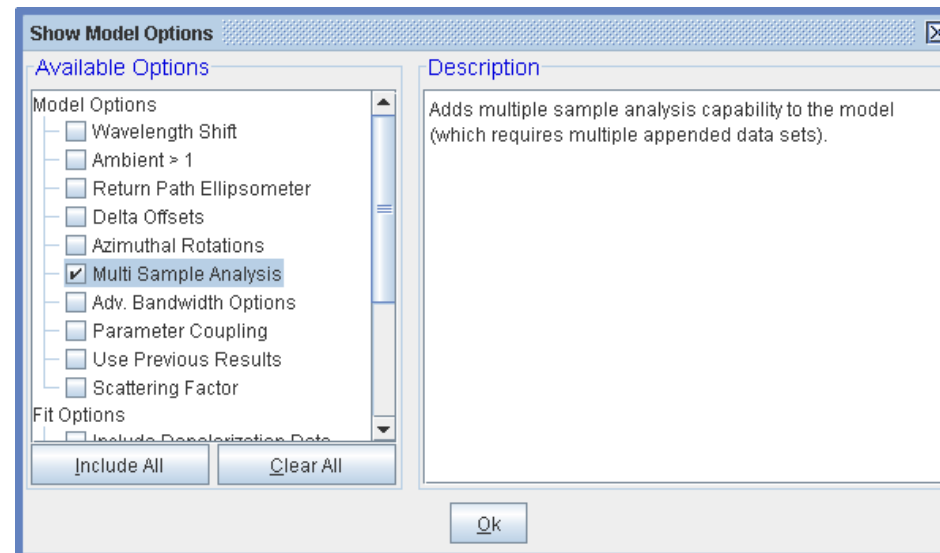
+ **MODEL Options**

+ **FIT Options**

+ **OTHER Options**

[Configure Options](#)

[Turn Off All Fit Parameters](#)



## Add Fit Parameter

- **MODEL Options**

Include Substrate Backside Correction = [OFF](#)

Model Calculation = [Ideal](#)

- **Multi Sample Analysis**

[Add Fit Parameter](#) [Delete All Parm](#)s

<u>Data Set</u>	<u>Thickness # 1</u>
<u>#1</u>	<a href="#">100.00 nm</a>
<u>#2</u>	<a href="#">100.00 nm</a>
<u>#3</u>	<a href="#">100.00 nm</a>

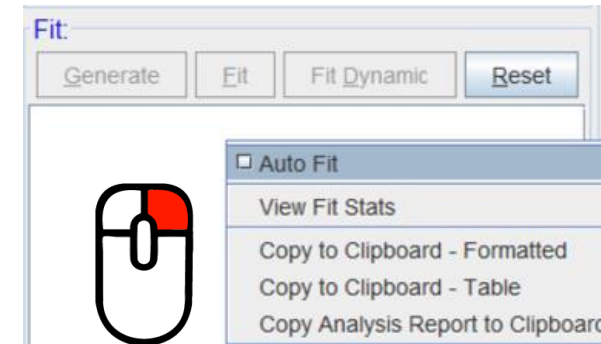
**Roll Mouse over each Fit  
Parameter and choose which  
to fit**



# CHECK MODEL AT MULTIPLE POINTS

- Test model on different areas of map.
- Thickness Pre-Fit is helpful when thickness greatly varies.
- Do all optical constant parameters need to vary?
- Turn Fit Parameters reset ON to avoid parameter lost due to singularities at some locations

**Configure Options>**  
“More Fit Options”



Hint: Turn off “Auto-Fit”.

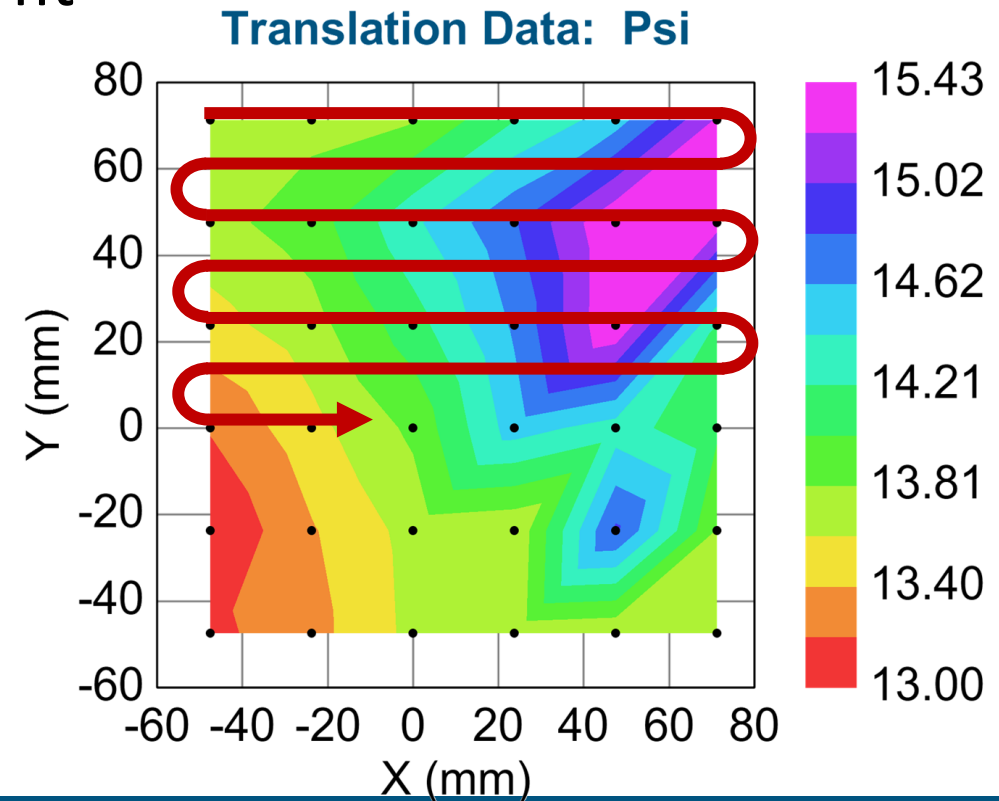
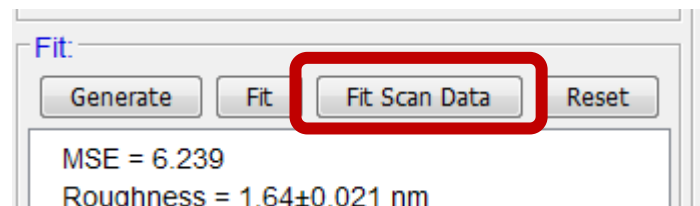
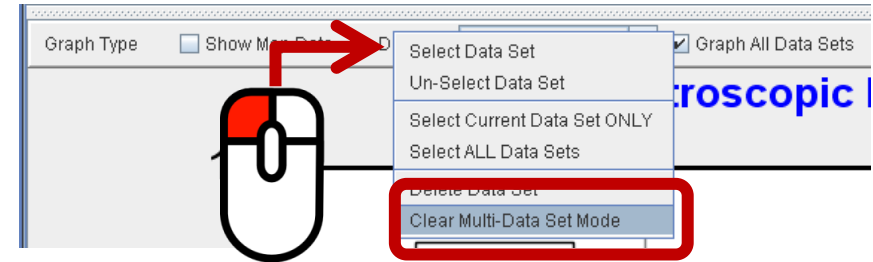
## **FIT Options**

- + Perform Thickness Pre-Fit = [ON](#)
- Use Global Fit = [OFF](#)
- Fit Weight = [N.C.S](#)
- Limit Wvl. for Fit = [ON](#) Range = [400.0 nm - 1000.0 nm](#)
- Limit Angles for Fit = [ON](#) Included Angles = [65](#)
- Max. Acceptable MSE = [100.000](#)
- Skip Data Points in Fit = [5](#) Max. Fit Iterations = [50](#)
- Auto Fit Parameter Reset = [OFF](#)



# FITTING THE ENTIRE MAP

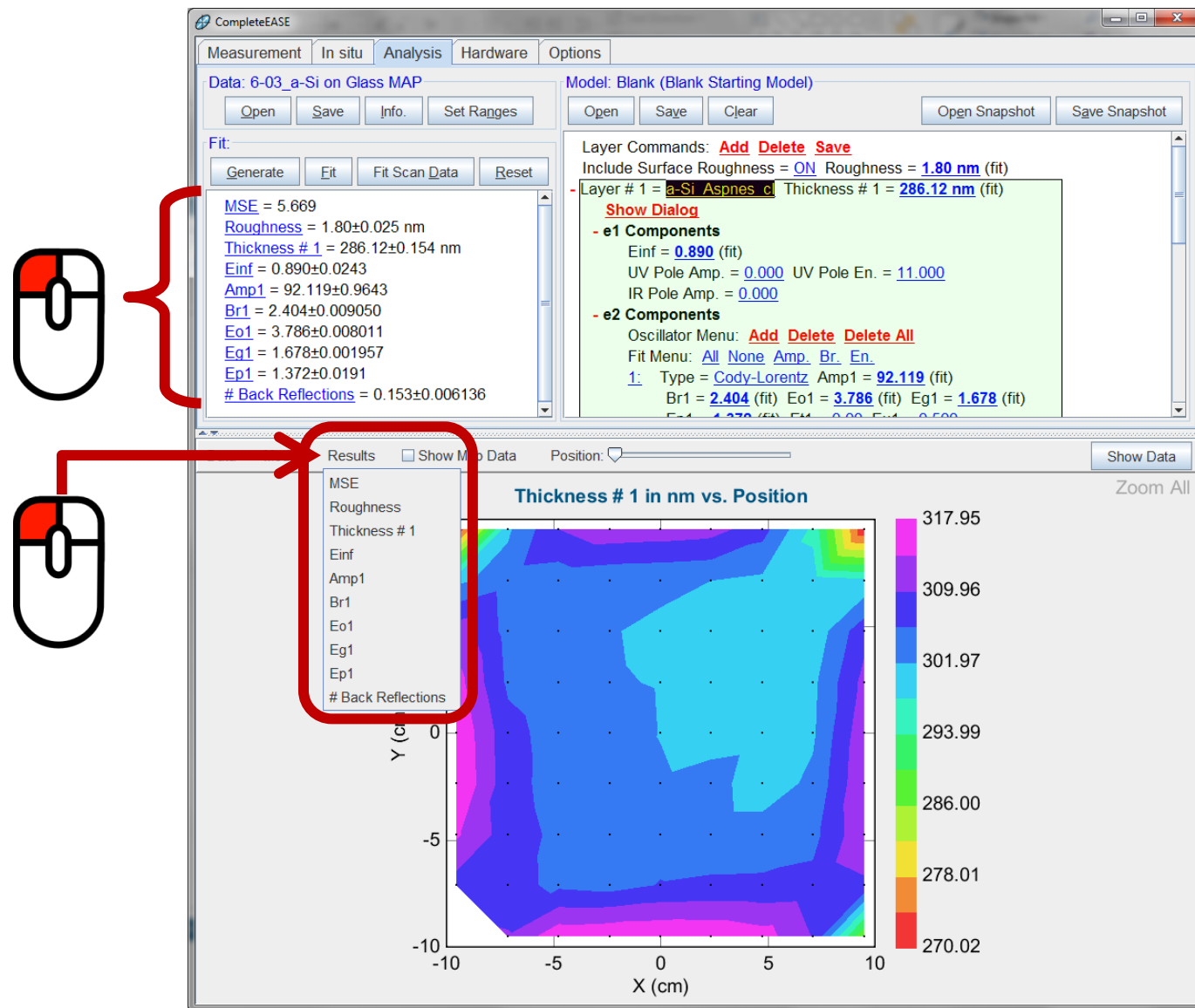
- Clear Multi-Data Set Mode before fitting entire map
- “Fit Scan Data” performs sequential fit for a every data point on map

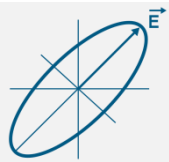




# VIEWING RESULTS

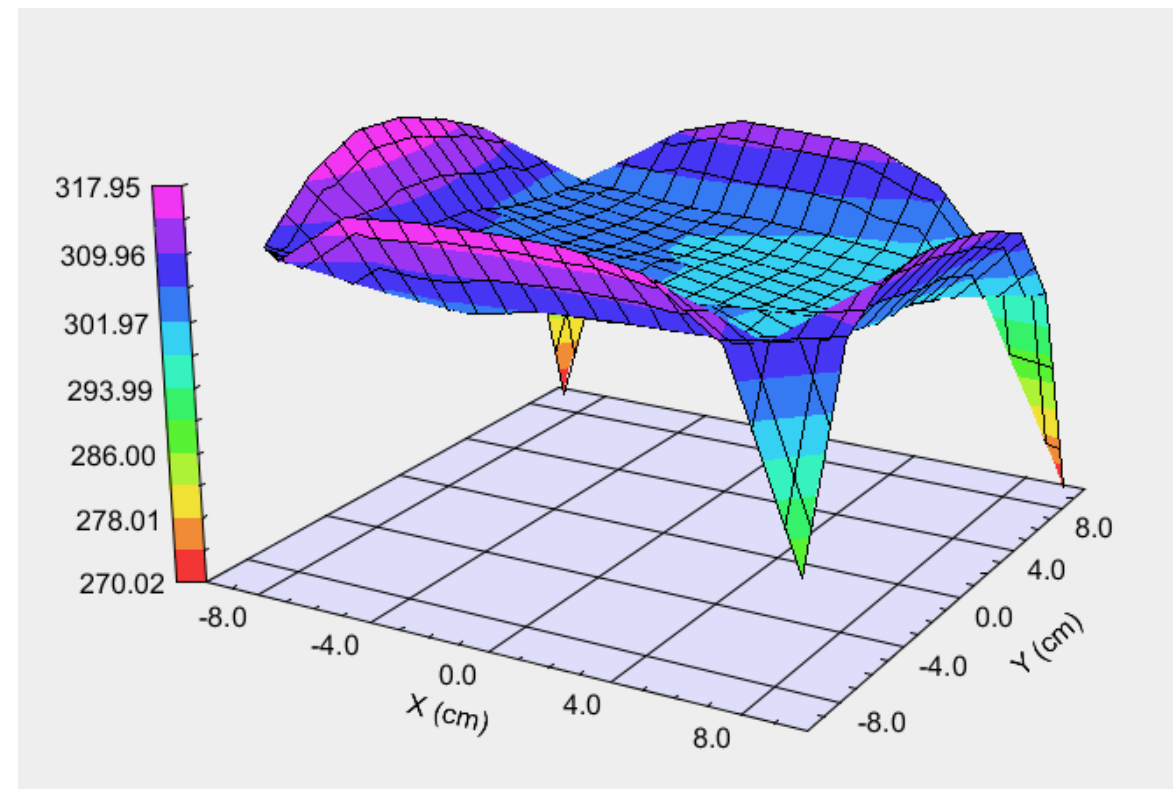
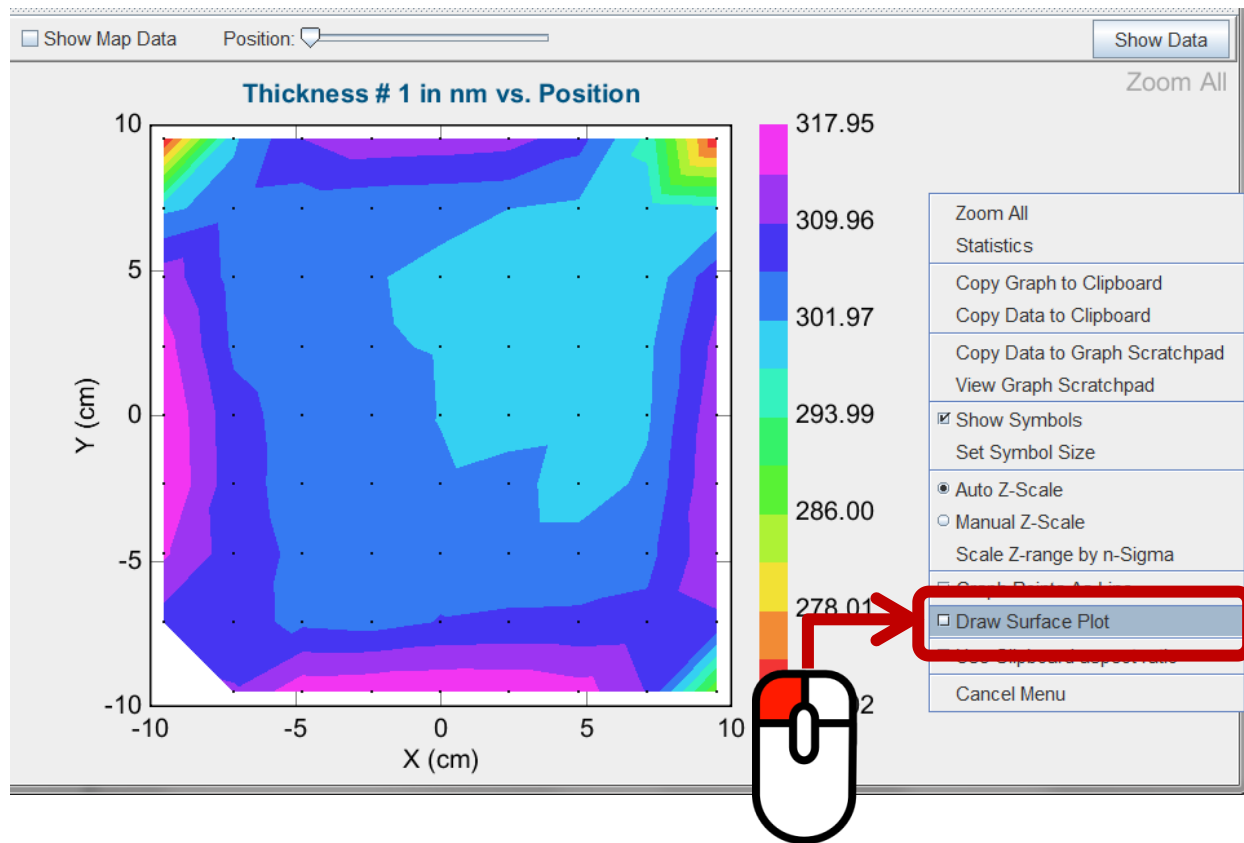
- 2 ways to graph results:
  - Click on fit parameters (in blue)
  - Select from “Results” drop-down menu





# SURFACE PLOTS

- Right-click outside graph > “Draw Surface Plot”



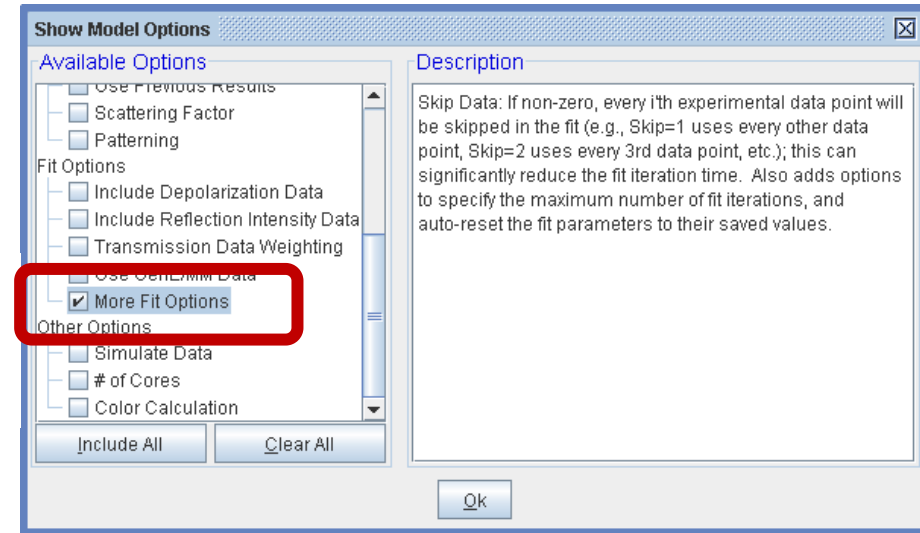




# REDUCE ANALYSIS TIME

- Skip Wavelengths
- Reduce Wavelength Range
- Reduce Angles
- Reduce fit parameters
- Turn-off Global fit

**Configure Options>**  
“More Fit Options”



## **-FIT Options**

- + Perform Thickness Pre-Fit = ON  
Use Global Fit = OFF  
Fit Weight = N.C.S
- Limit Wvl. for Fit = ON Range = 400.0 nm - 1000.0 nm  
Limit Angles for Fit = ON Included Angles = 65  
Max. Acceptable MSE = 100.000
- Skip Data Points in Fit = 5 Max. Fit Iterations = 50  
Auto Fit Parameter Reset = OFF
- + Include Derived Parameters = ON



# MAPPING DATA SHORT-CUTS

Shortcut	Function
<b>CTRL-Click on Point</b>	Select / De-Select Point
<b>CTRL-ALT-Click on Point</b>	Delete Point
<b>CTRL-ALT-SHIFT-Click on Point</b>	Show camera image from point (when available)
<b>CTRL-Spacebar</b>	Switch view from single-point to map
<b>ALT-#</b>	Switch between Data Sets (when multiple selected)

## [6-02] CVD SiO<sub>2</sub> Map (on Si)

- Find a model to fit all the data from the map of this non-uniform coating.



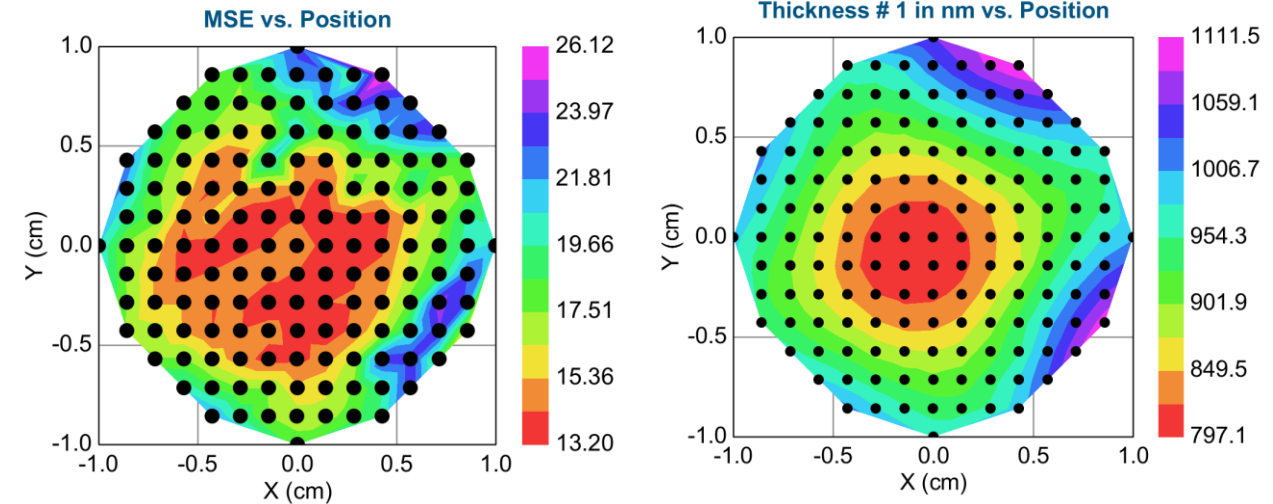
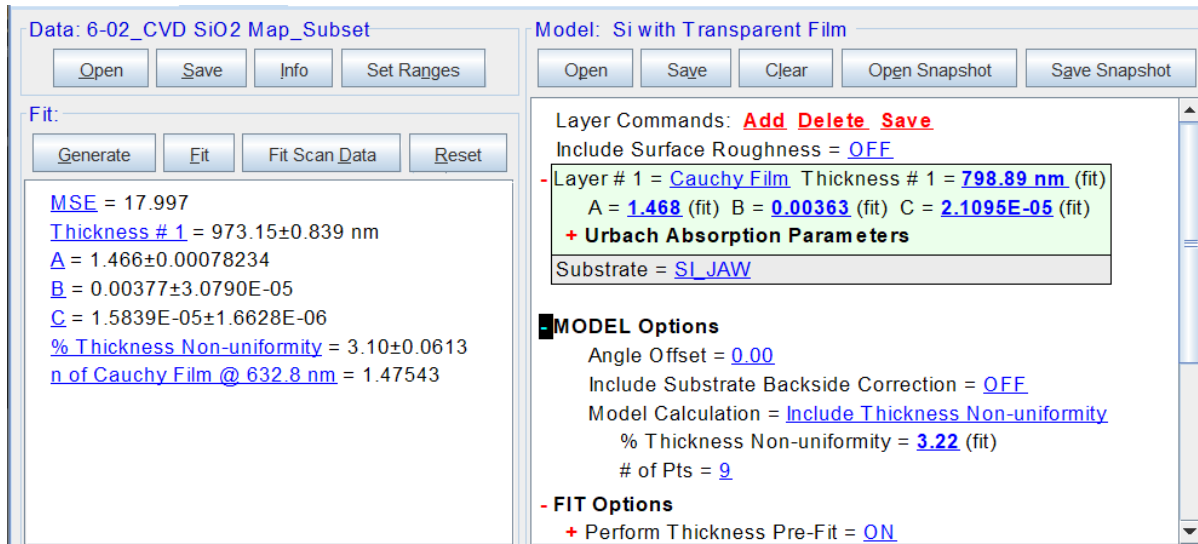
**Fit Thickness &  
Cauchy Parameters**



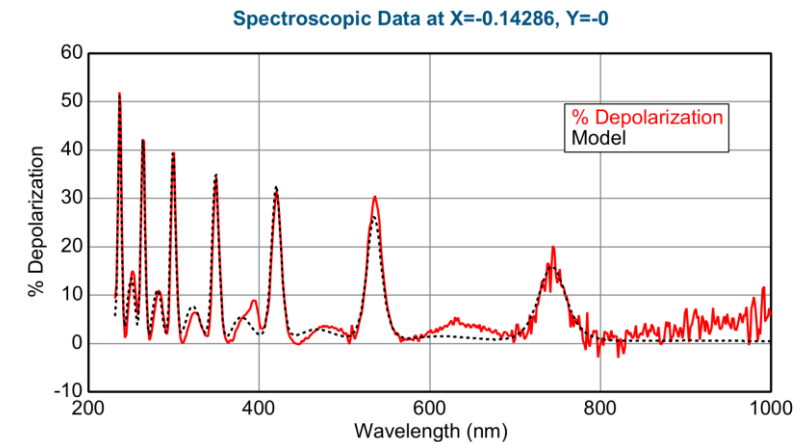
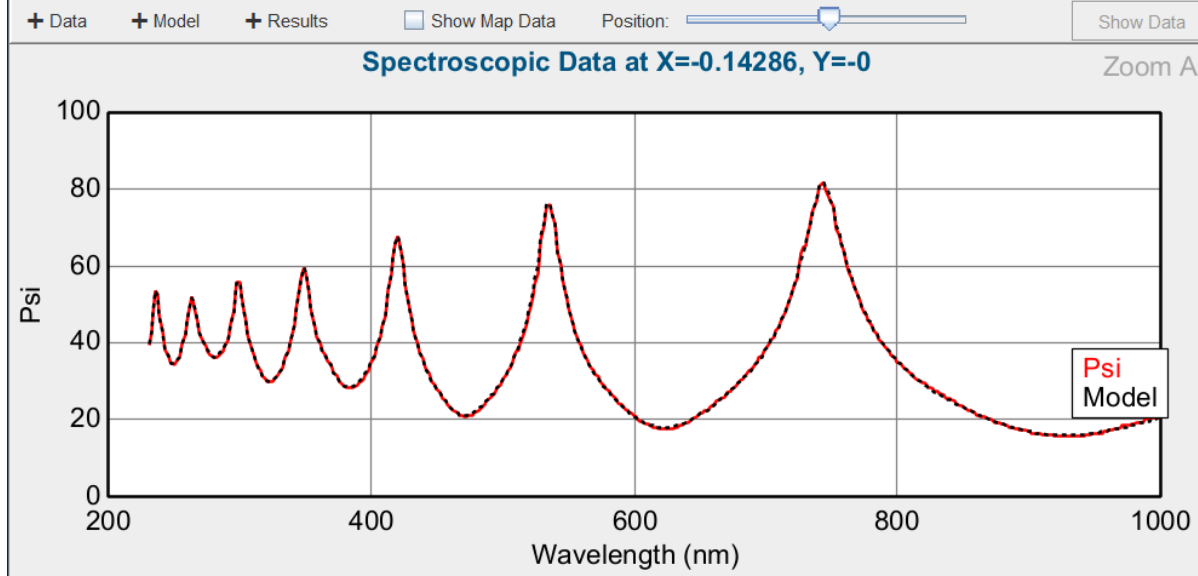
Add to improve MSE:  
Roughness?  
Index Grading?  
Anisotropy?  
Thickness Nonuniformity?



# 6-02 CVD SiO2 MAP: RESULTS



Parameter	Average	Std. Dev.	Slope	Minimum	Maximum	Range
Thickness # 1 in nm vs. Position	927.92	71.21		797.08	1111.55	314.47

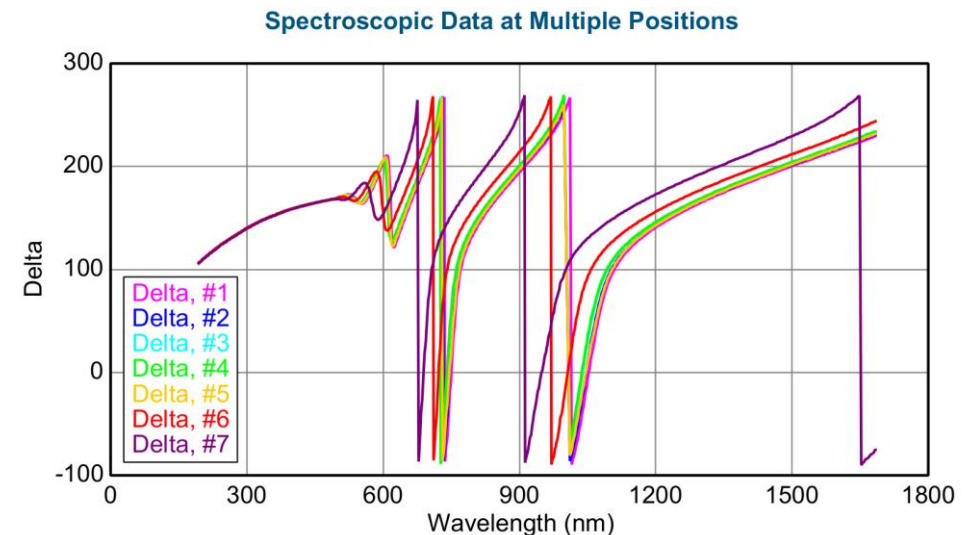
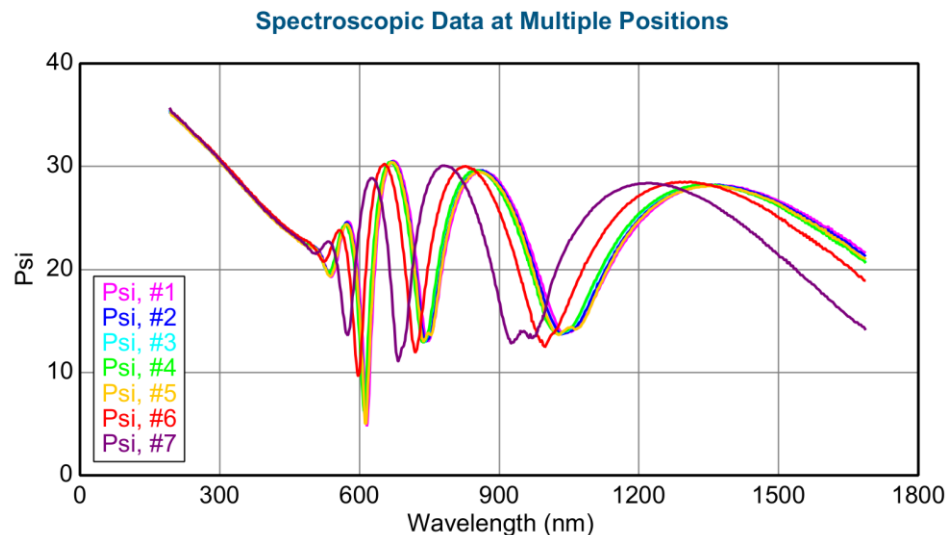


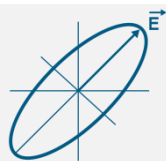
# [6-03] a-Si on 7059 Glass

- a-Si is coated over large glass panels for display applications. Thin film uniformity is checked with SE to ensure a great picture.

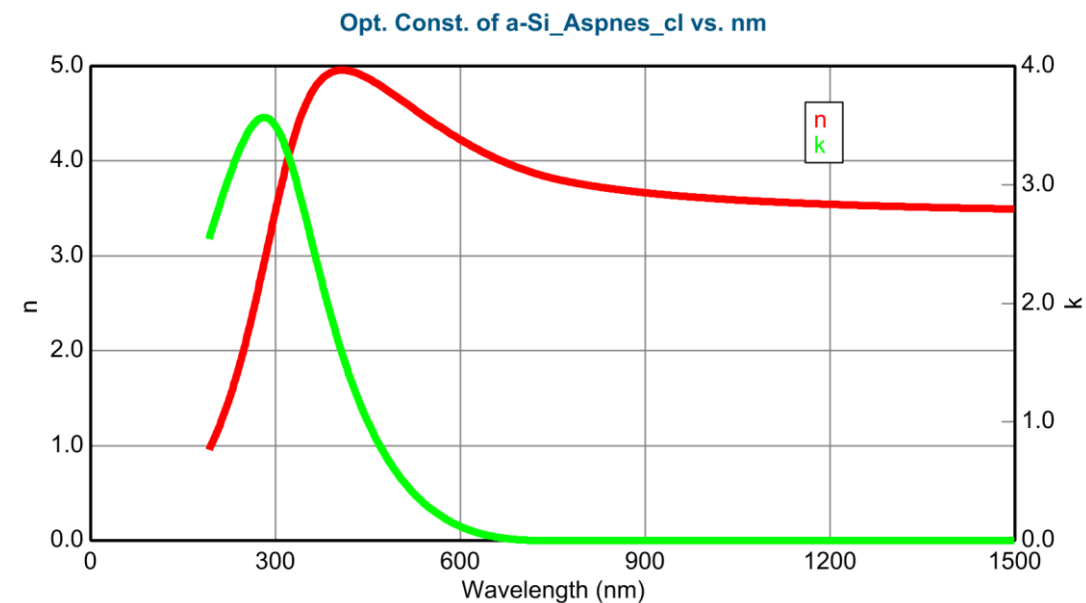
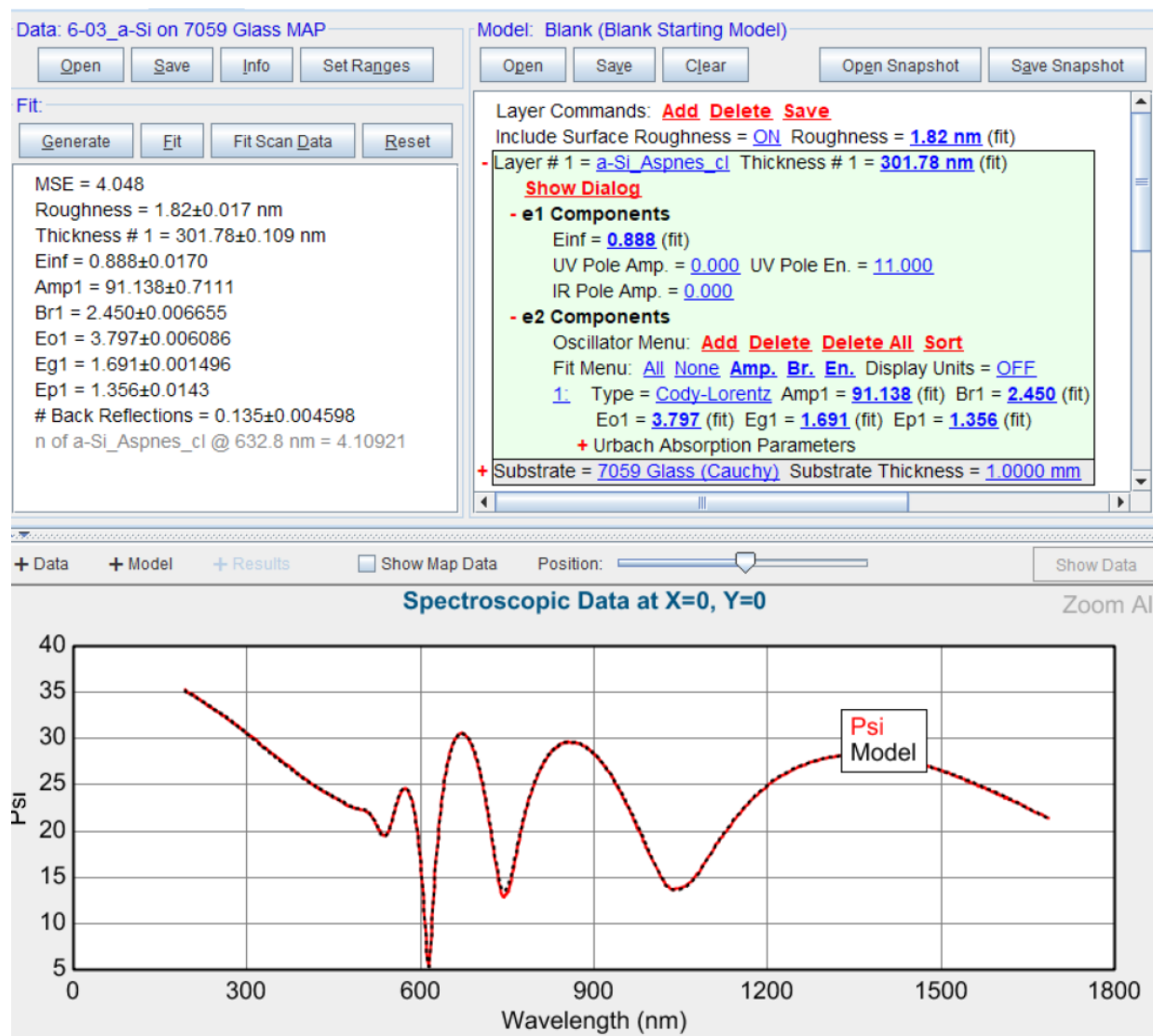


- Observe data variation – How to build a model that fits every data point?

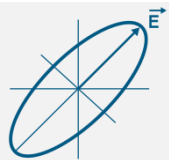




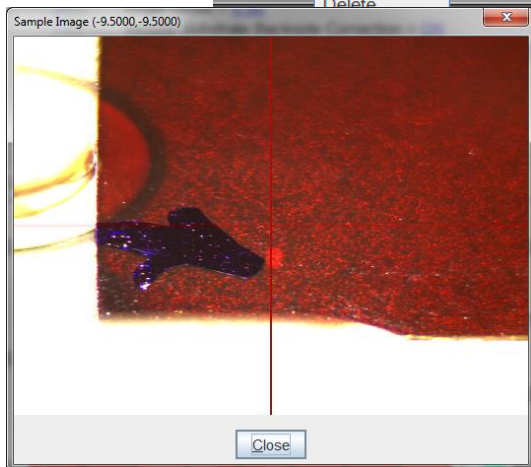
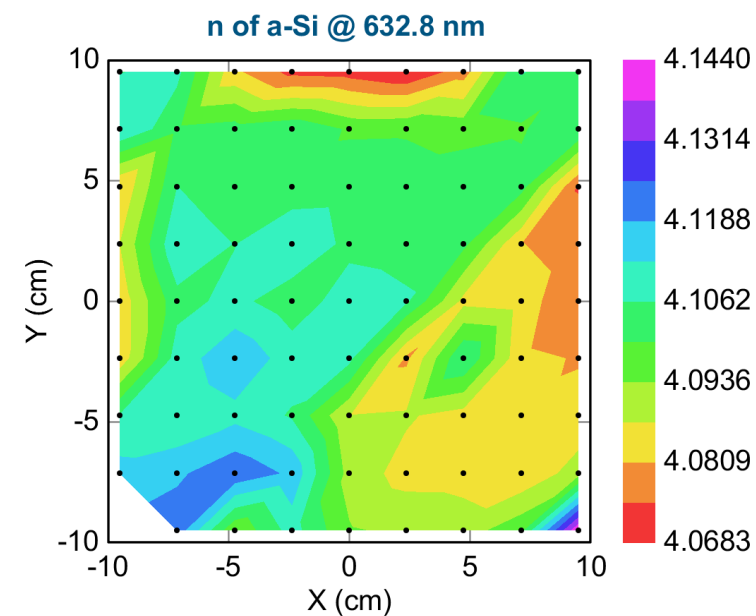
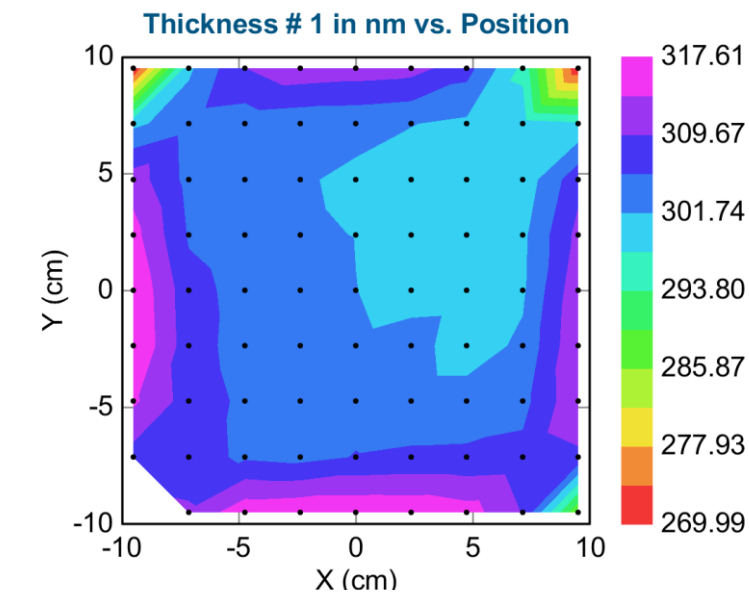
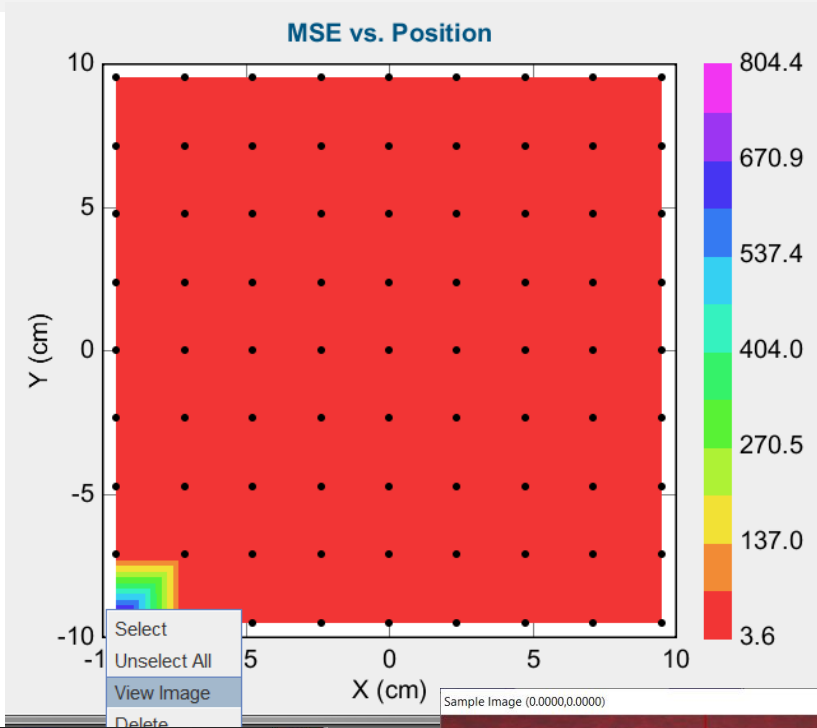
# 6-03 A-SI ON 7059 GLASS: CENTER RESULTS





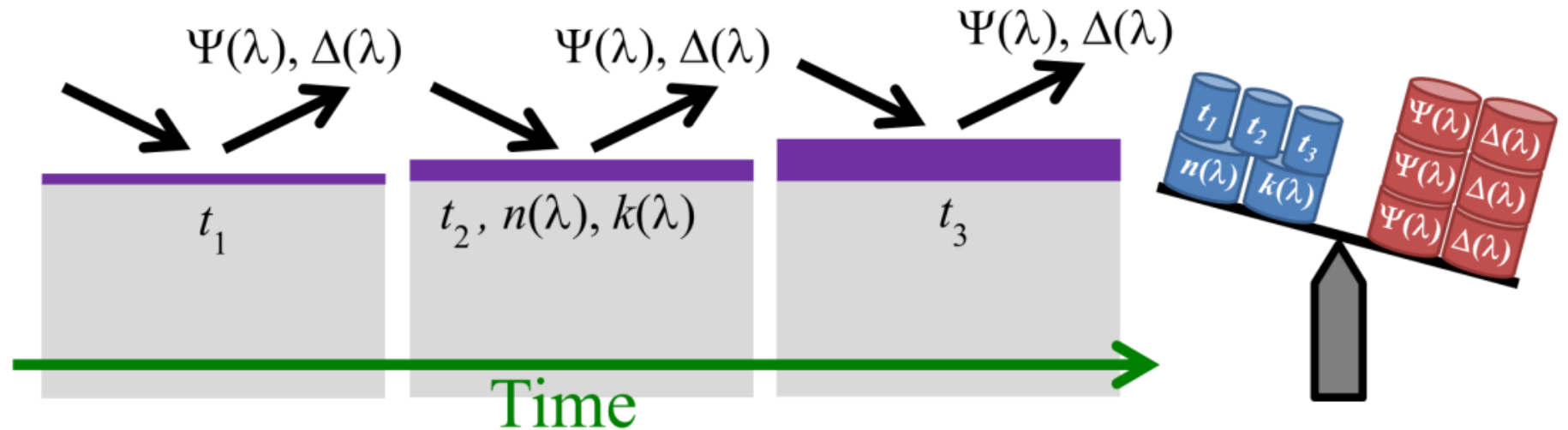


# 6-03\_A-SI ON 7059 GLASS - MAP



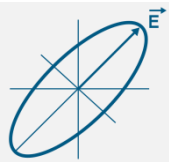
# Topic #3: Dynamic Data Analysis

- SE measurements are repeatedly collected during a process, such as film growth.



- Analyze all data versus time to characterize the process.

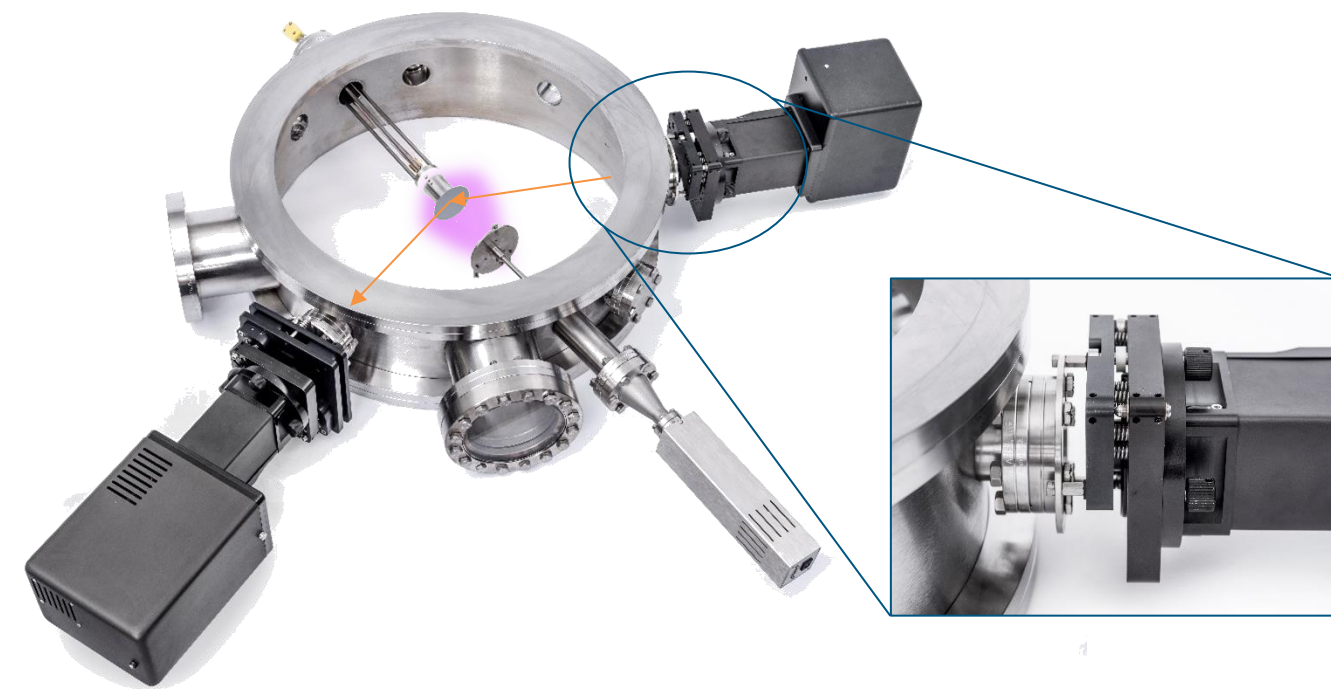
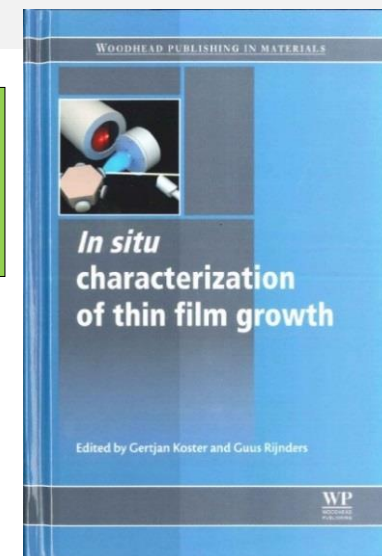




# IN SITU ELLIPSOMETRY

- Real-time monitoring and control
- Complete sample history
  - Before, during and after process
- Direct measurement of surfaces & interfaces

J.N. Hilfiker "In situ spectroscopic ellipsometry (SE) for characterization of thin film growth", chapter in *In situ characterization of thin film growth*, G. Koster and G. Rijnders, eds., Woodhead Publishing: Cambridge, UK (2011)

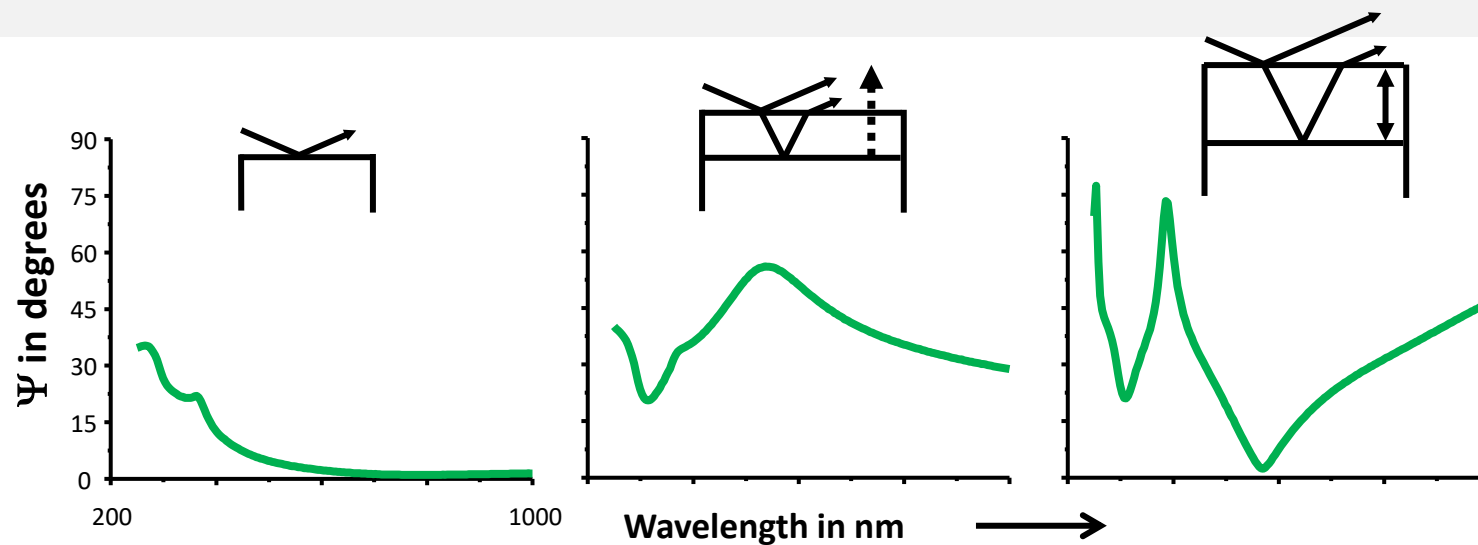


**Atomic Layer  
Deposition**

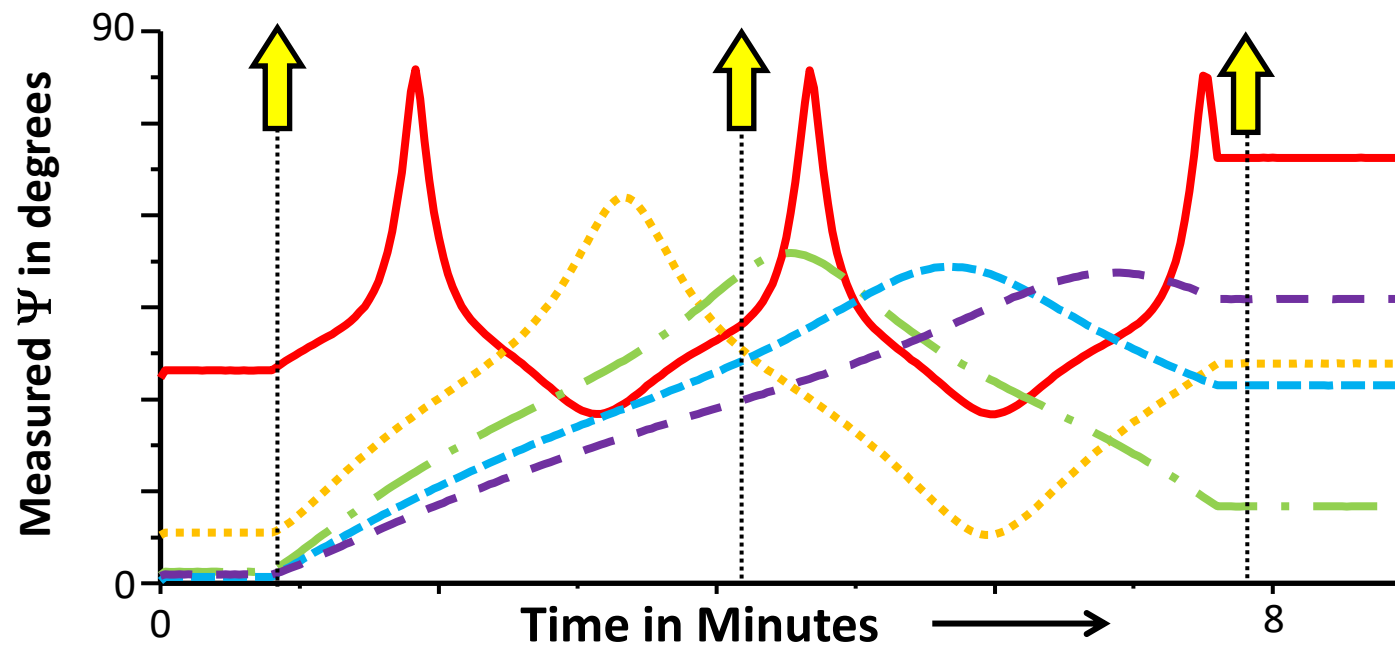


# IN-SITU SE DATA

**Spectral  
Data**



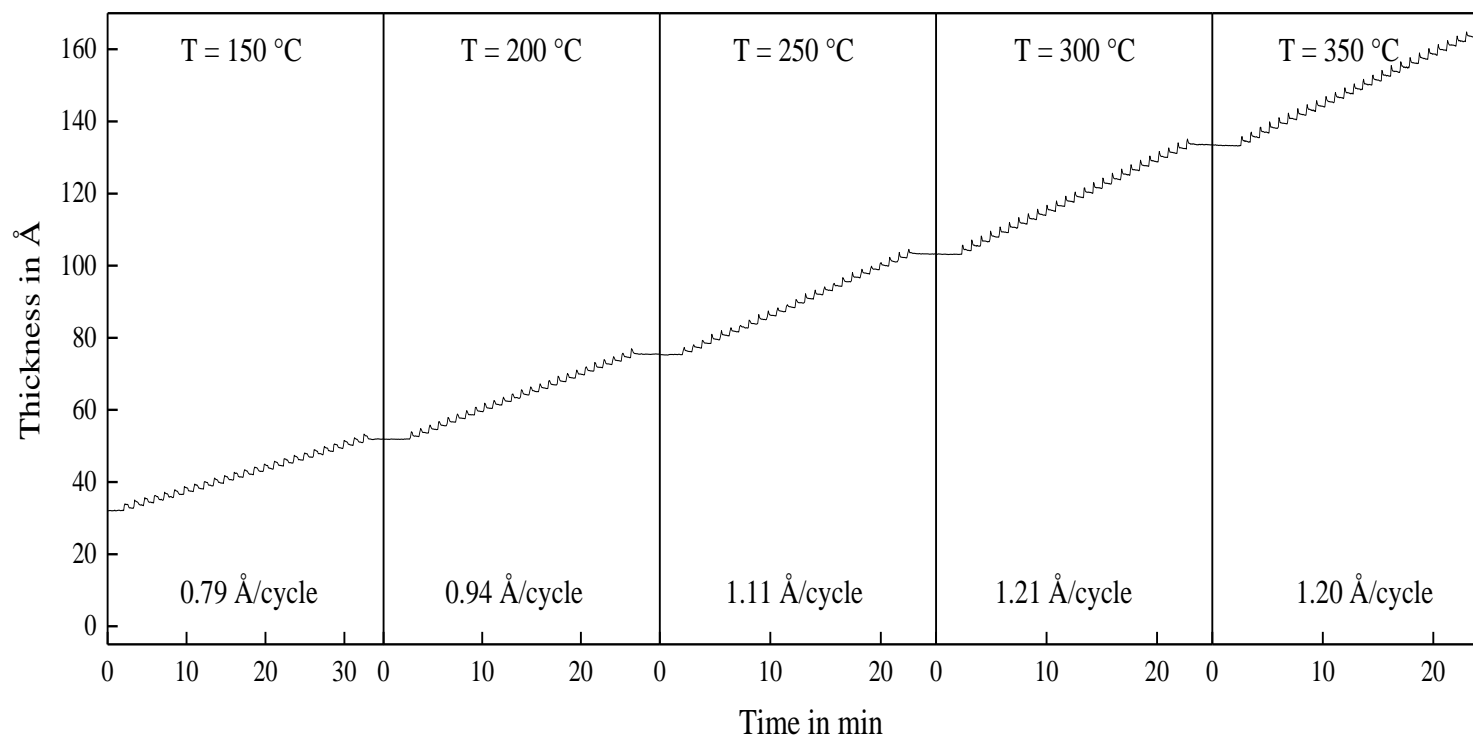
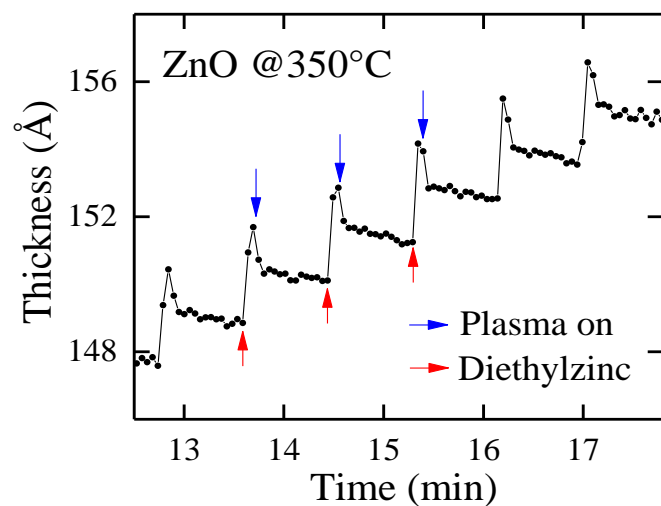
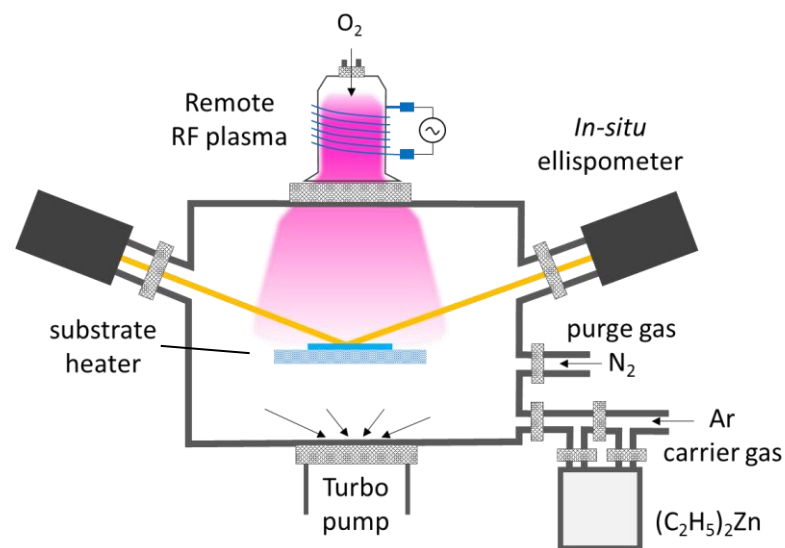
**Dynamic  
Data**





# ATOMIC LAYER DEPOSITION

## ■ Process optimization in one single run





# SHORT-CUTS FOR IN SITU DATA

Shortcut	Function
CTRL+Spacebar	Toggle view between single time-slice SE Data & Data vs. Time
ALT- (data set #)	Select specific data set (when multiple data sets selected)
CTRL+'Y'	Toggle double Y-axis
Left-click mouse (Dynamic Data Graph)	Select time-slice
CTRL-Left-click mouse (Dynamic Data Graph)	Add multiple time-slices for multi-time analysis
ALT+Left-click mouse (Dynamic Data Graph)	Set Virtual Interface time-slice (drag mouse to select time range)
CTRL+ALT+SHIFT+'U'	Display the <i>In situ</i> tab
CTRL+'U'	Select <i>In situ</i> tab
CTRL+'A'	Select <i>Analysis</i> tab

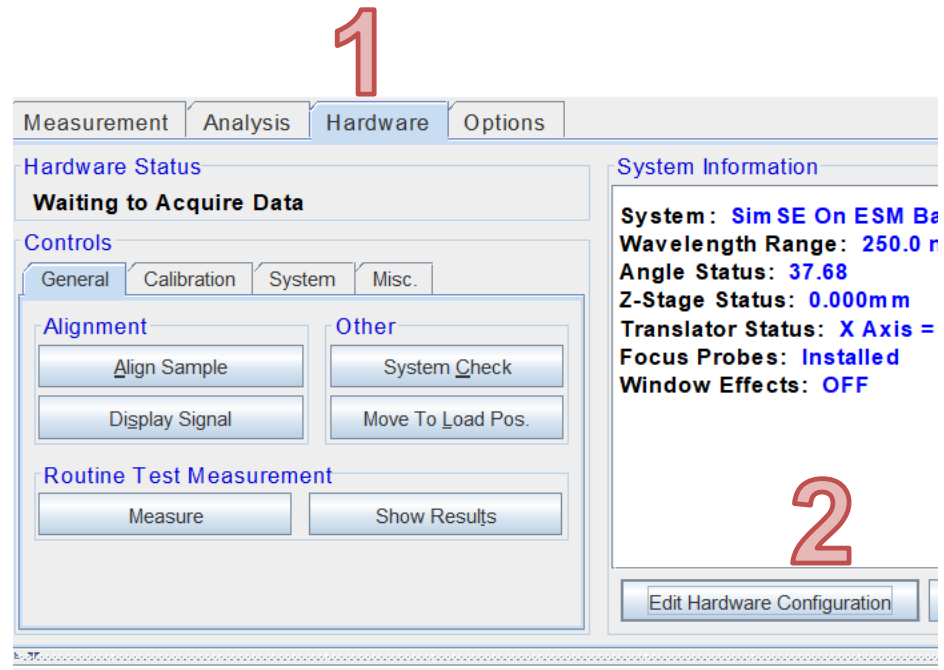


# BASIC IN SITU DATA ANALYSIS STRATEGY

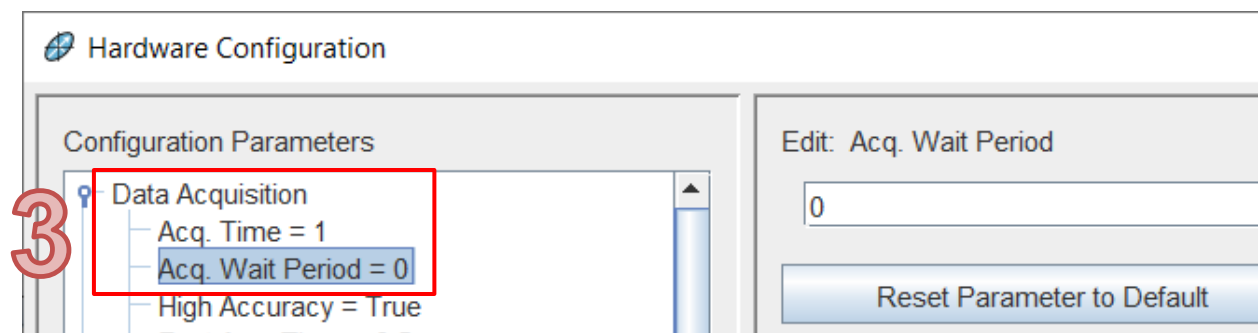
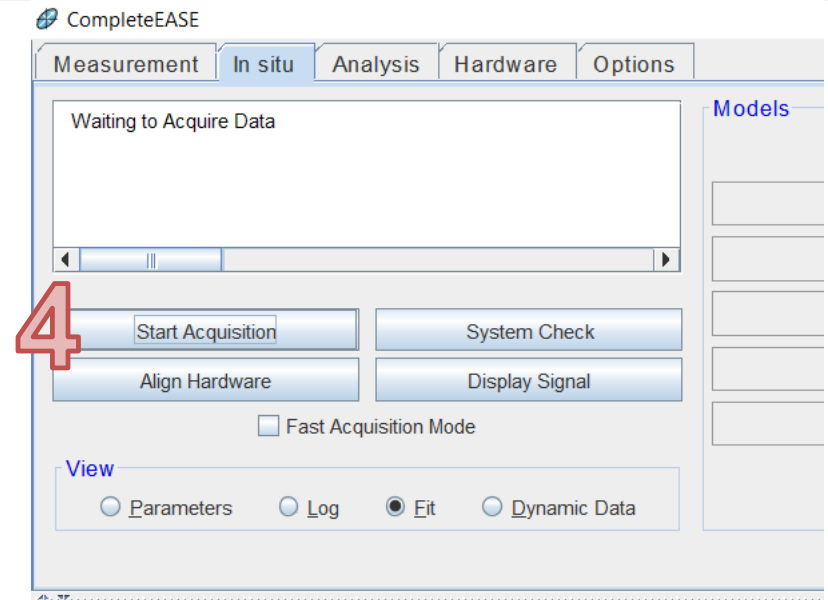
- Select early time-slice to:
  - Fit bare substrate (native oxide thickness, angle offset, temperature)
- Select late time-slice to:
  - Fit thin film optical constants
- Fix parameters except thickness and “Fit Dynamic”
  - Confirm initial model thickness is close prior to “Fit Dynamic”



# COLLECTING IN SITU DATA



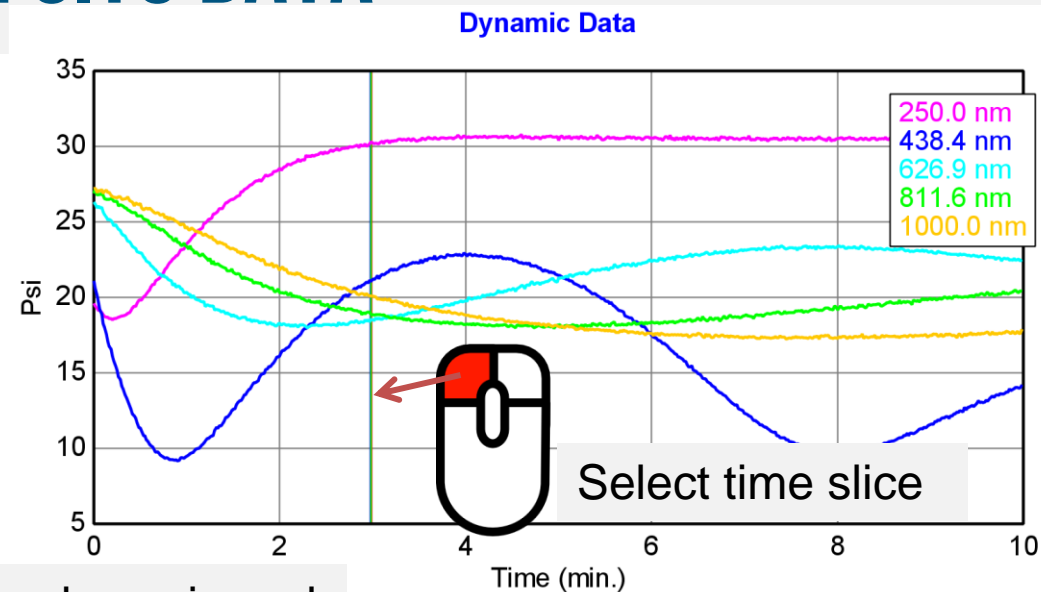
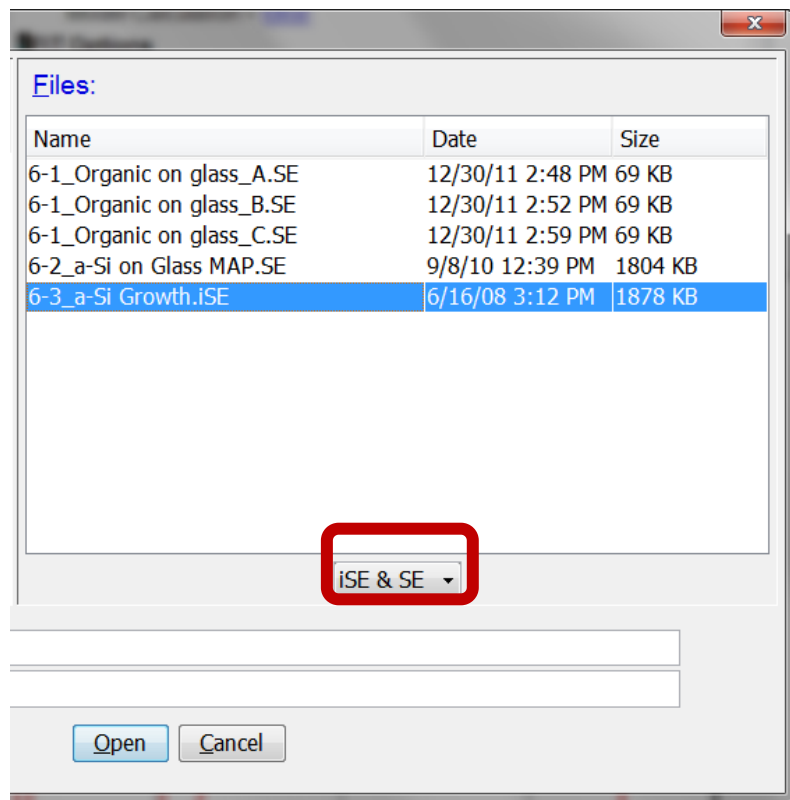
- Preset data acquisition time and intervals





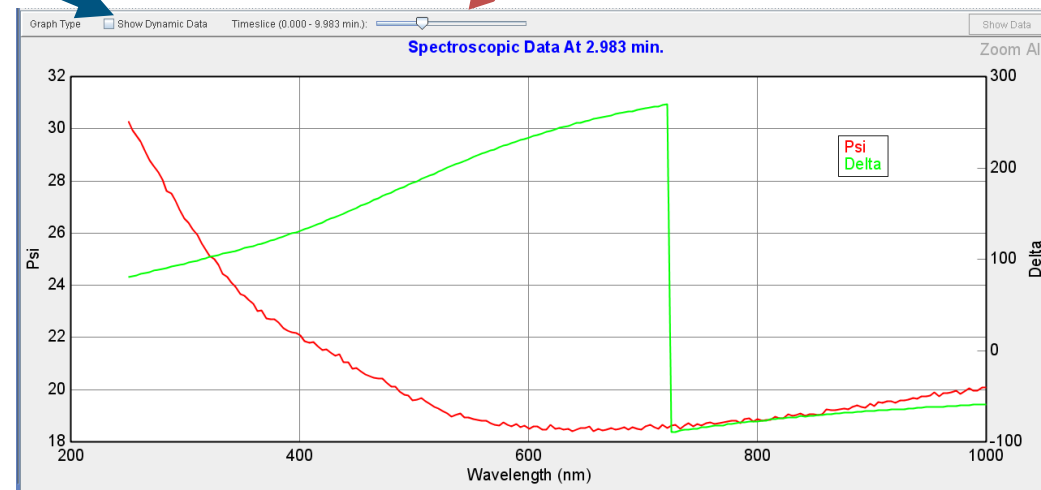
# OPEN AND VIEW IN SITU DATA

- Dynamic data is saved with “iSE” extension



Toggle bw dynamic and spectroscopic data

Bar to move through time slices

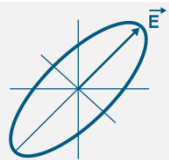




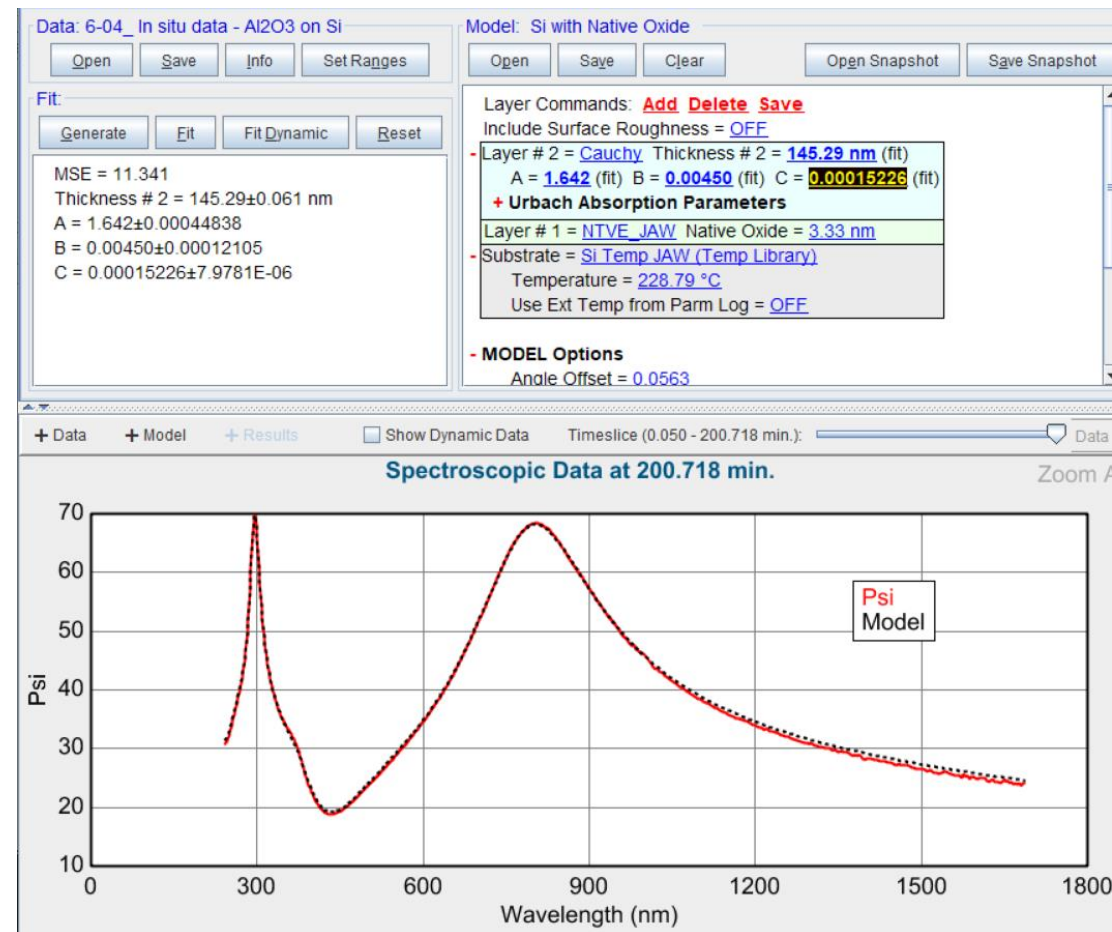
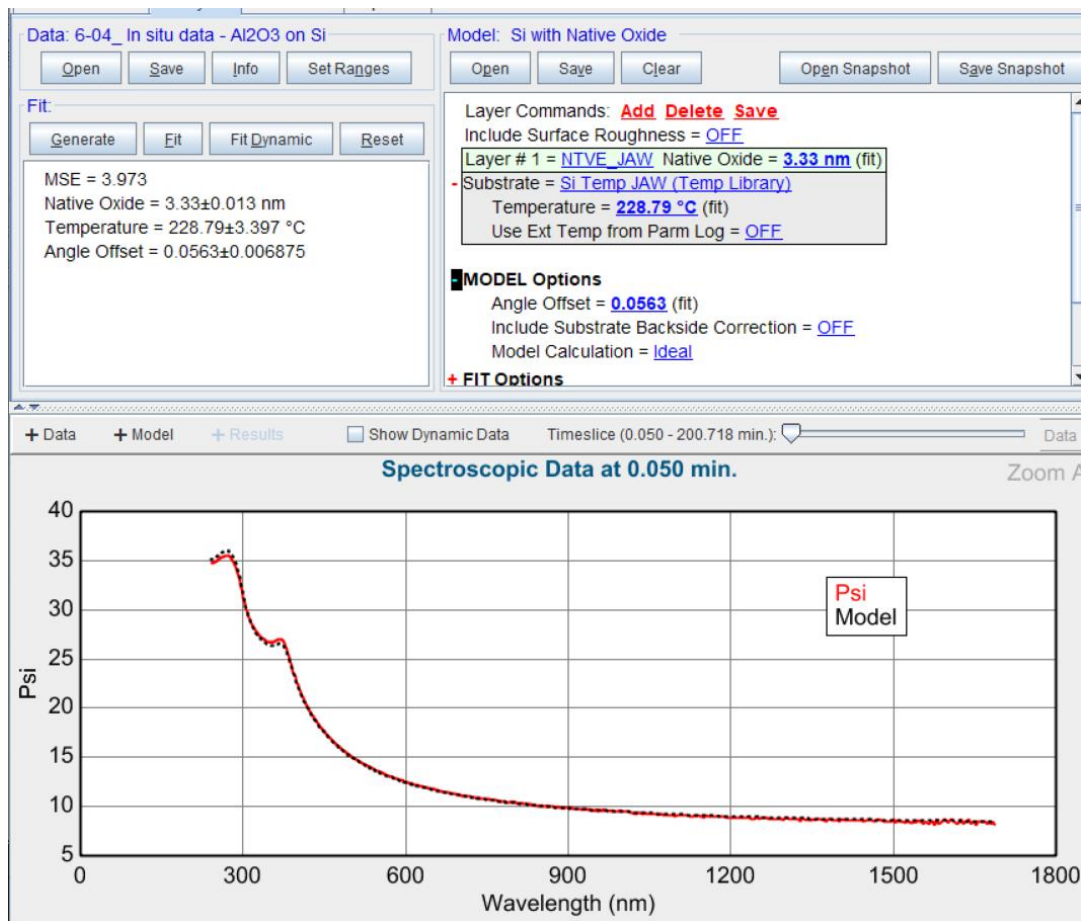
## [6-04] In situ data – $\text{Al}_2\text{O}_3$ on Si

- Determine Growth Rate from dynamic data of  $\text{Al}_2\text{O}_3$  on Si.





# FIT STRATEGY



- Determine sample baseline and system condition at the beginning
- Determine ALD layer refractive index when films become thick enough



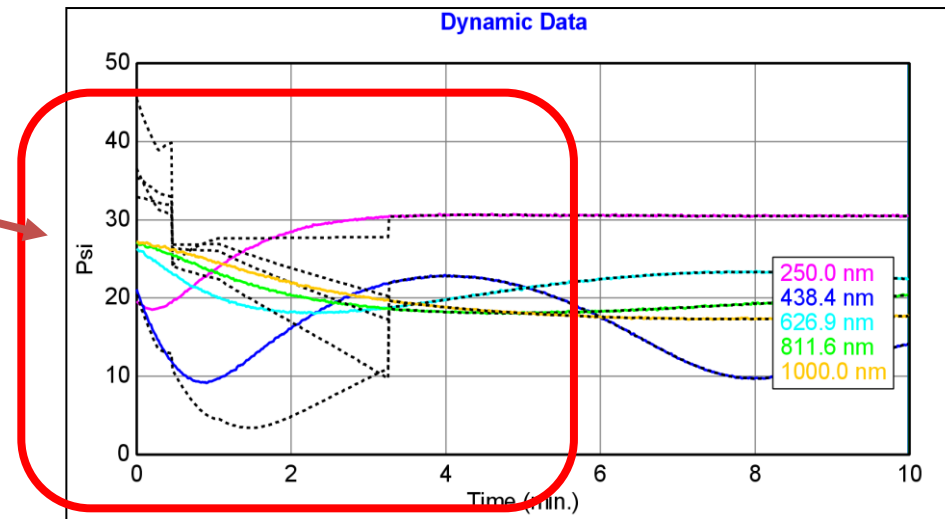
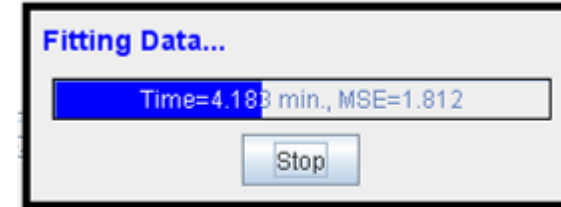
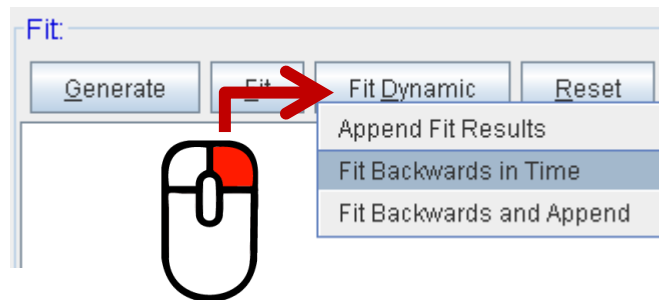
# DYNAMIC FIT

## 'Fit-Dynamic'

- a) Select 'Fit Dynamic'
- b) Can also "fit backwards in time" by right-clicking on 'Fit Dynamic'

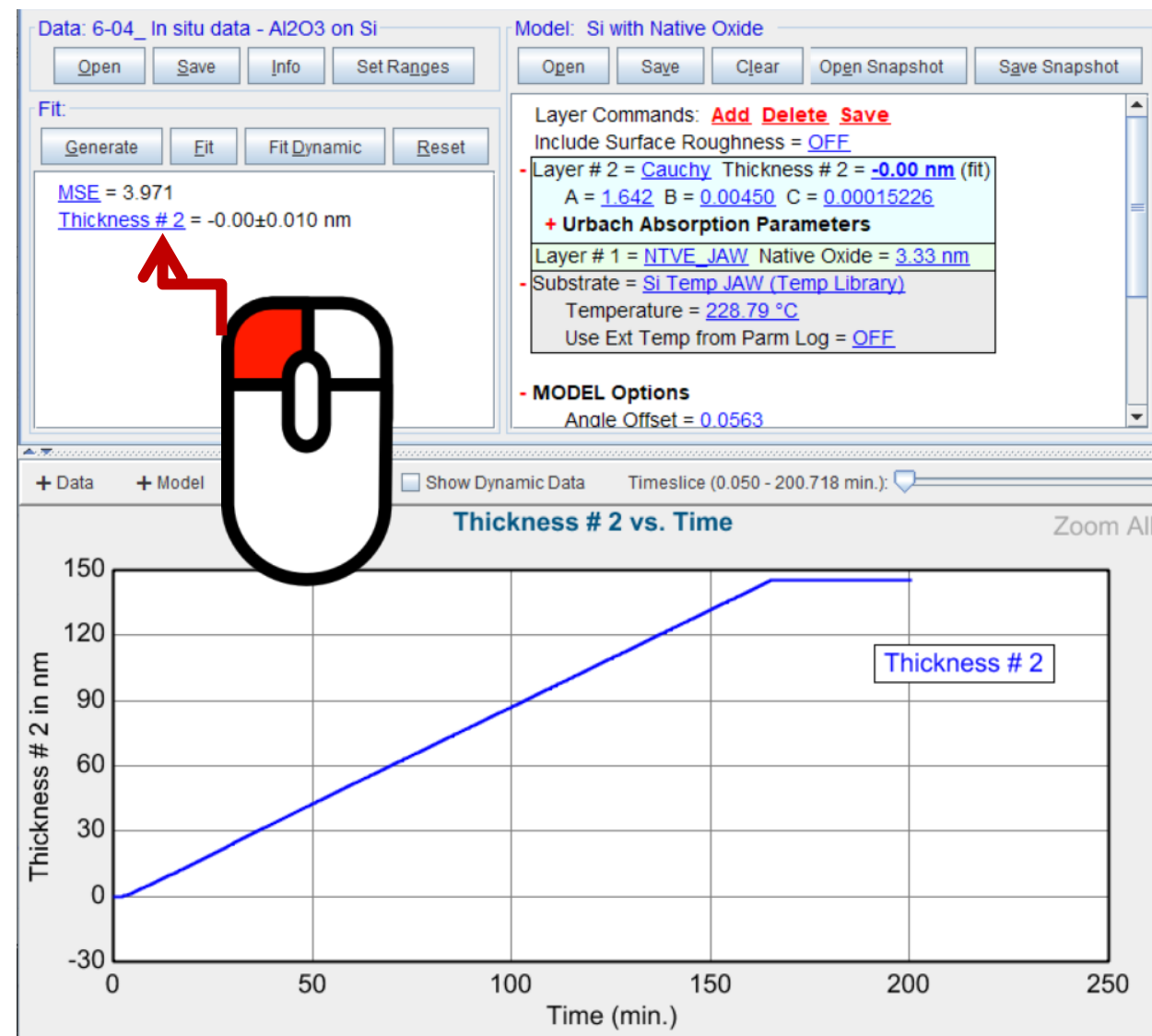
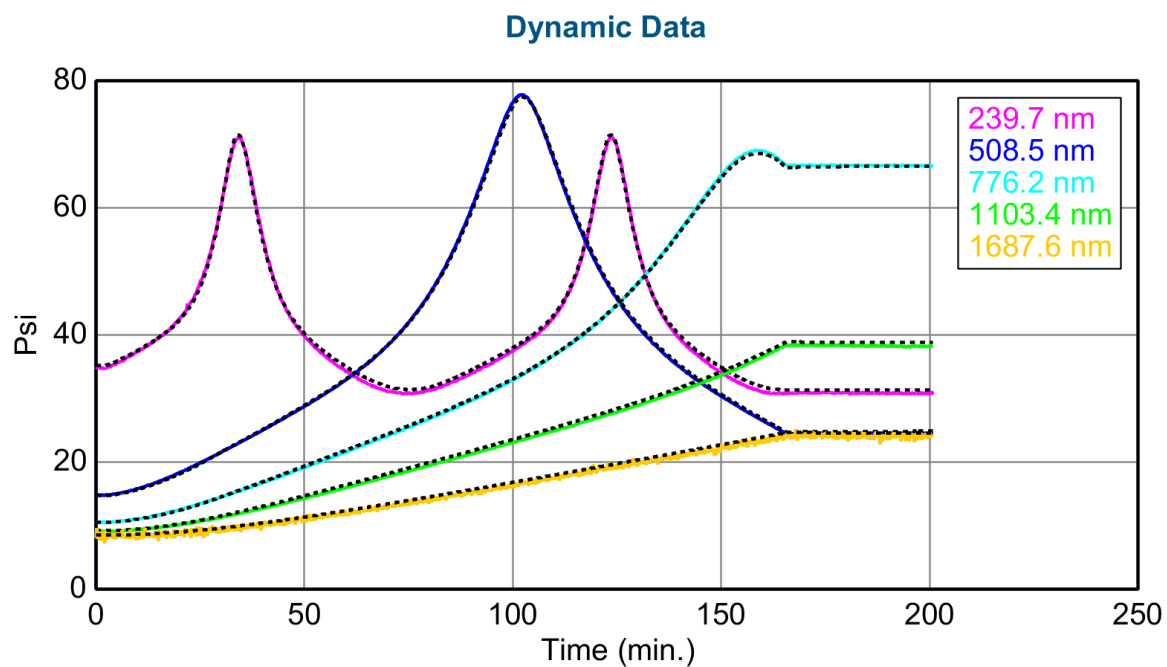


'Seed' fit parameters to good starting values or the Dynamic Fit will get lost



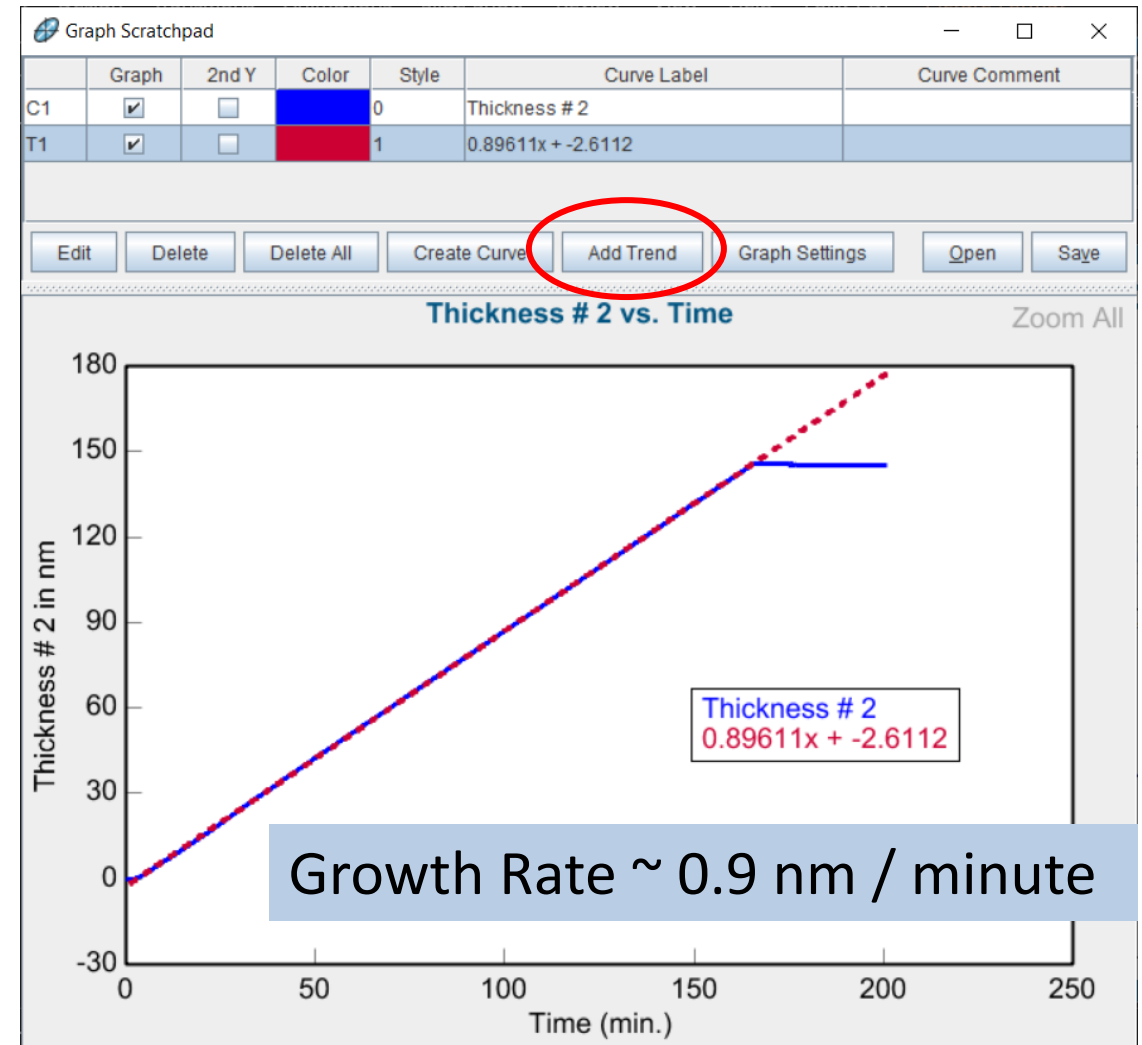
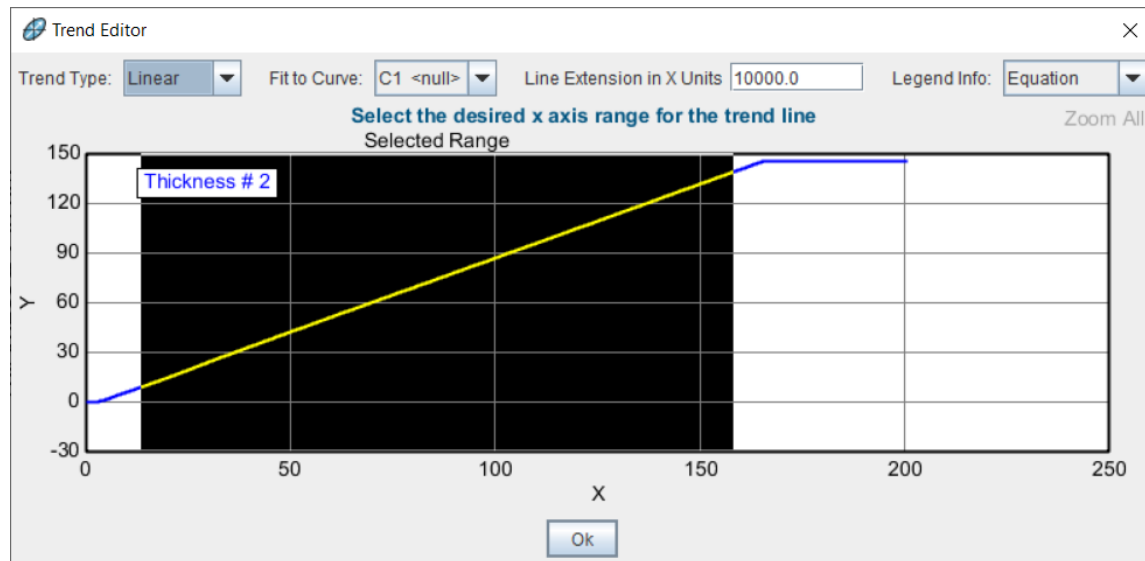


# DYNAMIC RESULTS



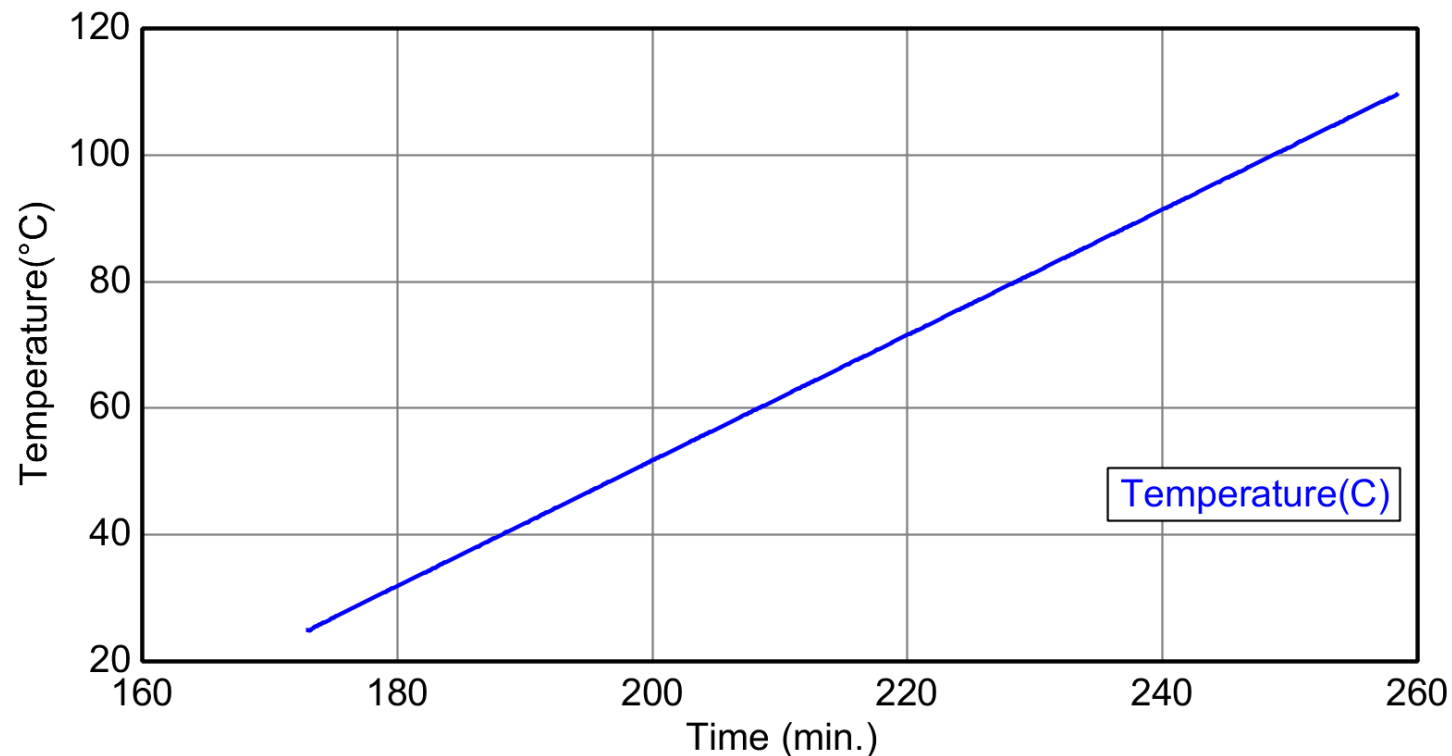


# GROWTH RATE FROM GRAPH SCRATCHPAD



## Example 6-05: Polymer on Si\_Tg

We created a novel polymer mixture and want to study the mechanical properties. We spin coat the polymer onto a Si wafer and use a heat cell to determine the glass transition temperature from the temperature dependence of the layer thickness.





# ANALYSIS STRATEGY

We will do these steps together:

1. Open dynamic data (.iSE extension)
2. Select the first time slice.
3. Build Model: Need to consider temperature effect on substrate
  - Use temperature library material file “Si\_Temp\_JAW(-160-500C)”
  - Use stored temperature readings
4. Fit Single Time Slice.
5. Fit Dynamic Data.
6. Graph results as function of Temperature using Advanced Graph Options in Fit window.
7. Use the Graph Scratch Pad to determine  $T_g$ .



-	Layer # 1 = <a href="#">Cauchy</a> Thickness # 1 = <a href="#">1921.60 nm</a> (fit) A = <a href="#">1.611</a> (fit) B = <a href="#">0.01283</a> (fit) C = <a href="#">0.0000</a> Show Urbach Absorption Parameters = <a href="#">OFF</a>
-	Substrate = <a href="#">Si_temp_jaw(-160_500C)</a> Temperature = <a href="#">25.00</a> Use Ext Temp from Parm Log = <a href="#">ON</a> (Library Ranges: 0.73 -6.45 eV, x=0.500 - 0.500, t=-160.000 - 500.000)

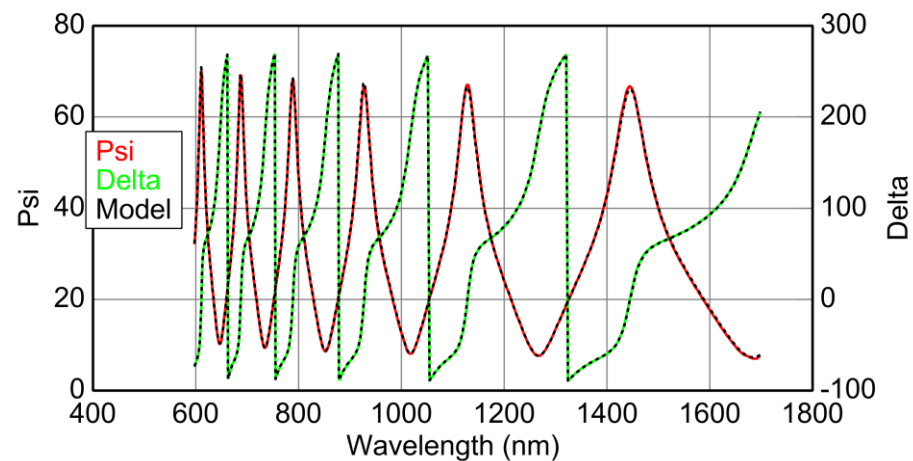




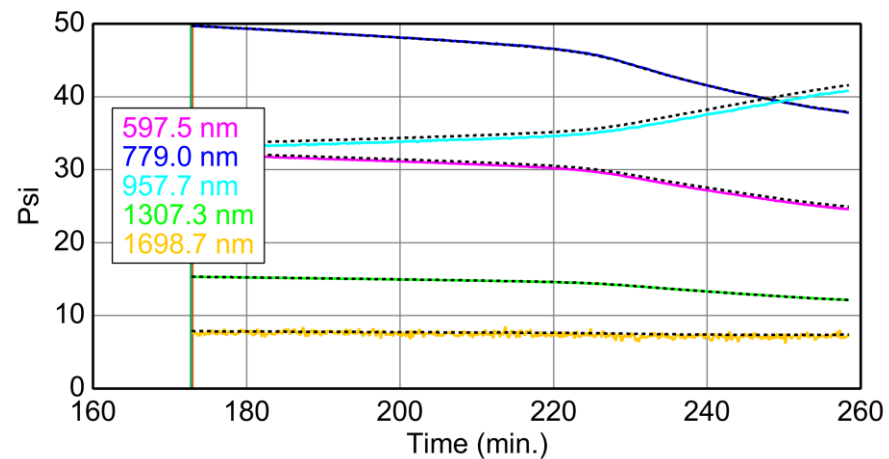
# 6-05: POLYMER ON SI\_TG - RESULTS



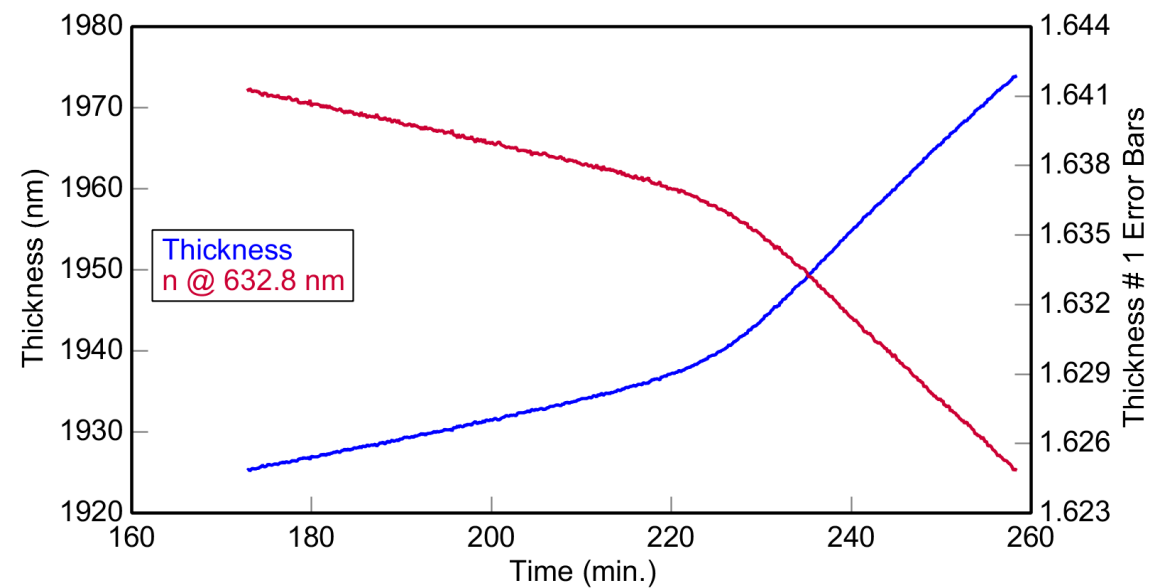
Spectroscopic Data At 172.843 min.

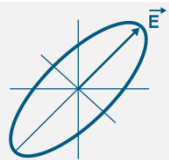


Dynamic Data



Thickness and Index vs. Time





# ADVANCED GRAPH CAPABILITIES

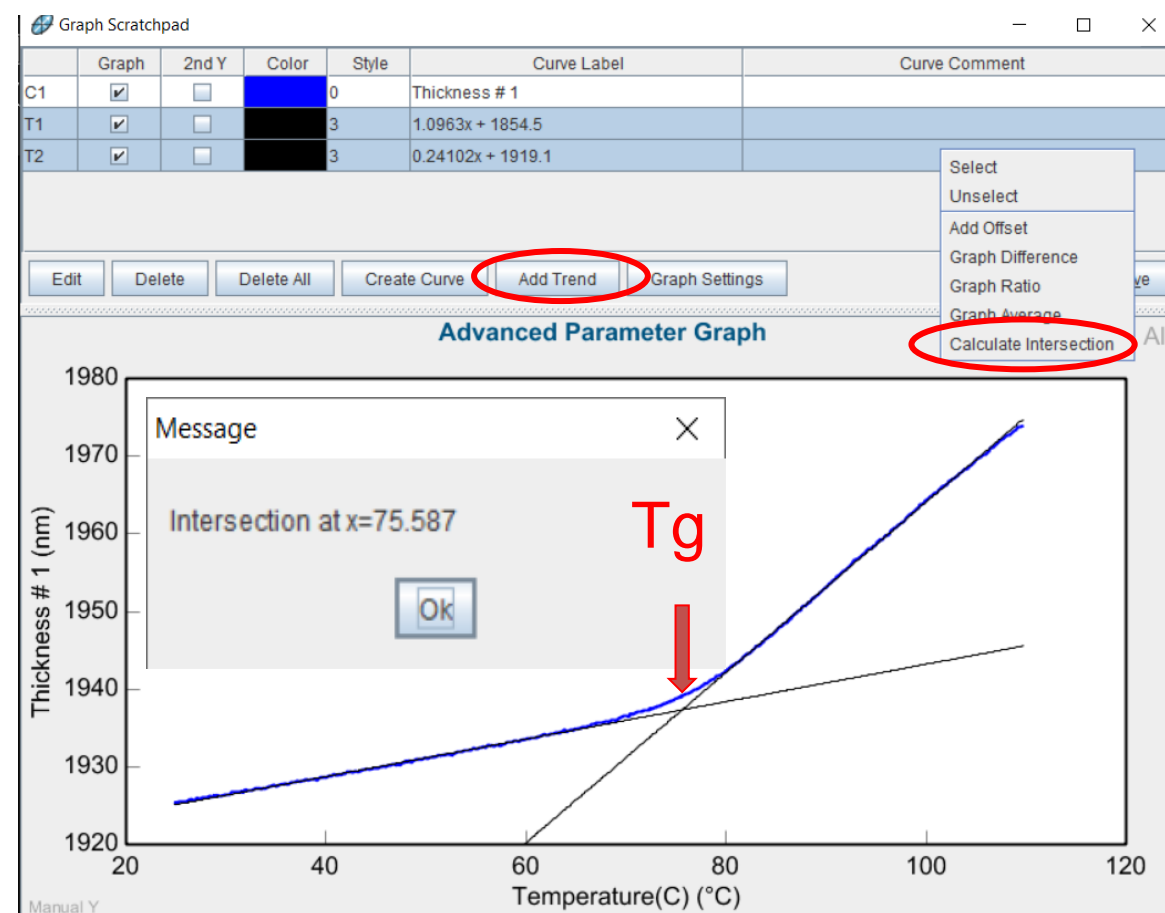
- Right Click in Fit Window to open Advanced Graph Options
- Plot thickness vs Temperature in Graphscratchpad
- Add trend lines and calculate T<sub>g</sub>

The Fit window displays the following statistics:

- MSE = 11.449
- Thickness # 1 = 1973.96 ± 1.086 nm
- A = 1.594 ± 0.00057333
- B = 0.01239 ± 3.5311E-05
- n of Cauchy @ 632.8 nm = 1.62484

The Advanced Graph Setup dialog shows the following parameters:

X-Axis Parameter	Y-Axis Parameter(s)
MSE	MSE
Absolute MSE	Absolute MSE
Thickness # 1	Thickness # 1
A	A
B	B
n of Cauchy @ 632.8 nm	n of Cauchy @ 632.8 nm
Temperature(C)	Temperature(C)
Time	



# Review

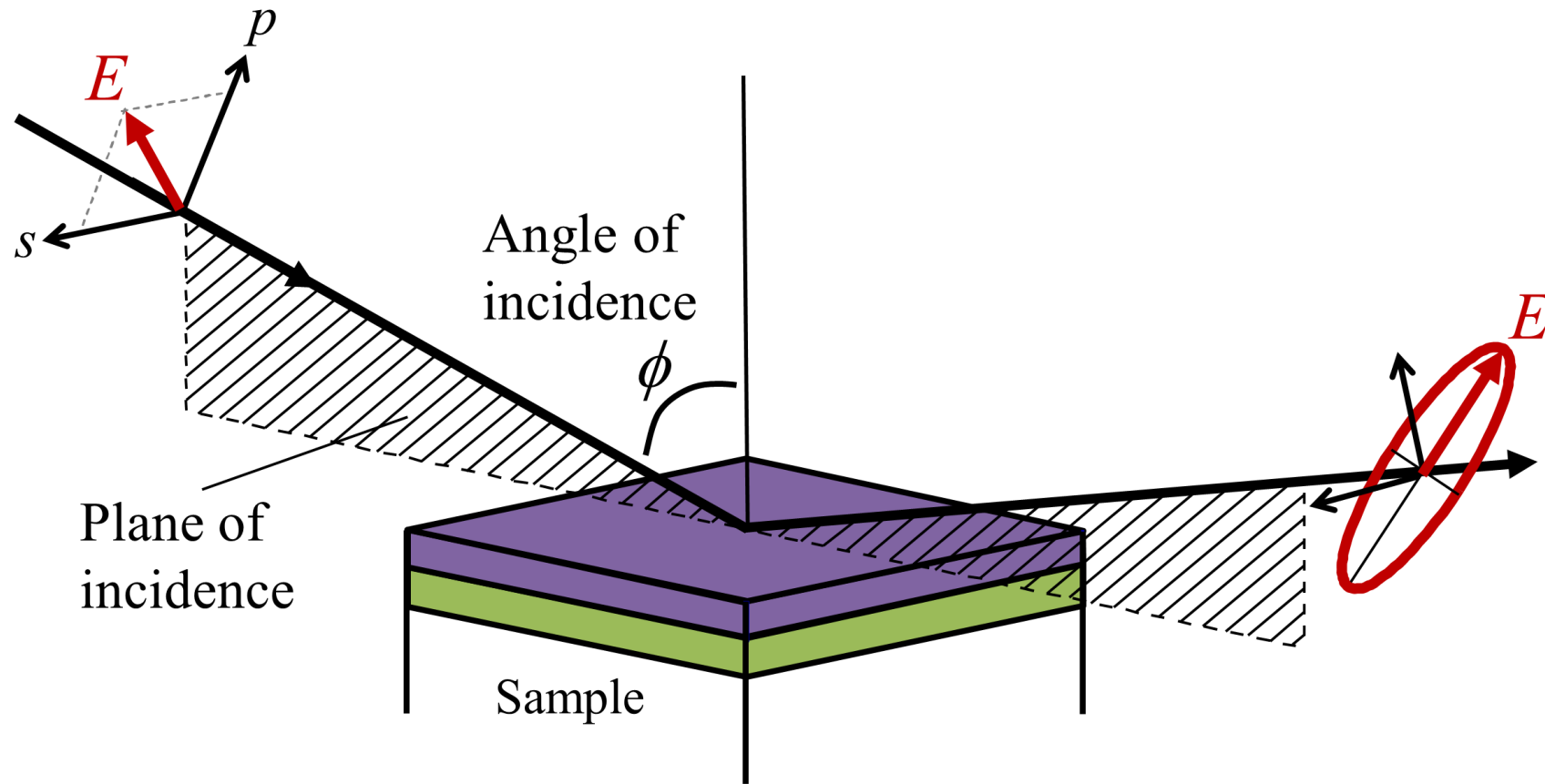
- Consider Key Concepts and how they fit together





# SPECTROSCOPIC ELLIPSOMETRY (SE)

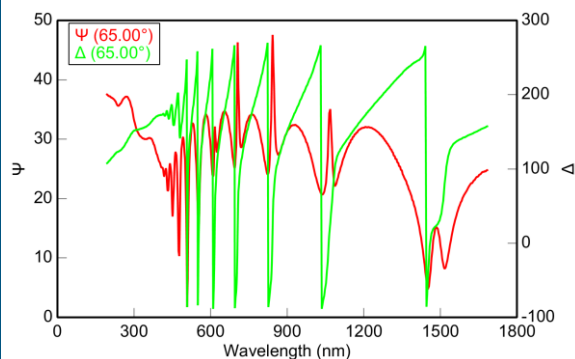
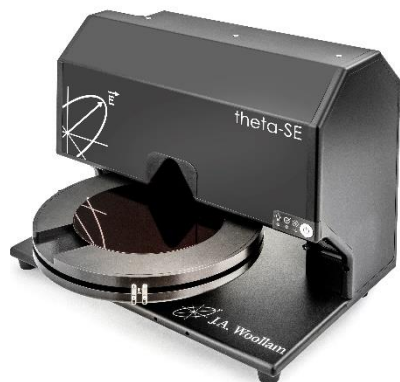
- Measures change in polarization.



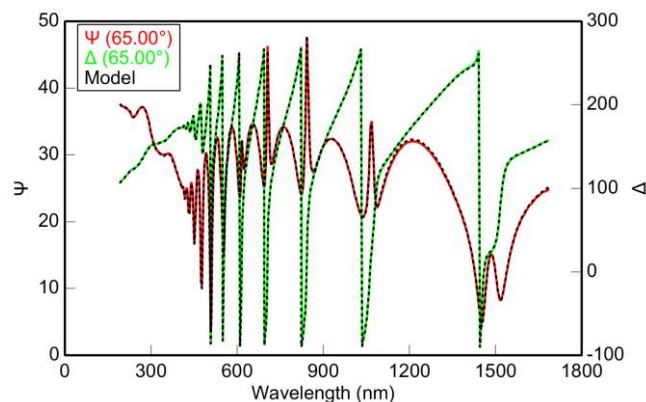


# Basics Of Ellipsometry

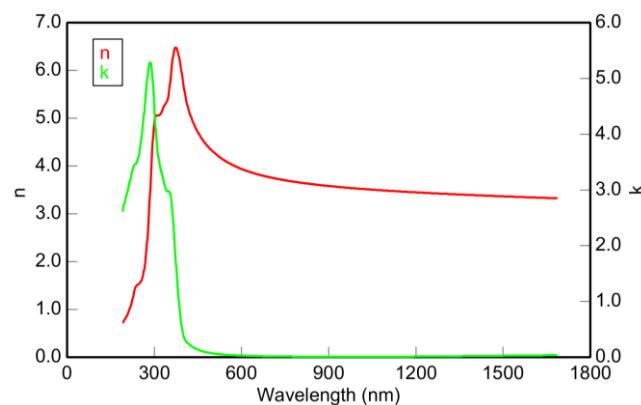
## Measurement



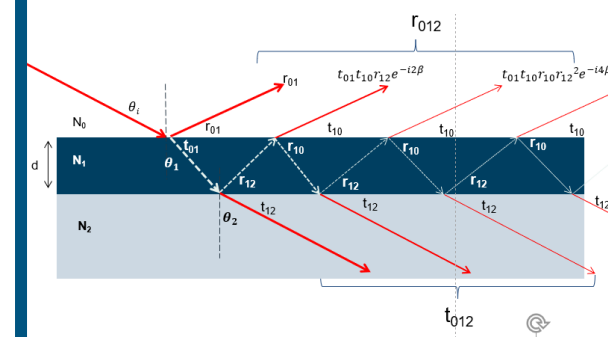
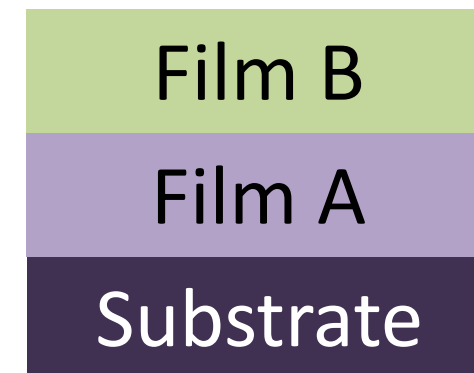
## FIT



## RESULTS



## MODEL



H.G. Tompkins and J.N. Hilfiker "Spectroscopic Ellipsometry: Practical Application to Thin Film Characterization" (2016) Momentum Press.



# MODEL EVALUATION

## Good Match

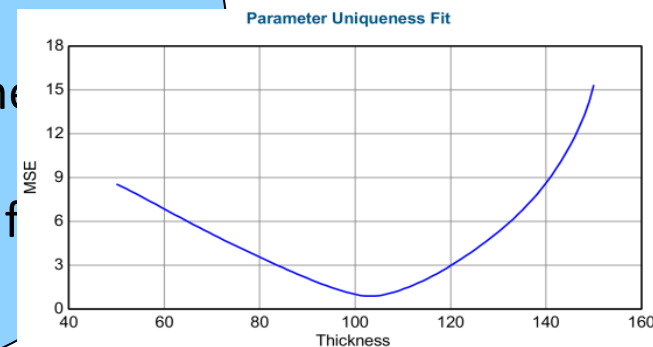
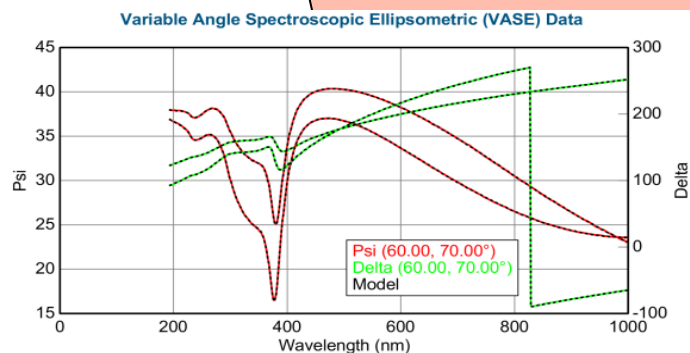
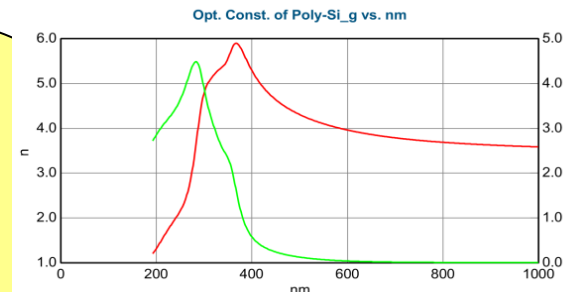
- Describes all significant features in the data
- Small MSE

## Physical results

- Positive  $\varepsilon_2$
- Positive thickness
- KK consistent index

## Unique answer

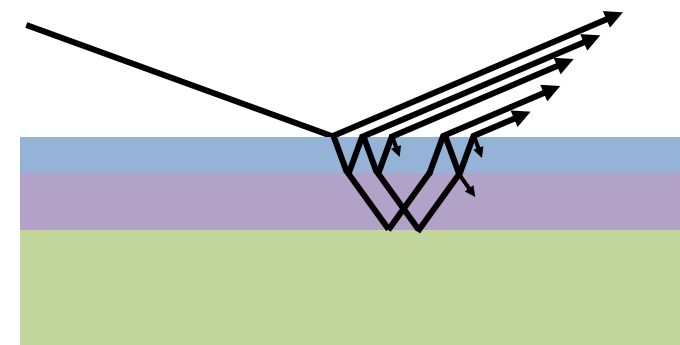
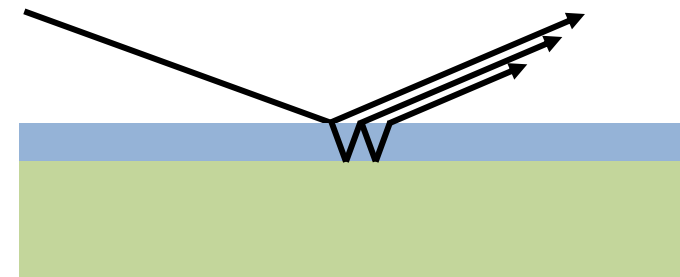
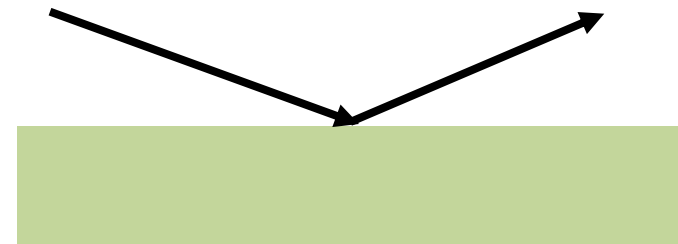
- Good sensitivity to fit parameters
- Low error bars
- Simplest model with fewest parameters



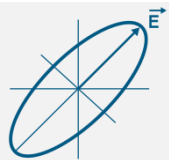


# WHAT ARE WE MEASURING?

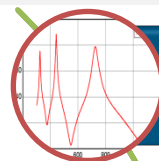
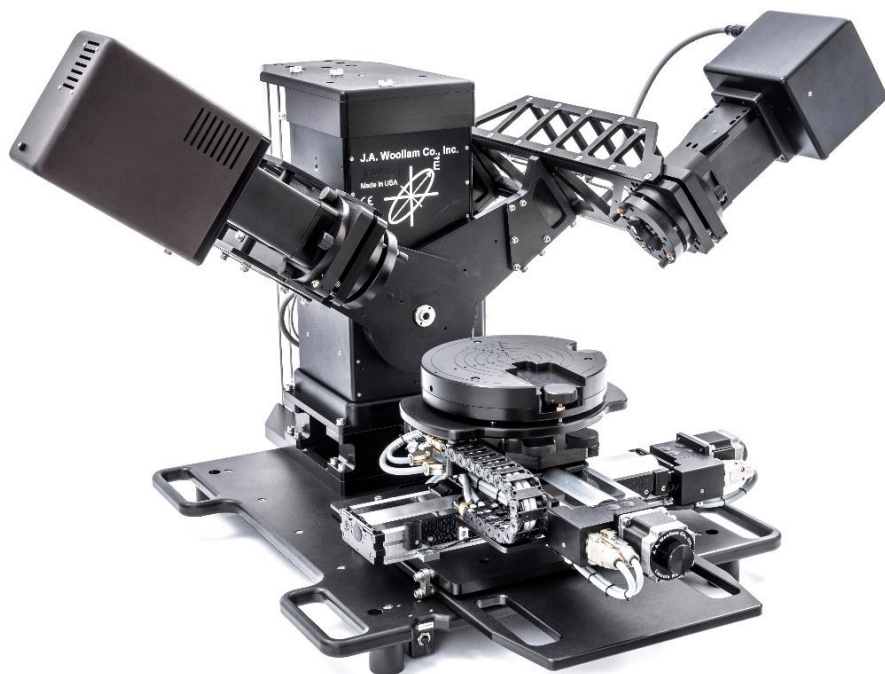
- Substrate
  - Ideal: Single surface reflection.
- Single-Layer
  - 1nm to 20  $\mu\text{m}$  of material on substrate
- Multi-Layer
  - More than one film with different  $n, k$



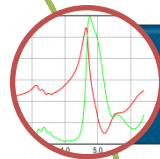




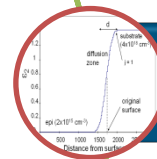
# WHAT DOES ELLIPSOMETRY DO?



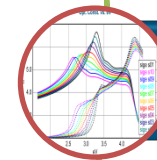
Layer thickness and Uniformity



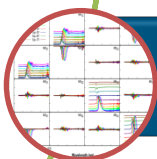
Refractive Index / Optical Constants



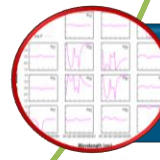
Grading and Roughness



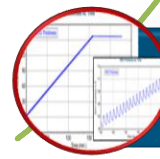
Composition / Bandgap /  
Conductivity/ Porosity /Crystallinity



Anisotropy



Retardance/ Chirality



In-situ Monitoring / Dynamic Properties



# DATA CONTENT → MATERIAL PROPERTIES

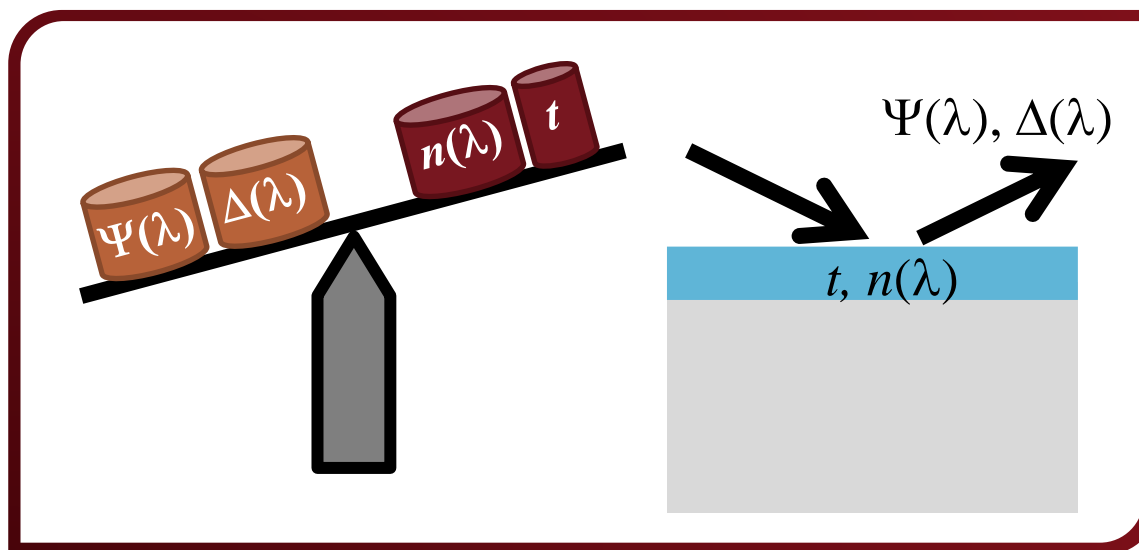
## Measurement information

- Total content:  $2\lambda$ .
- Multiple angles may add extra information.

## Material properties

- Film thickness
- Optical Constants
  - Transparent ( $n$ ):  $1\lambda$
  - Absorbing ( $n$  &  $k$ ):  $2\lambda$

- Measurement content needs to solve all unknown sample properties





# MODELING DIFFERENT MATERIALS

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

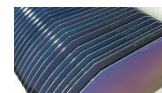
$$\tilde{\epsilon} = \epsilon_1 - i\epsilon_2$$

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

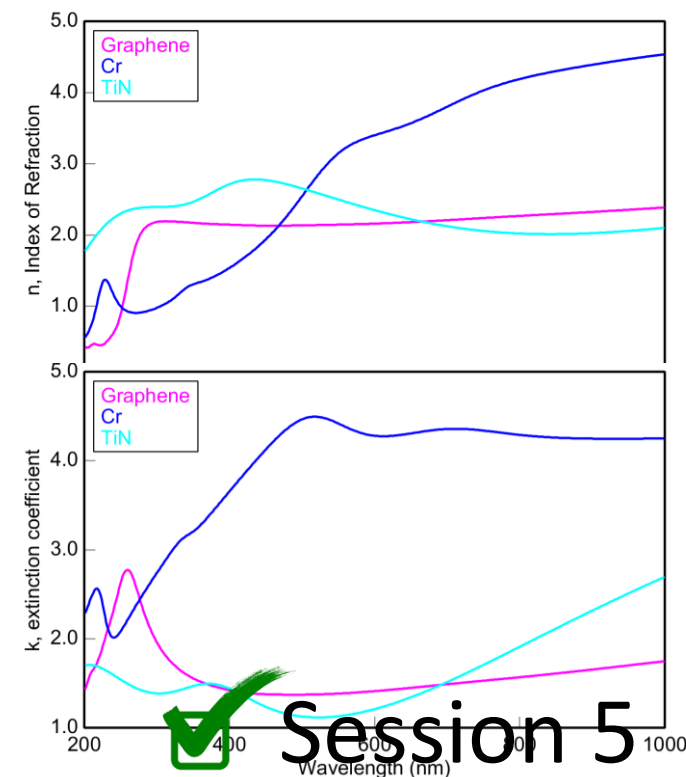
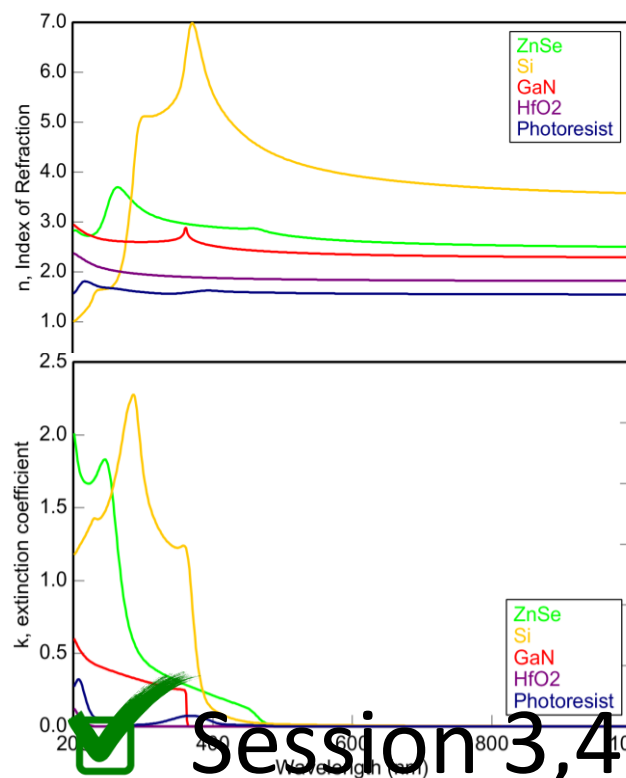
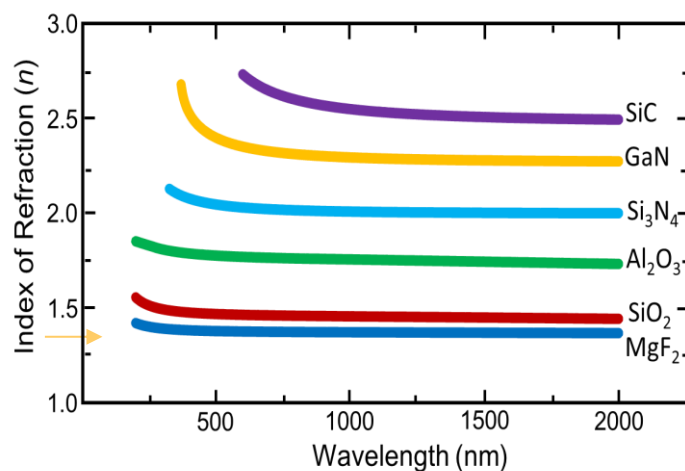
Transparent



Semi-absorbing



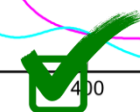
Absorbing



Session 2



Session 3,4



Session 5

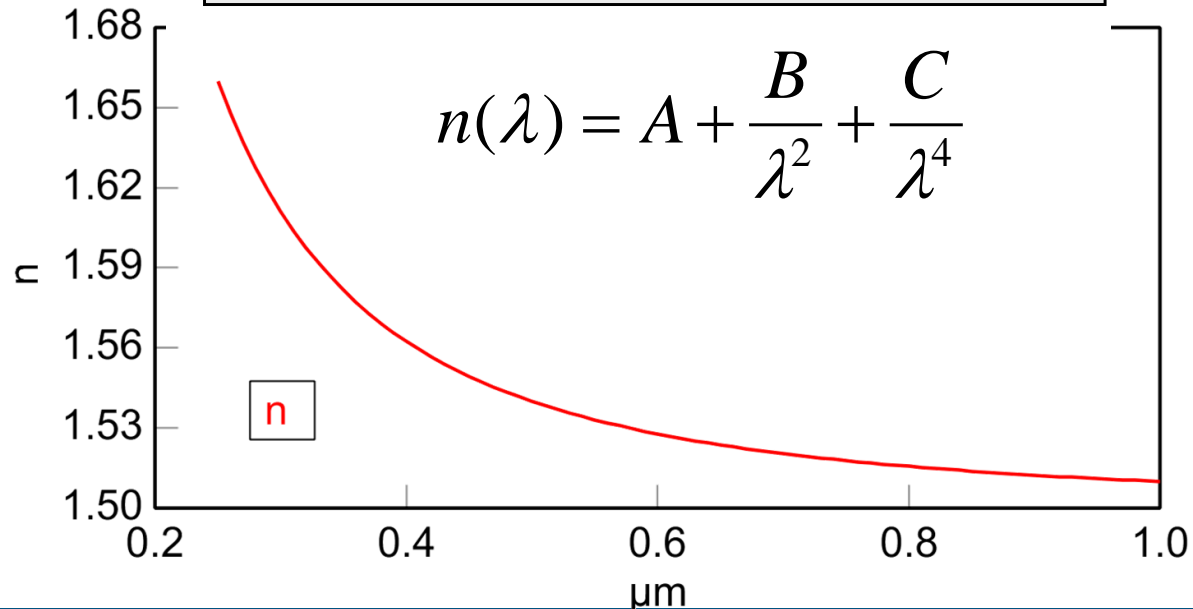


# TRANSPARENT MATERIALS

## Cauchy

- Empirical equations
- Easy to use

- Substrate = [Cauchy](#)  
A = [1.450](#) B = [0.01000](#) C = [0.0000](#)  
Show Urbach Absorption Parameters = [OFF](#)



## Sellmeier

- Embedded in Genosc
- Works better for materials presenting absorptions at longer wavelengths

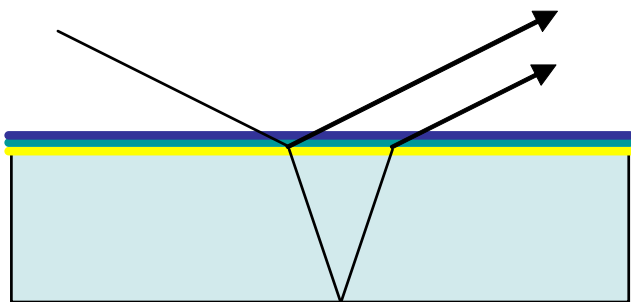
Include Surface Roughness = [ON](#) Roughness = [13.44 Å](#) (fit)

- Substrate = [Gen-Osc](#)  
**Show Dialog**

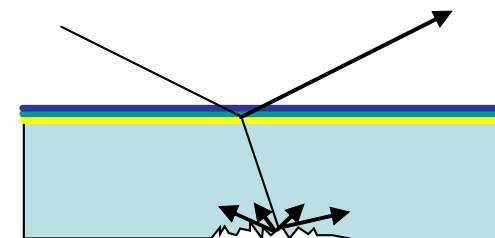
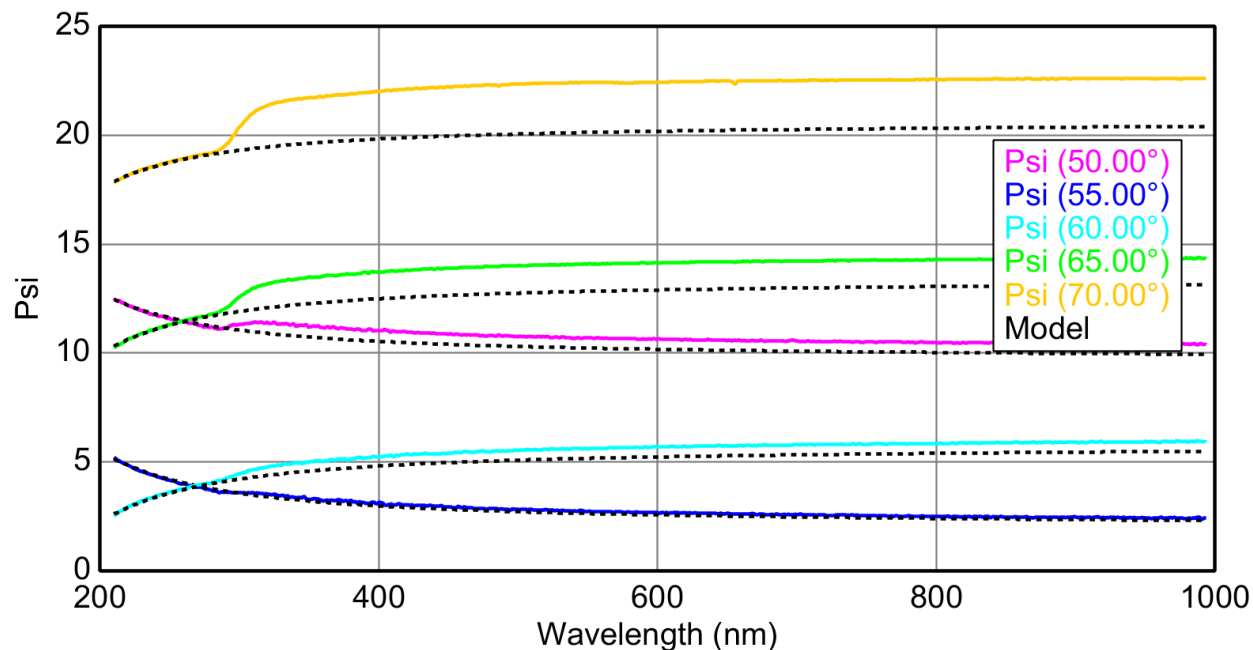
- **e1 Components**  
Einf = [1.466](#) (fit)  
UV Pole Amp. = [92.7823](#) (fit) UV Pole En. = [10.665](#) (fit)  
IR Pole Amp. = [0.0200](#) (fit)
- **e2 Components**  
Oscillator Menu: [Add](#) [Delete](#) [Delete All](#) [Sort](#)  
Fit Menu: [All](#) [None](#) [Amp.](#) [Br.](#) [En.](#) Display Units = [OFF](#)  
(There are no oscillators added.)



# TRANSPARENT SUBSTRATES



Backside Reflection



## - MODEL Options

Angle Offset = 0.00

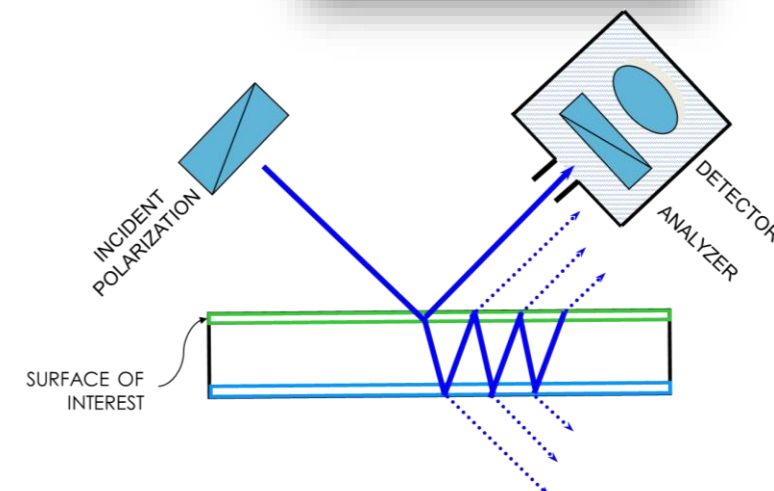
Include Substrate Backside Correction = ON

Transmission SE Data = OFF Reverse Direction =

# Back Reflections = 0.881 (fit)

% 1st Reflection = 100.00

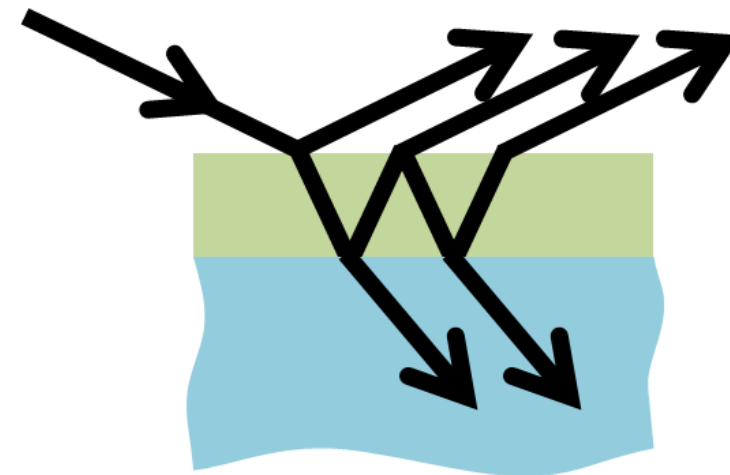
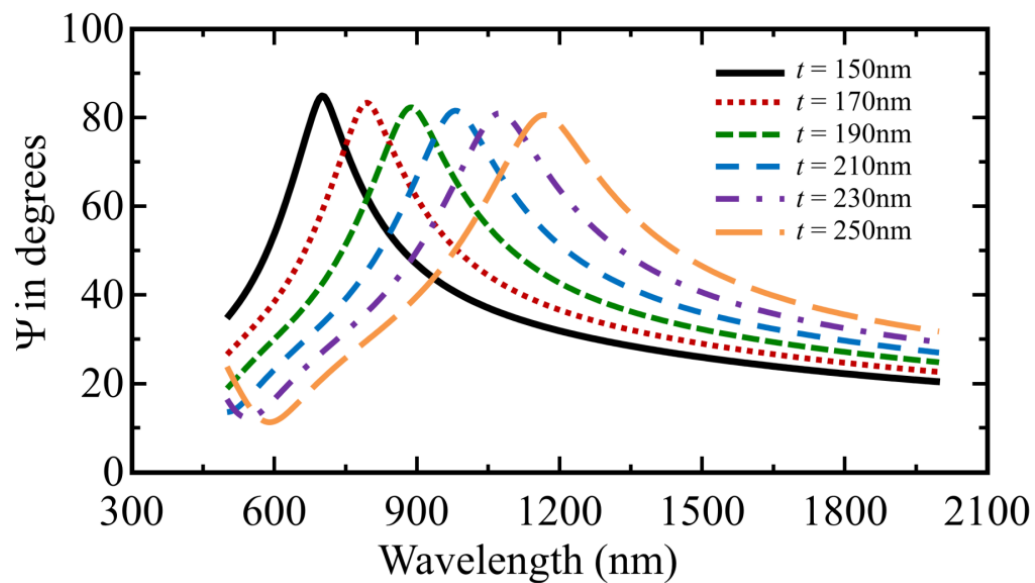
Model Calculation = Ideal



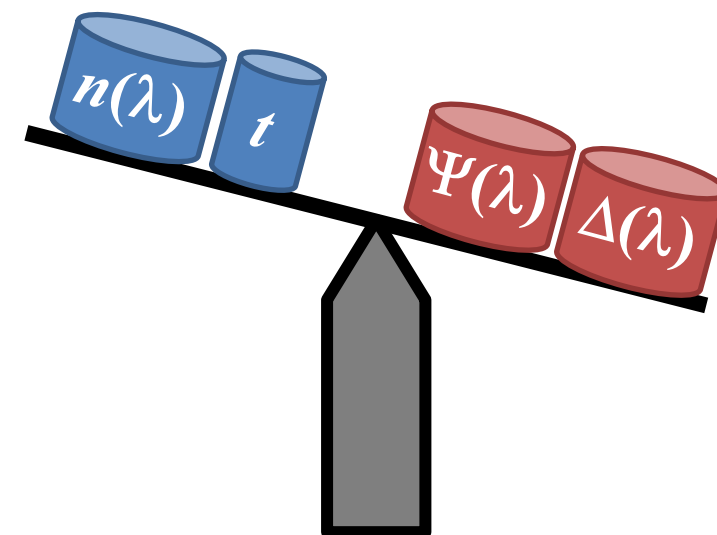
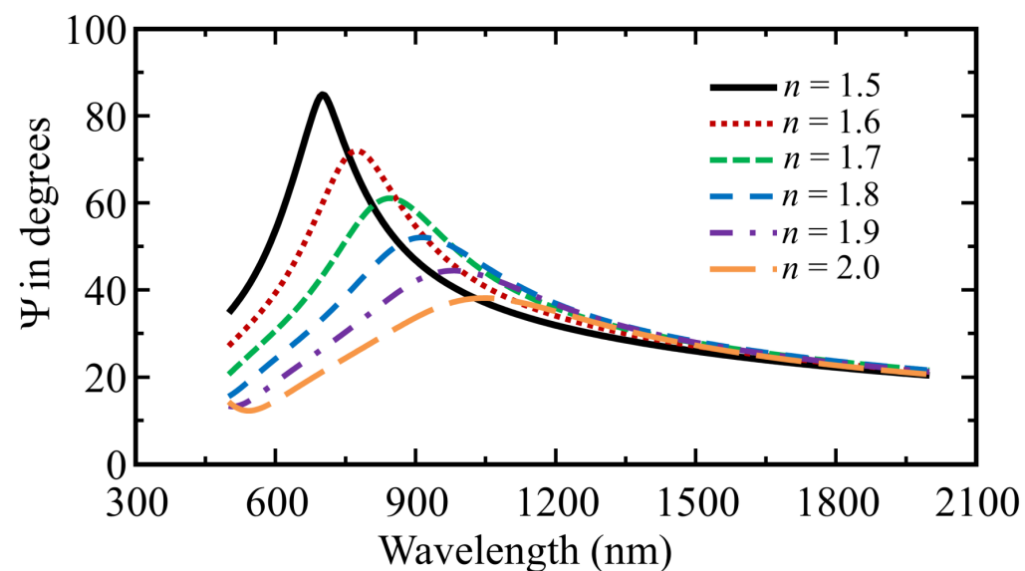


# TRANSPARENT THIN FILMS

Thickness Shifts  
interference

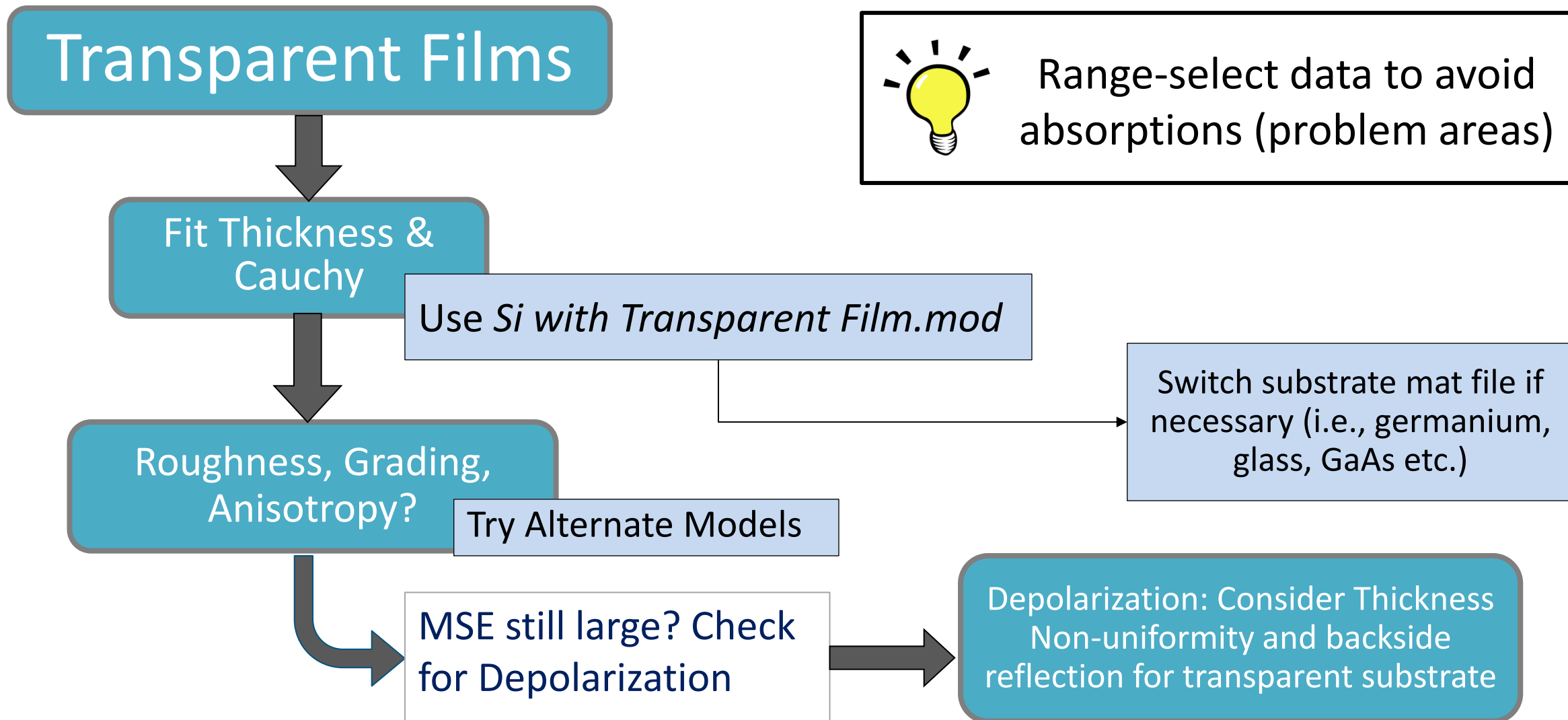


Index of Refraction  
affects amplitude  
and shifts peak





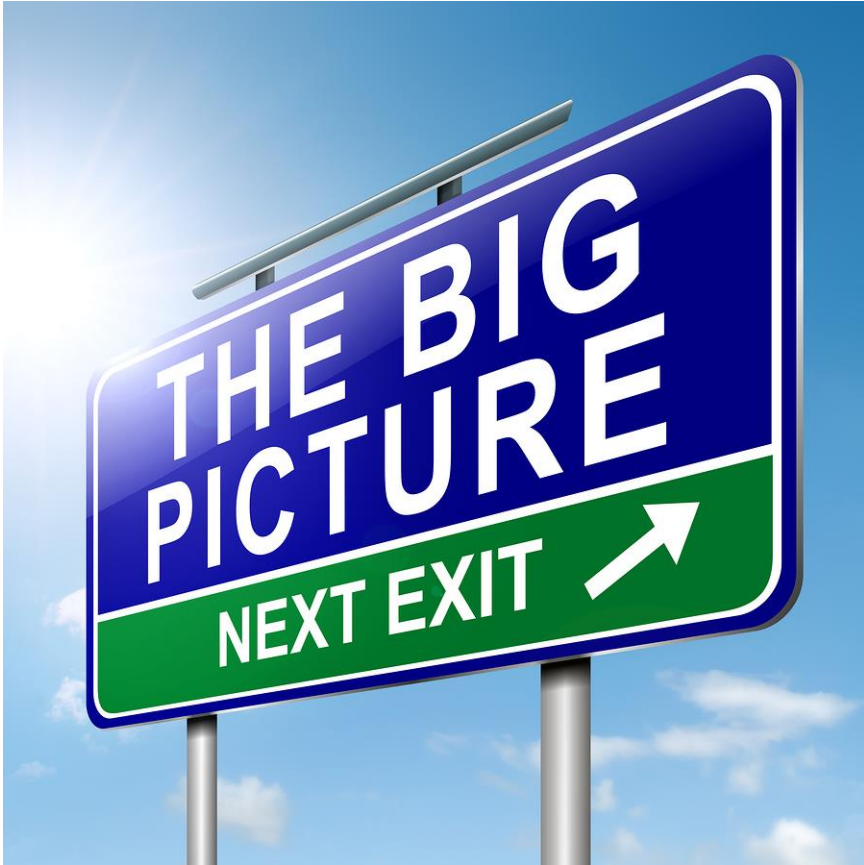
# TRANSPARENT FILMS







# MATERIALS THAT ABSORB



- We will apply the **B-Spline** and **Gen-Osc** layers to describe absorbing materials to fit their optical constants (both  $n$  and  $k$ ).
- Benefits:
  - Smooth, continuous functions
  - Can constrain to “physical” shapes

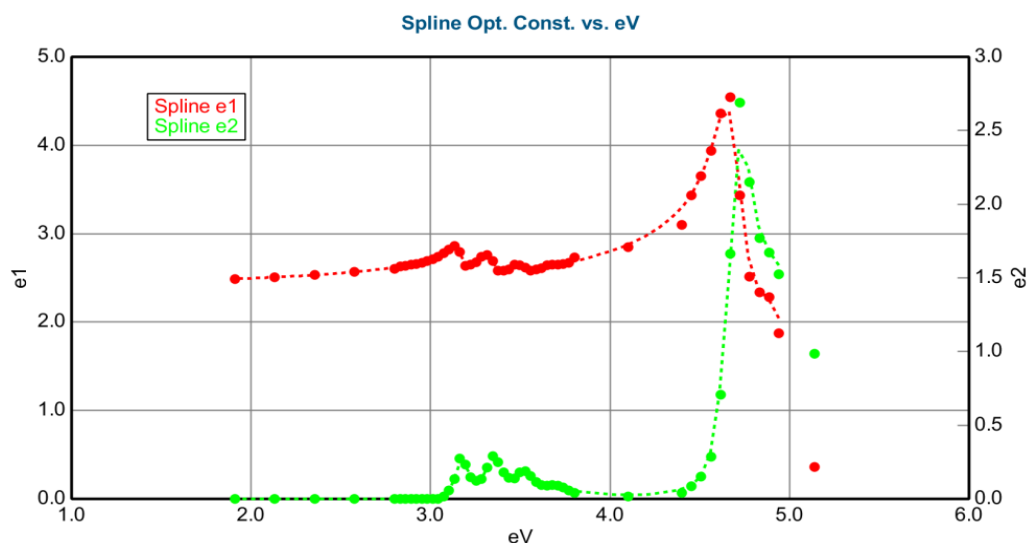


# MODELING ABSORPTION

## B-spline

- Interpolation functions to best describe the shape of optical constants

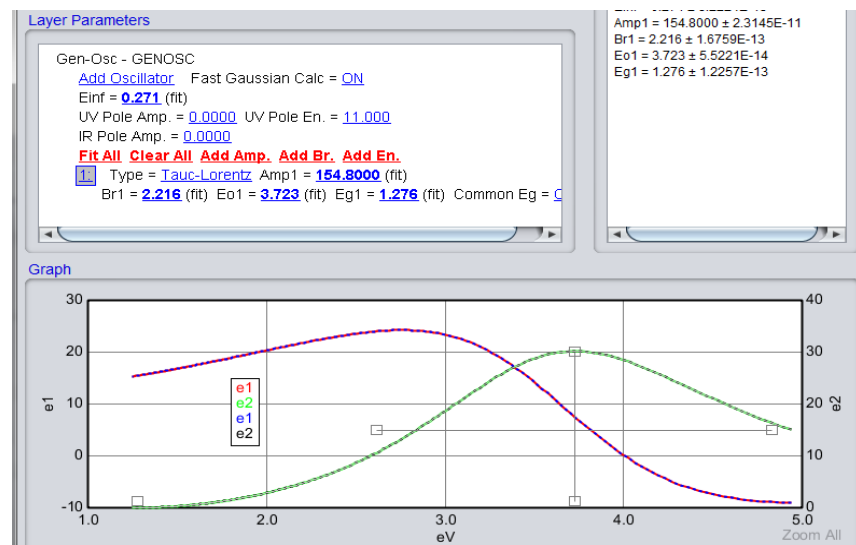
Layer # 1 = [B-Spline](#) Thickness # 1 = [64.74 nm](#)  
 Init. values:  $n = 1.500$   $k = 0.000$  Starting Mat = [B-Spline](#)  
 Resolution (eV) = [0.200](#) 53 Pts. (1.242-4.940 eV) [Draw Node Graph](#)  
 Fit Opt. Const. = [ON](#)  
 Use KK Mode = [OFF](#)  
 Query remote system for Opt. Const. = [OFF](#)  
 Show Advanced Options = [OFF](#)



## Gen-Osc

- Combine physically motivated Oscillator functions to describe physical nature of optical constants with minimal parameters

Layer # 1 = [Gen-Osc](#) Thickness # 1 = [64.74 nm](#)  
[Add Oscillator](#) [Show Dialog](#) Fast Gaussian Calc = [ON](#)  
 E<sub>inf</sub> = [0.271](#) (fit)  
 UV Pole Amp. = [0.0000](#) UV Pole En. = [11.000](#)  
 IR Pole Amp. = [0.0000](#)  
[Fit All](#) [Clear All](#) [Add Amp.](#) [Add Br.](#) [Add En.](#)  
 1: Type = [Tauc-Lorentz](#) Amp1 = [154.8000](#) (fit)  
 Br1 = [2.216](#) (fit) Eo1 = [3.723](#) (fit) Eg1 = [1.276](#) (fit) Common Eg = [OFF](#)





# MODEL COMPARISON

Metals

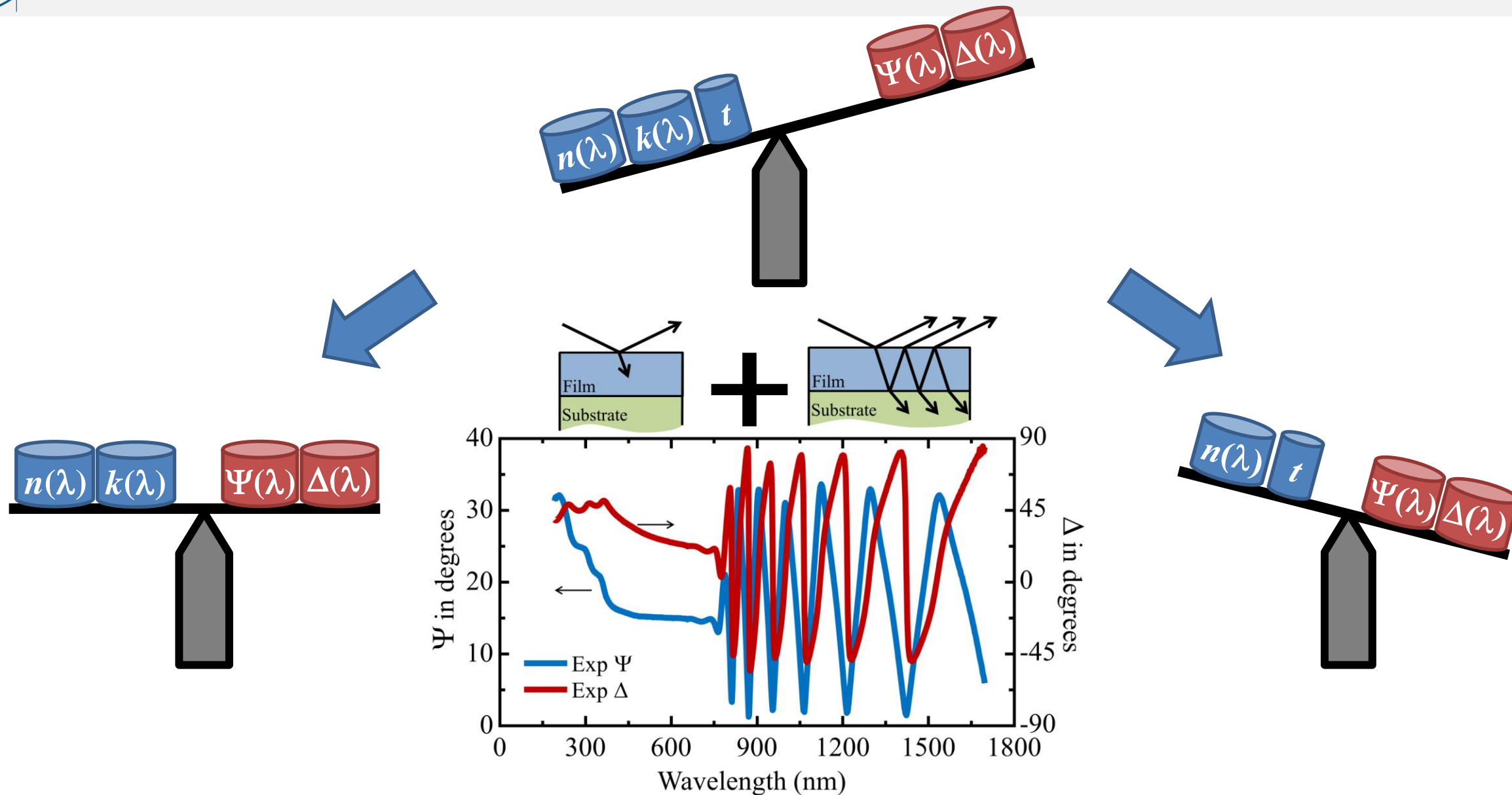
Organics  
Semiconductors

Dielectrics  
Semiconductors

Model	Advantages	Disadvantages
<b>B-Spline</b>	<ul style="list-style-type: none"> <li>▪ Easy extension of transparent region.</li> <li>▪ Computationally efficient.</li> </ul>	<ul style="list-style-type: none"> <li>▪ Most Fit Parameters.</li> <li>▪ No physical basis – just “curve fitting”.</li> <li>▪ Can get lost.</li> </ul>
<b>KK B-Spline</b>	<ul style="list-style-type: none"> <li>▪ Fewer Fit Params. than B-Spline</li> <li>▪ May avoid getting lost.</li> <li>▪ Kramers-Kronig consistent.</li> </ul>	<ul style="list-style-type: none"> <li>▪ No physical basis for <math>\epsilon_2</math> – just “curve fitting”.</li> <li>▪ More Fit Params than Gen-Osc.</li> </ul>
<b>Gen-Osc</b>	<ul style="list-style-type: none"> <li>▪ Fewest Fit parameters.</li> <li>▪ Kramers-Kronig consistent</li> </ul>	<ul style="list-style-type: none"> <li>▪ Can be tedious.</li> <li>▪ May not capture all features in the data.</li> <li>▪ Oscillators lose physical meaning –become curve fitting.</li> </ul>



# STRATEGY: FILMS WITH ABSORBING REGION





# SIMPLIFIED AND AUTOMATED B-SPLINE PROCEDURE

III

Fit Transparent Region with Cauchy

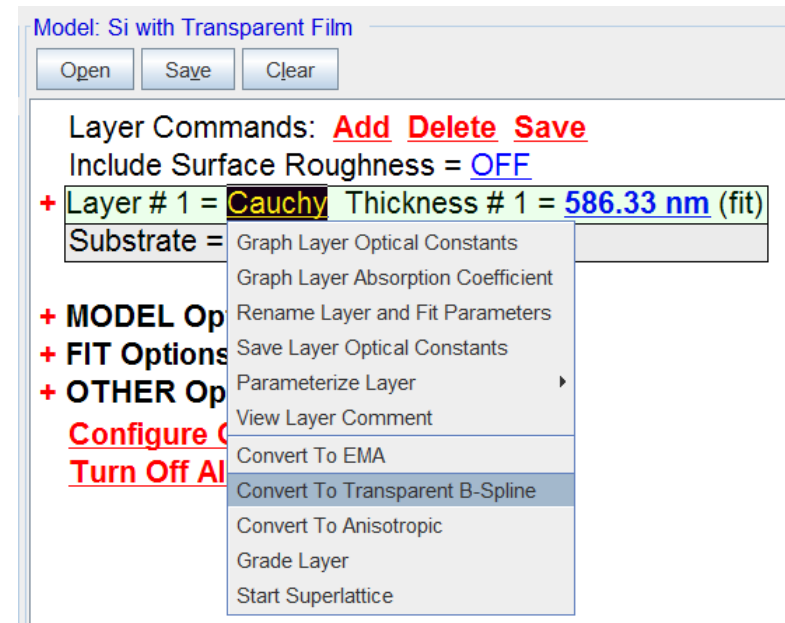


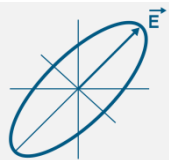
Right-Click on Cauchy ►  
“Convert to Transparent B-Spline”



Optimize Node Resolution, Roughness,  
Grading,...

CAUCHY ►  
Convert to  
Transparent B-Spline





# Gen-Osc Layer

- Substrate = [Gen-Osc](#)

**Show Dialog**

## - e1 Components

Einf = [1.000](#)

UV Pole Amp. = [0.000](#) UV Pole En. = [11.000](#)

IR Pole Amp. = [0.000](#)

## - e2 Components

Oscillator Menu: [Add](#) [Delete](#) [Delete All](#)

Fit Menu: [All](#) [None](#) [Amp.](#) [Br.](#) [En.](#)

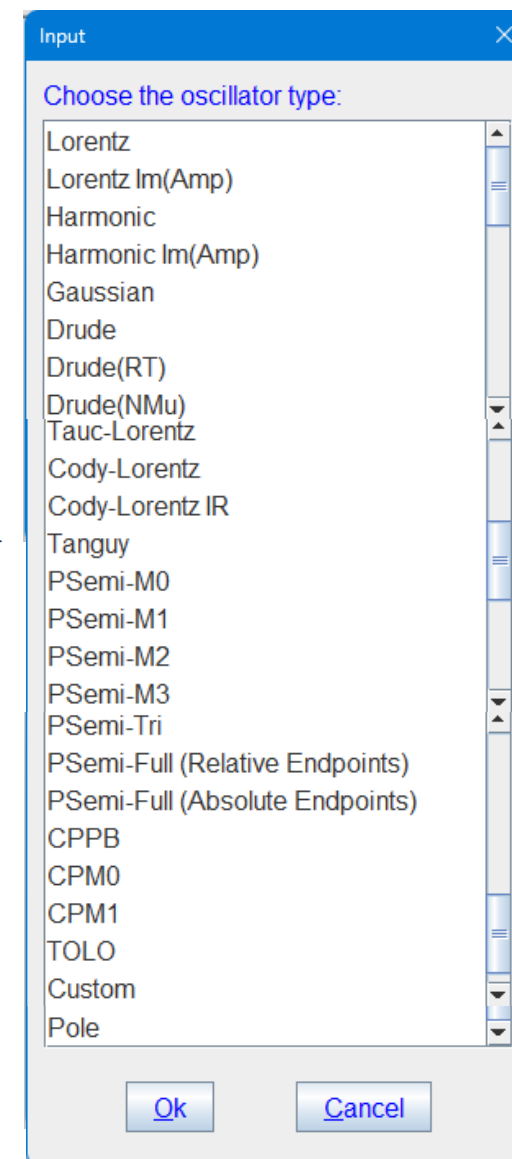
1: Type = [Gaussian](#) Amp1 = [10.000000](#) Br1 = [0.1000](#) En1 = [3.000](#)

## e1 - Einf & Poles:

Describes the effect on  $\epsilon_1$  from out-of-range absorptions

## e2 - Oscillator List:

Describe absorptions within the analysis range, affecting  $\epsilon_2$  and KK transformed  $\epsilon_1$  shape





# CHOOSING THE BEST APPROACH



II

Build Gen-Osc from  
Tabulated Reference

III

Cauchy ► B-Spline



Build Gen-Osc from  
B-Spline  $n, k$

I



Fit Data with  
Pre-built Gen-Osc

Fit Data with Gen-  
Osc



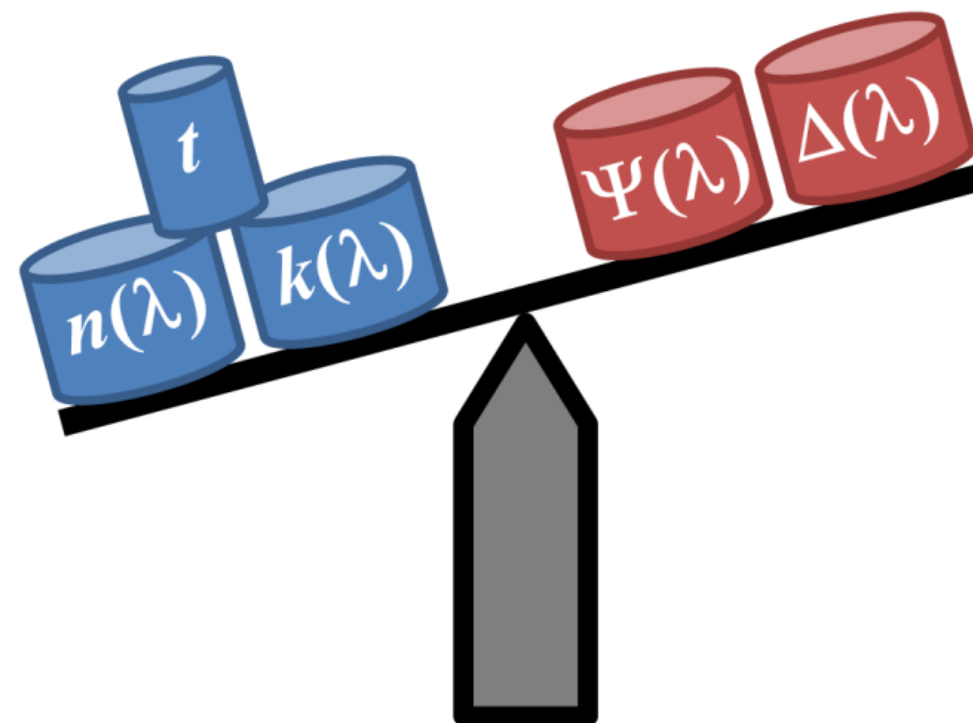
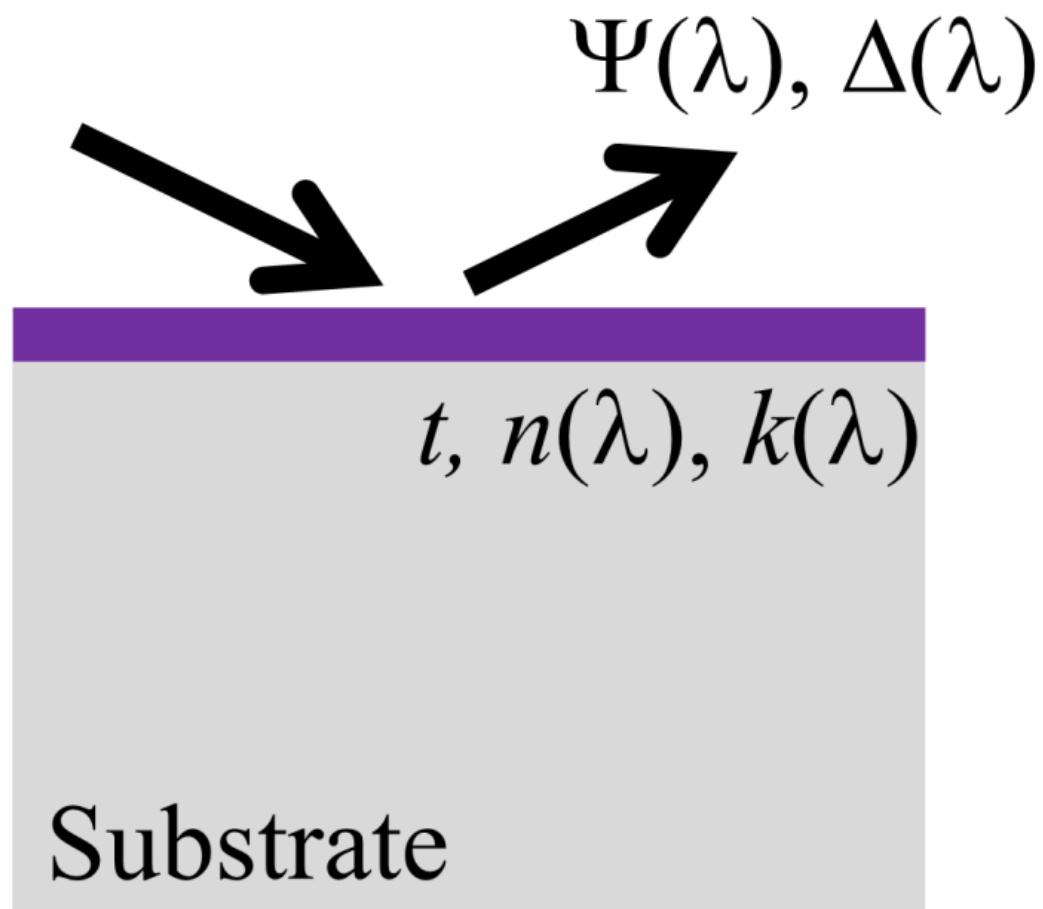
Fit Data with Gen-  
Osc





# ABSORBING MATERIAL CHALLENGE

- Need to determine thickness,  $n$  and  $k$ !





# STRATEGIES

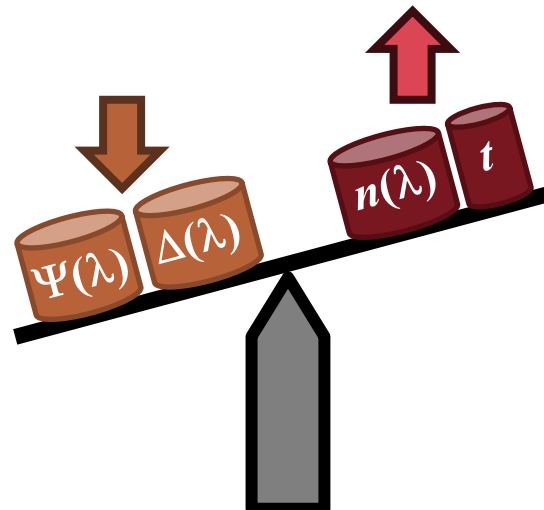
## Increase measurement content

- Multi-angle interference enhancement
- SE + Transmission
- Multi-sample
- In situ (Real-Time)

## ■ OTHER TECHNIQUES

## Reduce sample unknowns

- Opaque materials
- Transparent wavelengths
- Dispersion equation

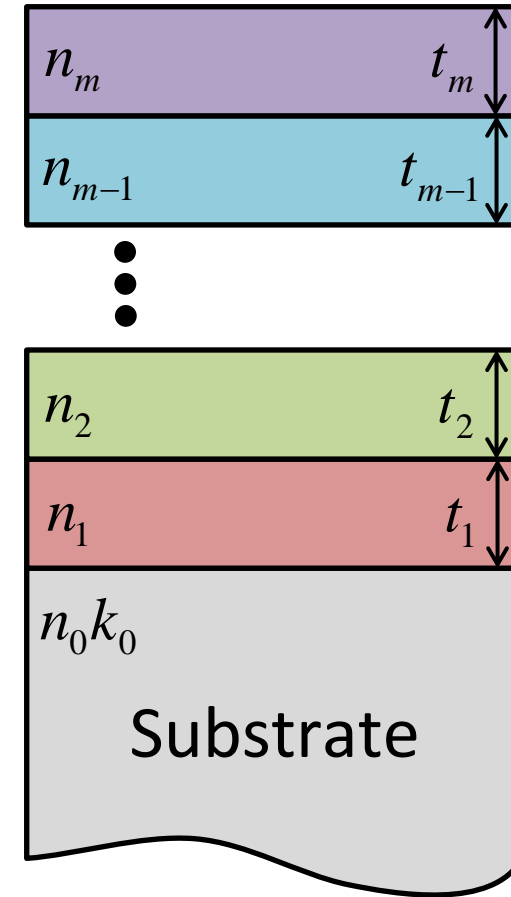
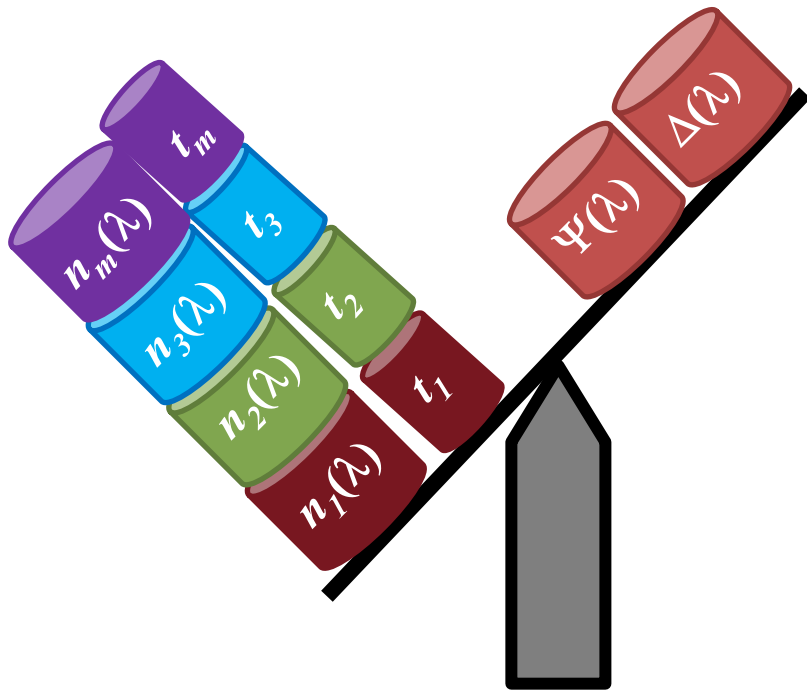


J.N. Hilfiker, et al. "Survey of methods to characterize thin absorbing films with spectroscopic ellipsometry" *Thin Solid Films* **516** (2008) 7979-7989.



# MULTILAYER STACK CHALLENGE

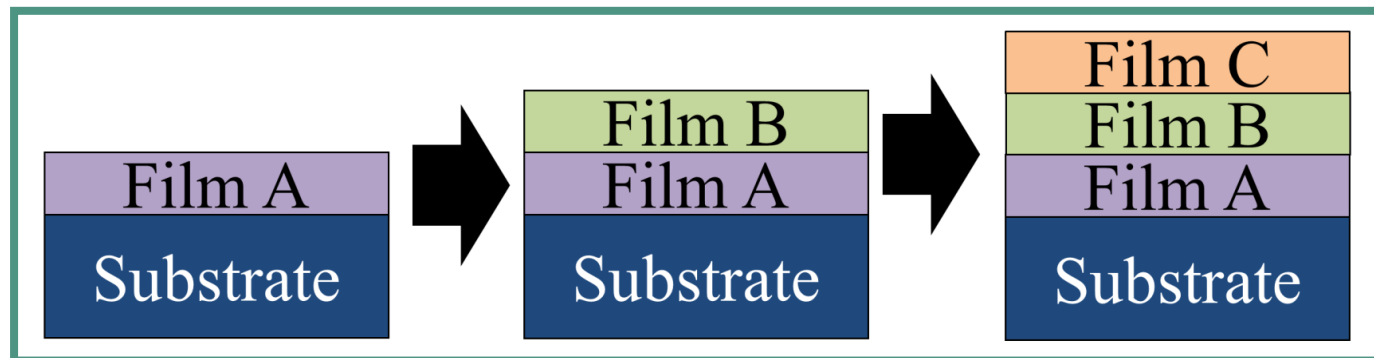
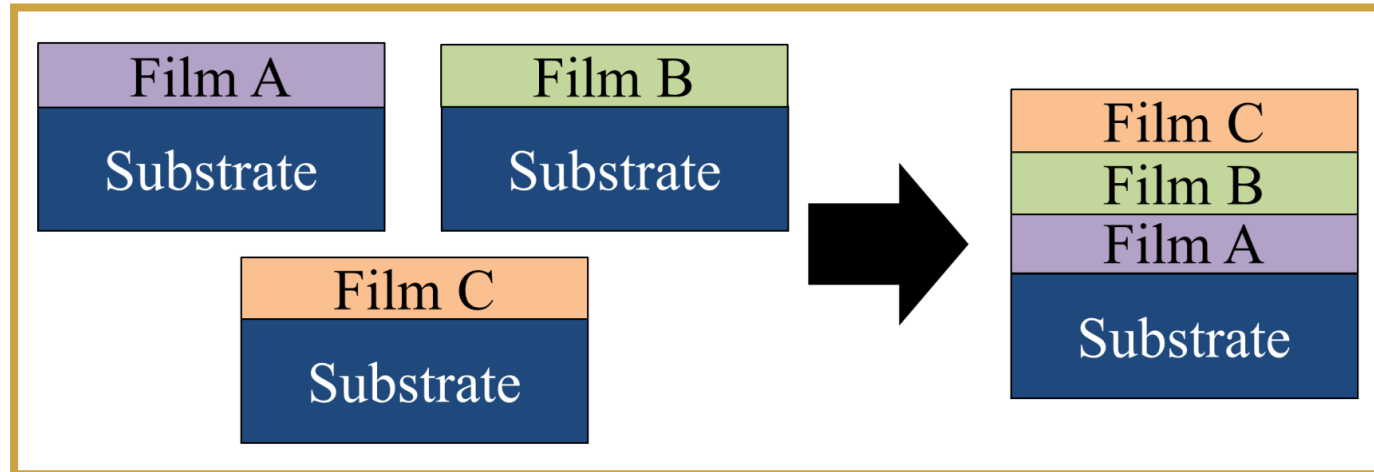
- Multilayer applications lead to excessive unknowns!





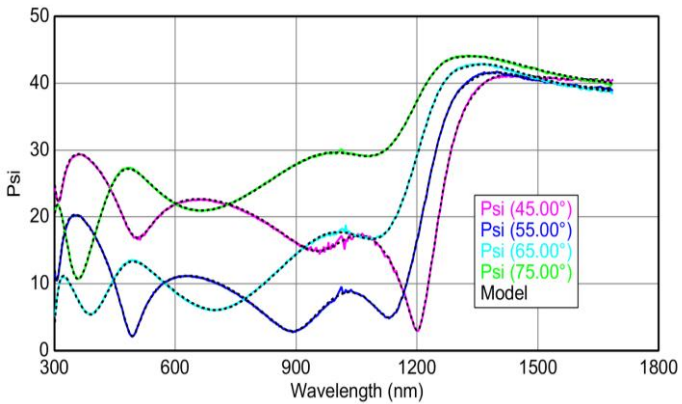
# MULTILAYER STACKS

- Solution: Determine optical constants from single layers.

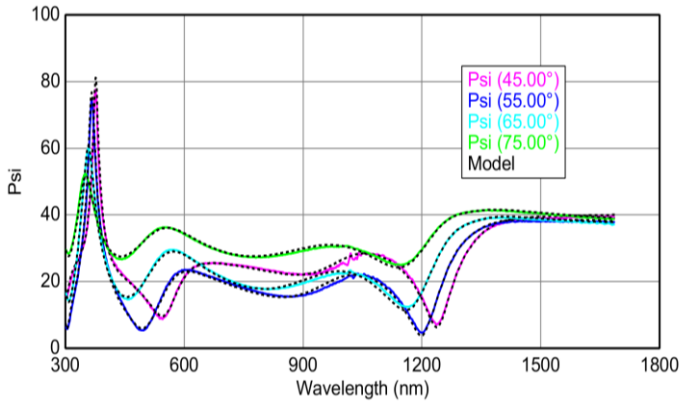




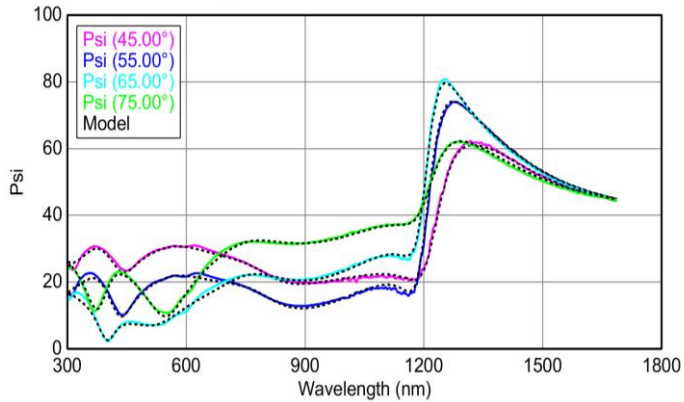
# MULTILAYERS - OLED



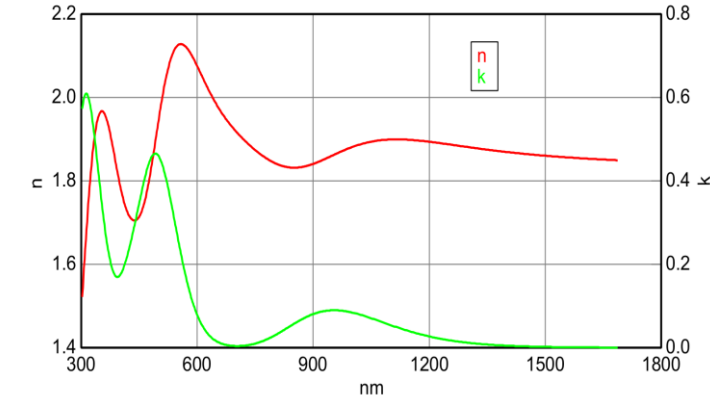
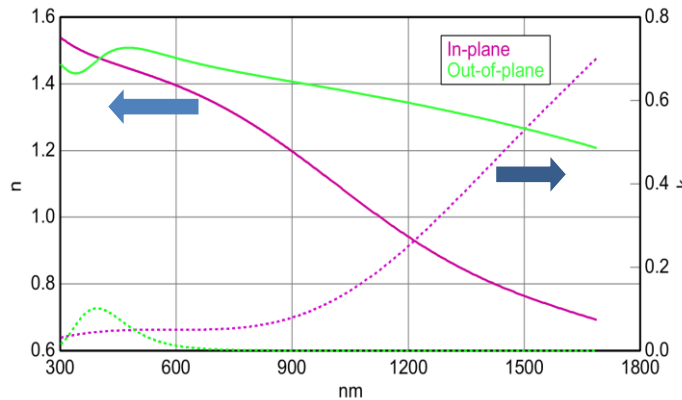
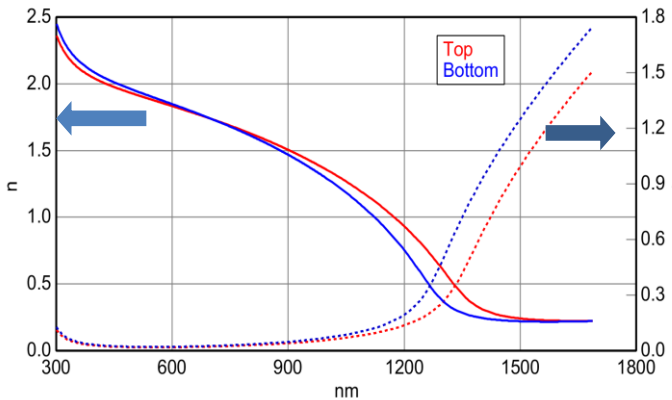
Opt. Const. of ITO



Opt. Const. of PEDOT



Opt. Const. of Active Layer





# FINAL PRACTICE SET

## [6-06] Quiz: Dielectric on Si

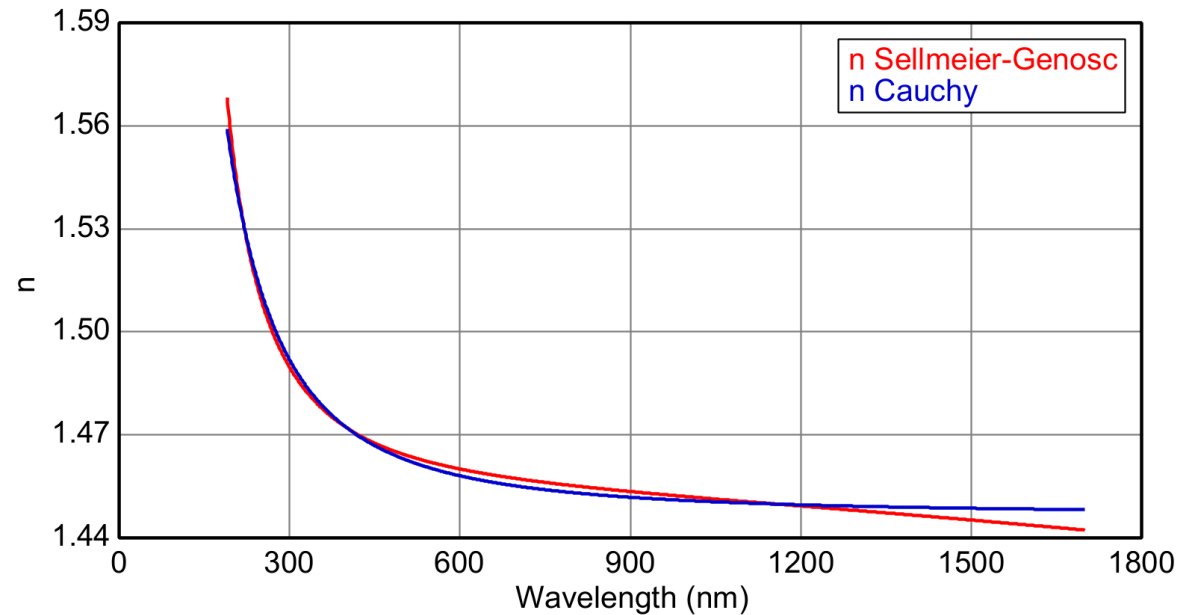
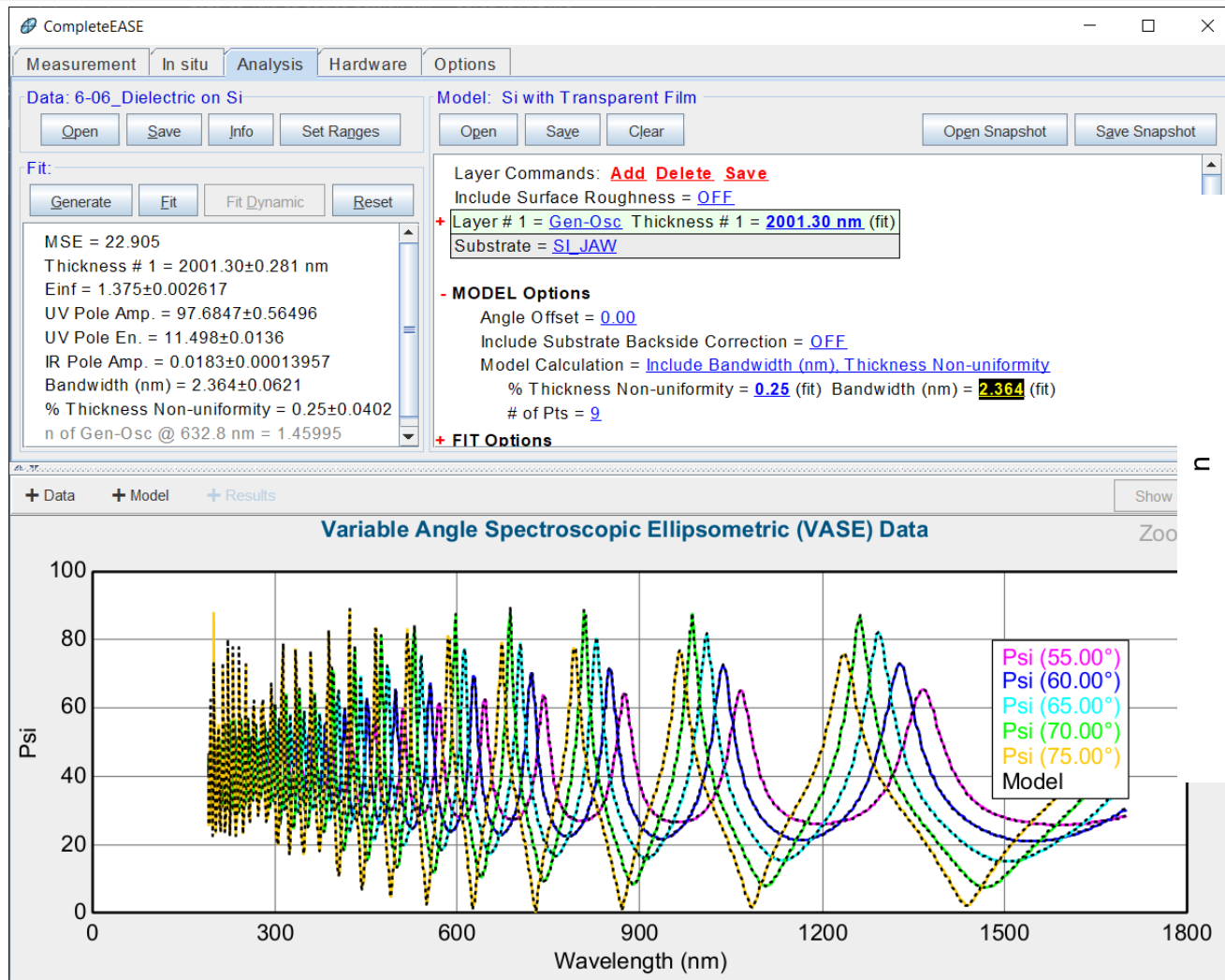
- Determine thickness and optical constants over full wavelength range.

What Model Approaches  
to use?





# 6-06 DIELECTRIC ON SI: RESULTS



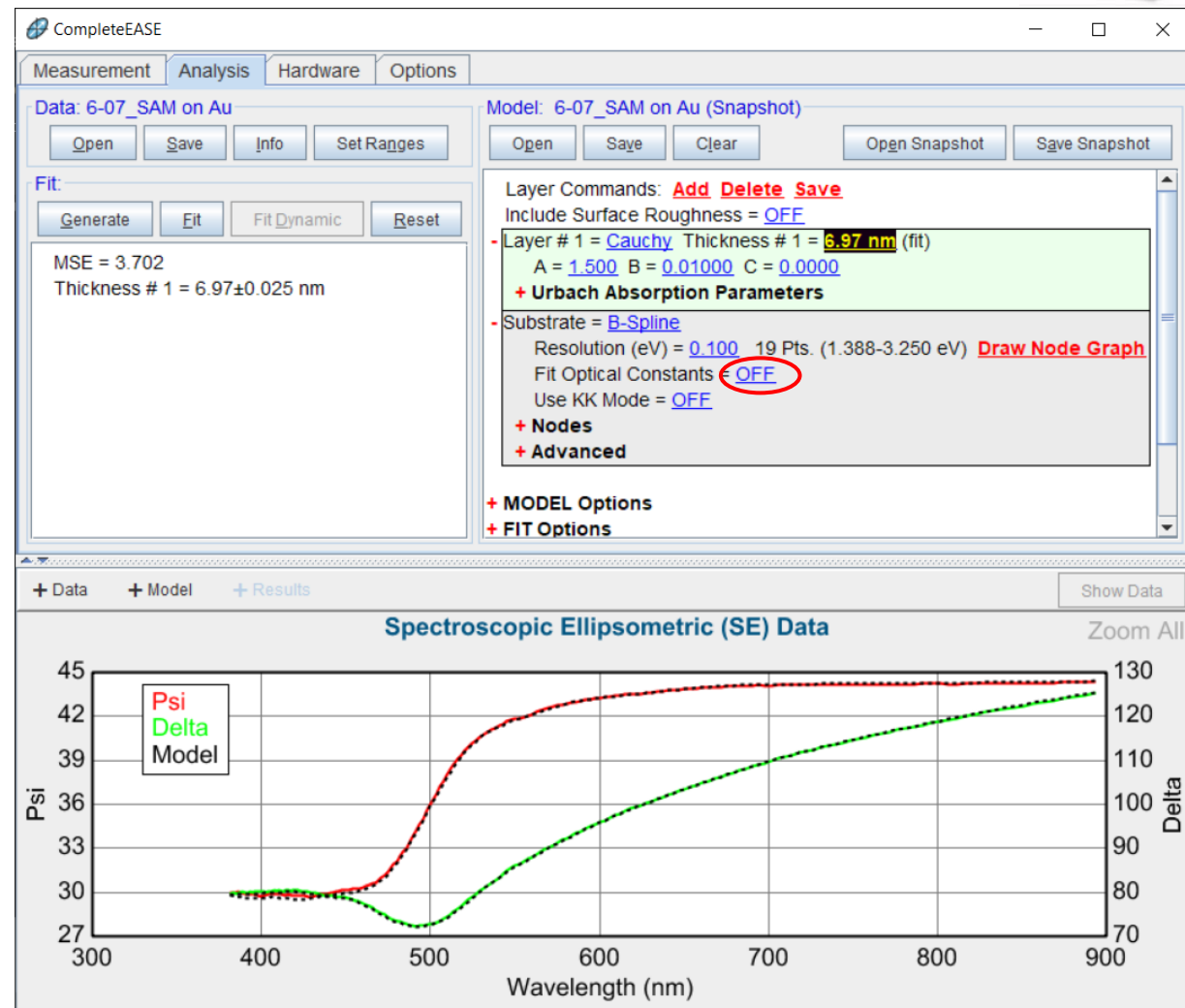
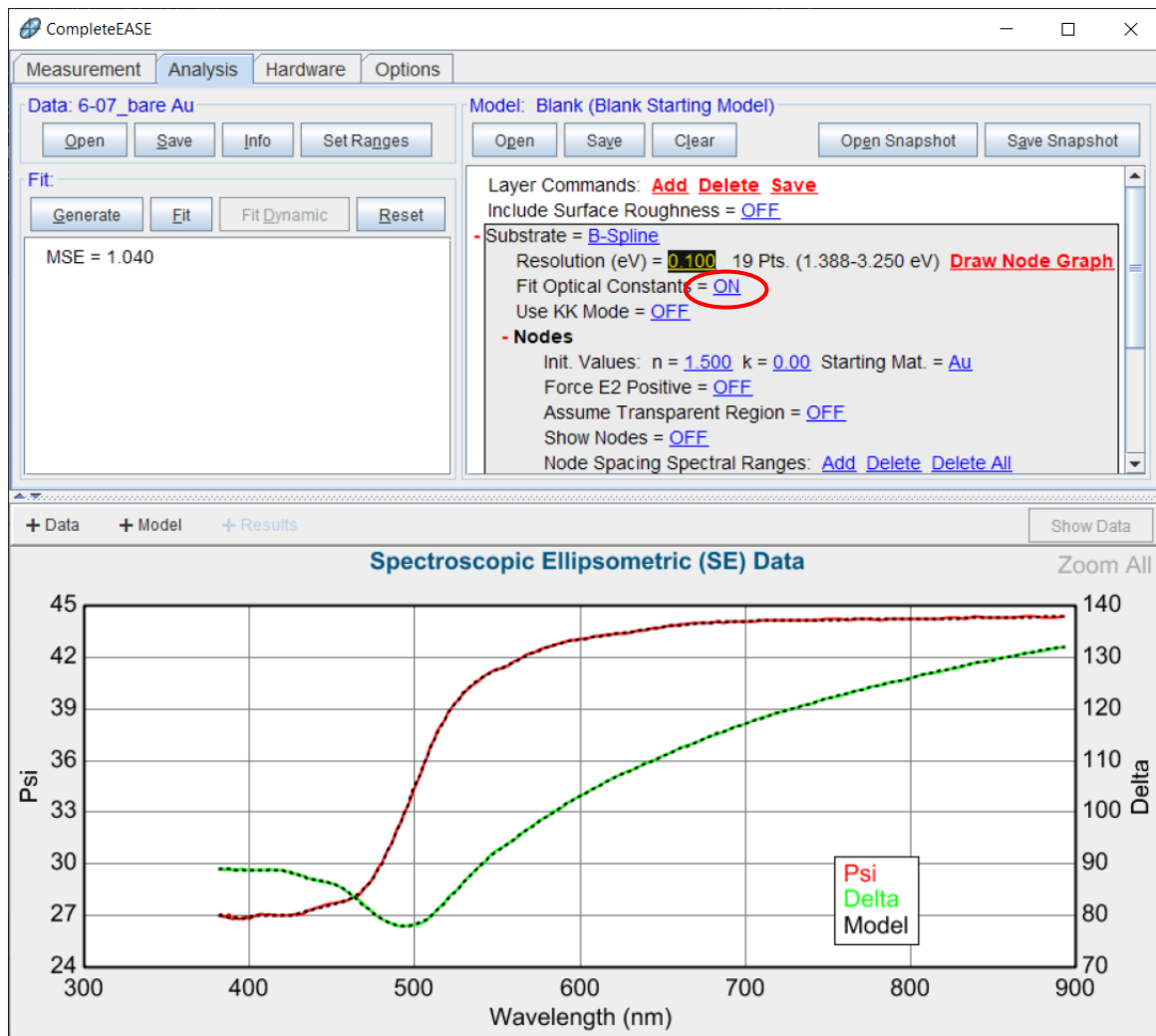
## [6-07] Quiz: Self-Assembled monolayer on Au

- **Determine thickness of SAM layer.**

What Model Approaches  
to use?



# 6-07 SAM ON AU: RESULTS



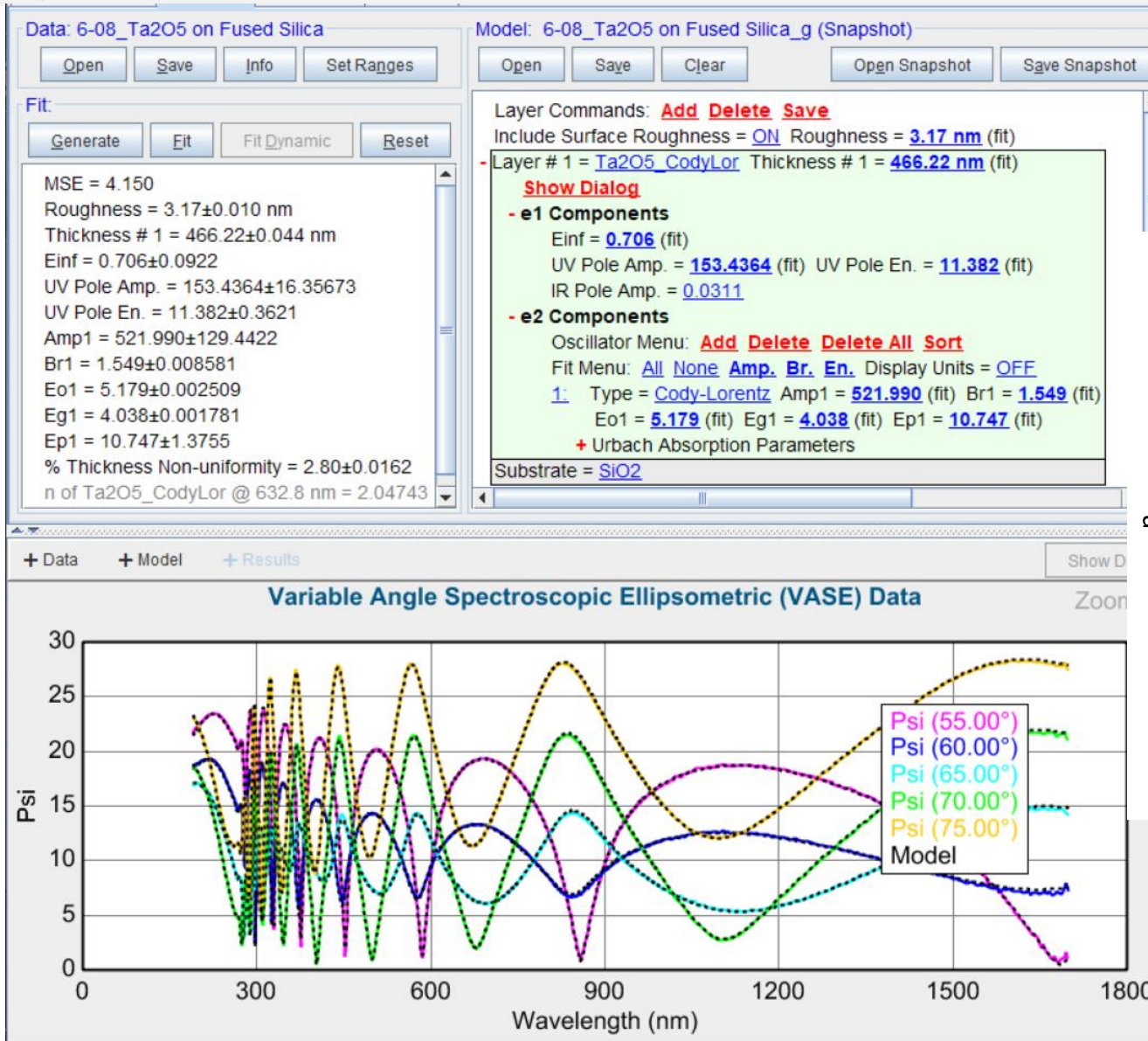
## [6-08] Quiz: Ta<sub>2</sub>O<sub>5</sub> on Fused Silica

- Use “SiO2.mat” for substrate
- Determine optical constants for Ta<sub>2</sub>O<sub>5</sub> film

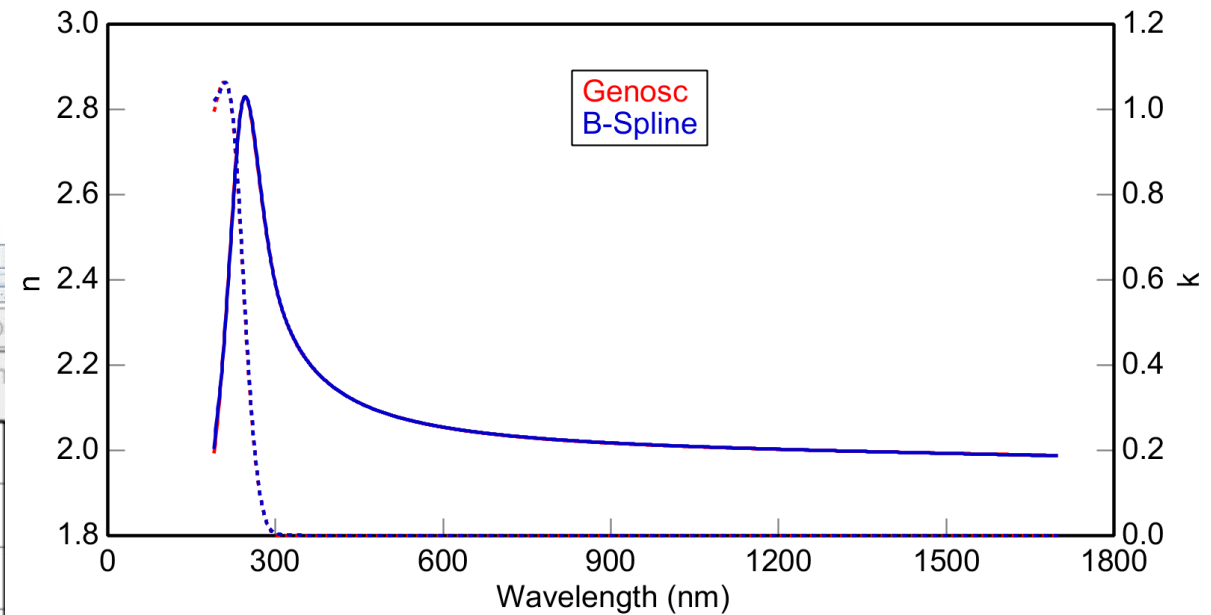
What Model Approaches  
to use?



# 6-08 TA<sub>2</sub>O<sub>5</sub> ON FS: RESULTS



Optical Constants of Ta2O5



A word cloud featuring the phrase "Thank You" in numerous languages, centered on a solid blue background. The words are rendered in white, with varying font sizes and orientations. The largest and most prominent words are "Thank" and "You". Other visible words include "Maake", "Asante", "Shukria", "Dhanyavadagalu", "Manana", "Dankon", "Kiitos", "Mauruuru", "Biyan", "Dank Je", "Suksama", "Vinaka", "Dankscheen", "спасибо", "kösönöm", "Dziakuje", "Juspaxar", "Arigato", "Chokrane", "Diolch i Chi", "Gratias Tibi", "Terima Kasih", "Grazie", "Taiku", "Najis Tuke", "Matur Nuwun", "Gracias", "cảm ơn bạn", "Tack", "Kop Khun Khap", "Paldies", "Obrigado", "Eskerrik Asko", "Tingki", "Raibh Maith Agat", "Go", "Salamat", "Merci", "Di Ou Mèsi", "Hvala", "Děkuji", "Grazas", "धन्यवाद", "Dakujem", "Bedankt", "Ua Tsaug Rau Koj", "Nirringrazzjak", "Rahmat", "谢", "Xbala", "Danke", "Maake", "Kiitos", "Mauruuru", "Biyan", "Arigato", "Chokrane", "Diolch i Chi", "Gratias Tibi", "Terima Kasih", "Grazie", "Taiku", "Najis Tuke", "Matur Nuwun", "Gracias", "cảm ơn bạn", "Tack", "Kop Khun Khap", "Paldies", "Obrigado", "Eskerrik Asko", "Tingki", "Raibh Maith Agat", "Go", "Salamat", "Merci", "Di Ou Mèsi", "Hvala", "Děkuji", "Grazas", "धन्यवाद", "Dakujem", "Bedankt", "Ua Tsaug Rau Koj", "Nirringrazzjak", "Rahmat", "谢", "Xbala", "Danke".