ABSORBING FILMS USING B-SPLINE

SESSION 3

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COURSE OUTLINE

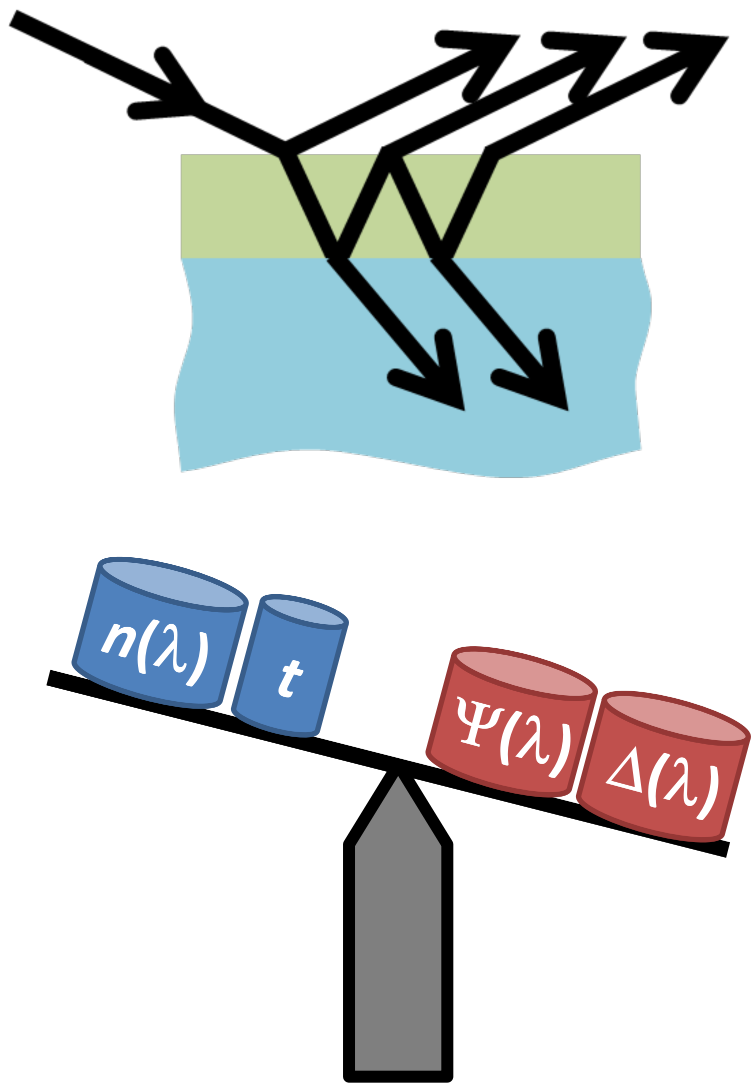
- Session 1: Introduction to CompleteEASE
- Session 2: Transparent Materials
- Session 3: Absorbing Films using B-Spline
- Session 4: Semi-Absorbing Films using Gen-Osc
- Session 5: Thin Absorbing Films & Multi-Sample Analysis
- Session 6: Advanced Topics and Review

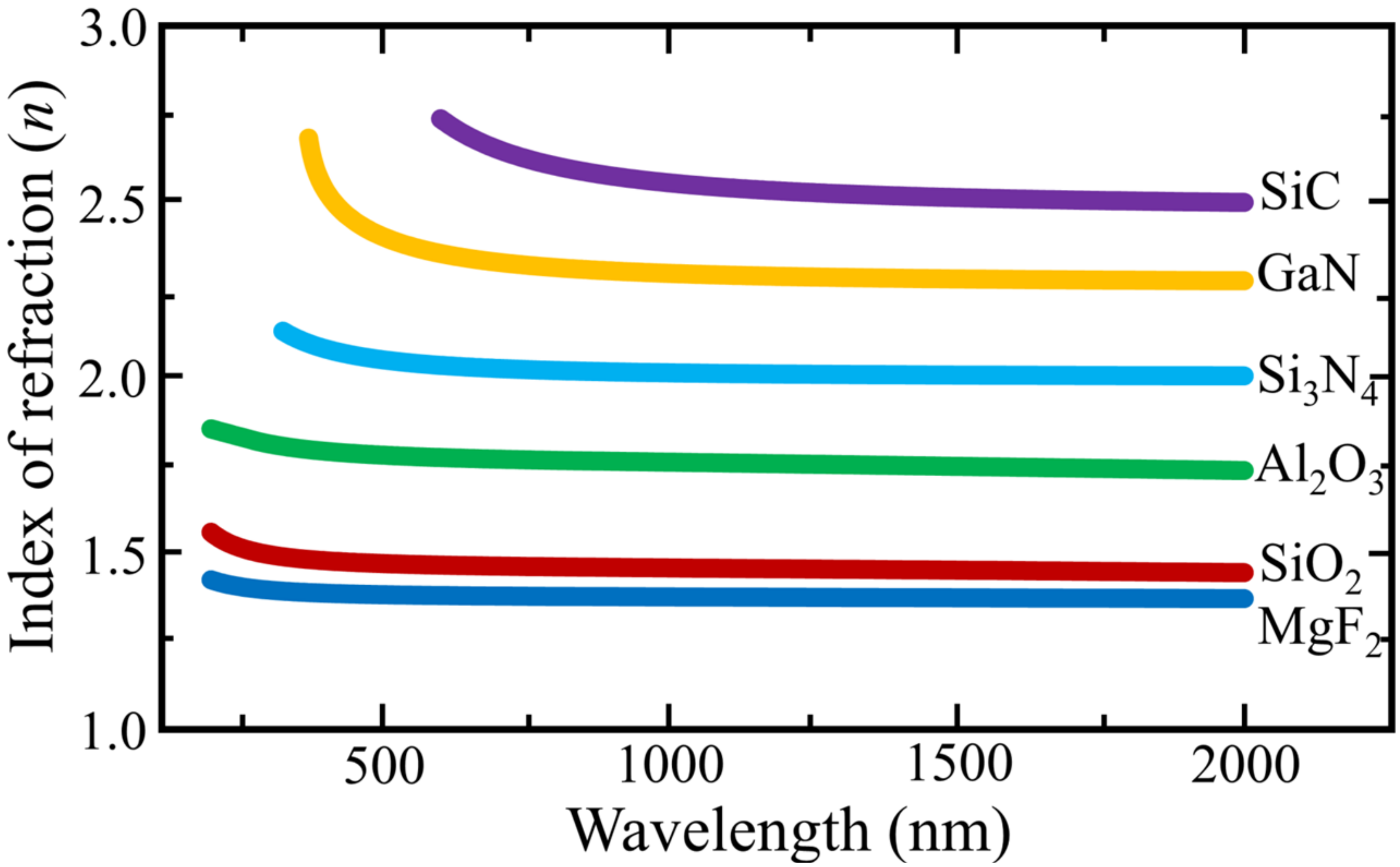
SESSION 3 OUTLINE

- Review of Transparent Materials
- B-Spline Math
- B-Spline Layer
- B-Spline for Absorbing Materials
  - Metal Films
  - UV Absorbing Films
- Kramers-Kronig (KK) B-Spline

QUICK REVIEW

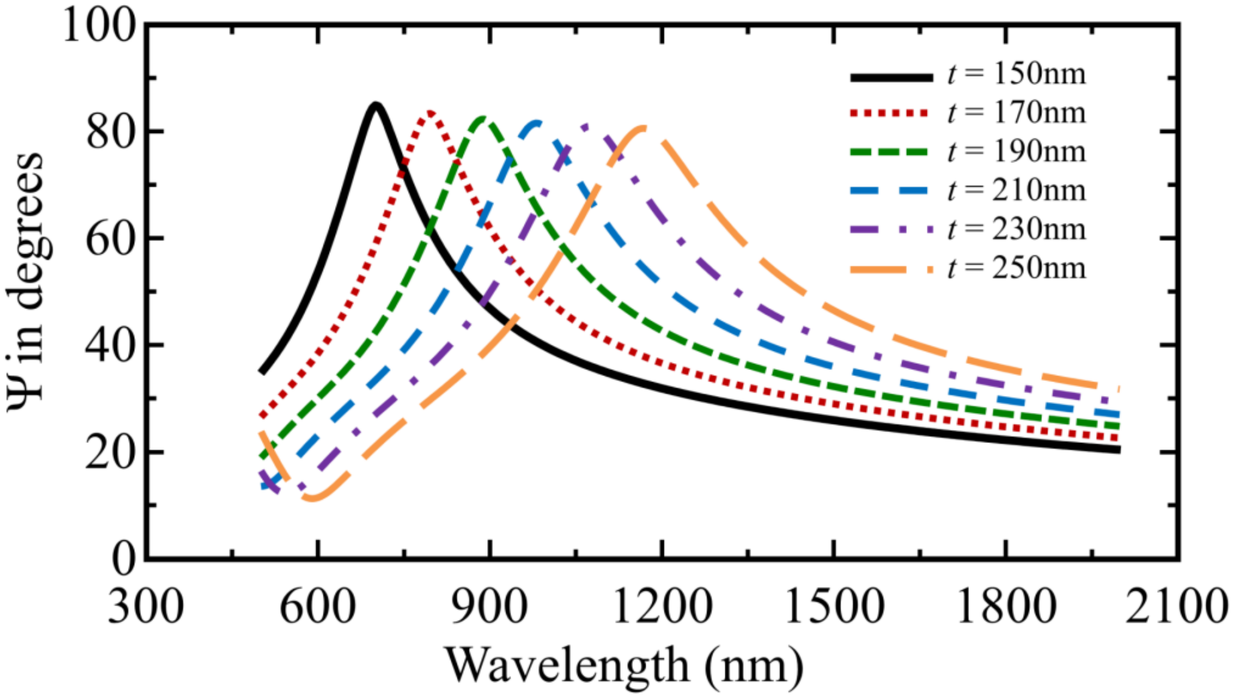
TRANSPARENT MATERIALS



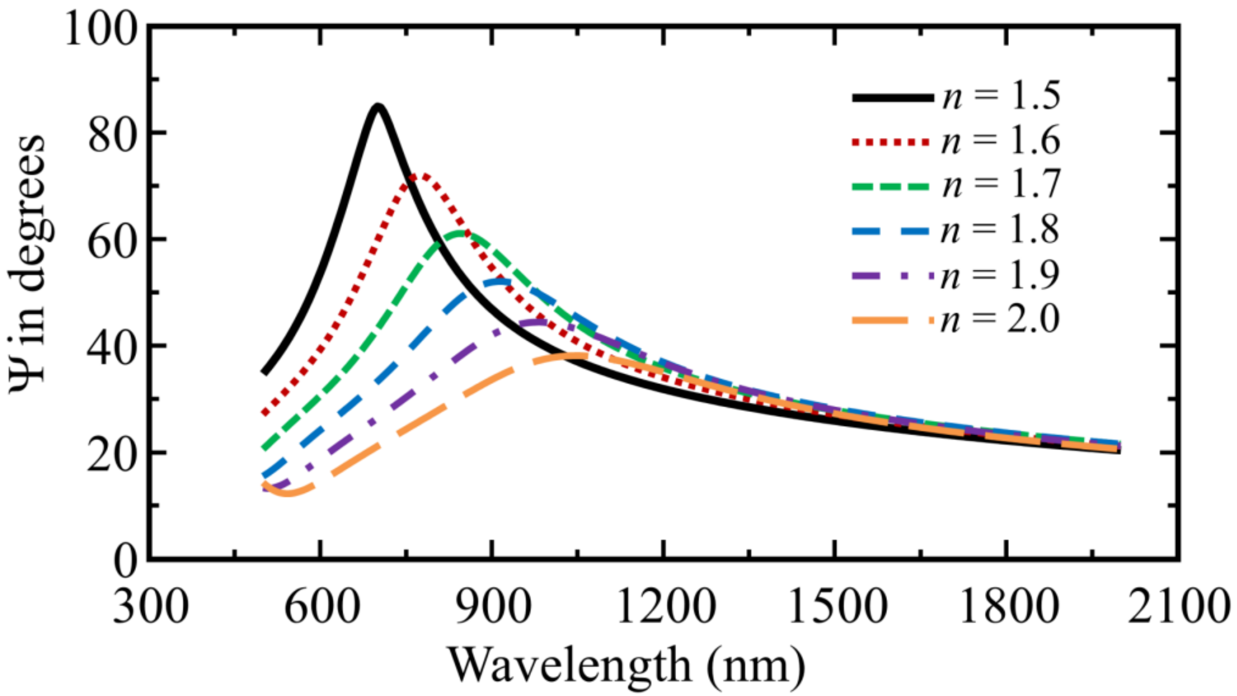


TRANSPARENT THIN FILMS

Thickness shifts interference

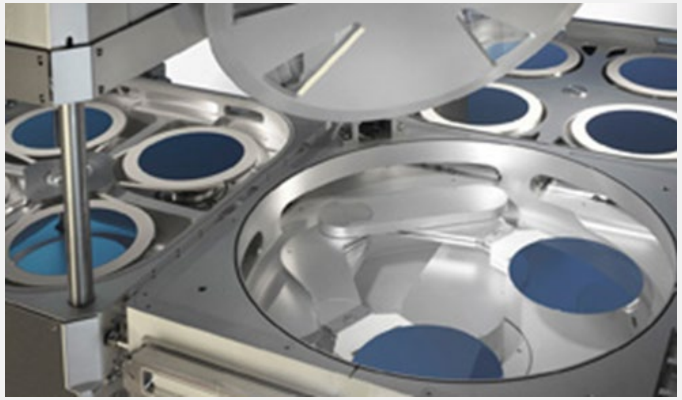


Index also affects amplitude



3-1_Oxynitride_on_Si.SE

- Determine thickness and index
- Review of procedure from Session 2



Estimate Thickness & Index

↓

Fit Thickness & Cauchy Parameters

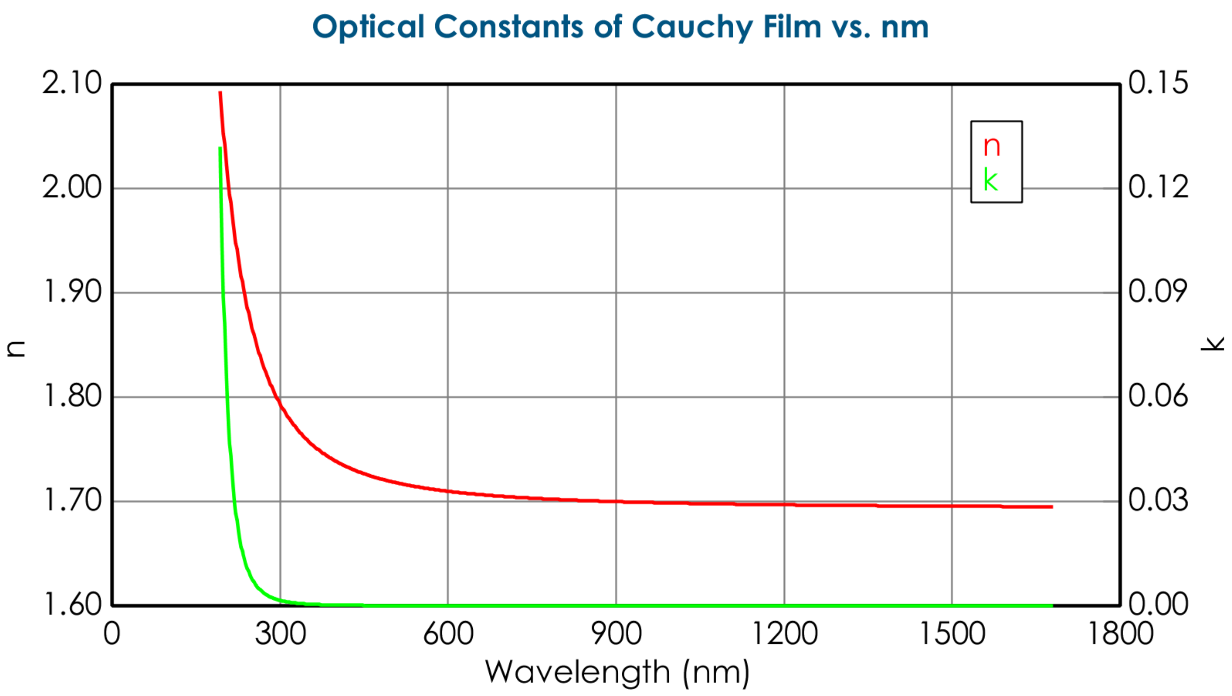
↓

Add roughness, grading, anisotropy, absorption?

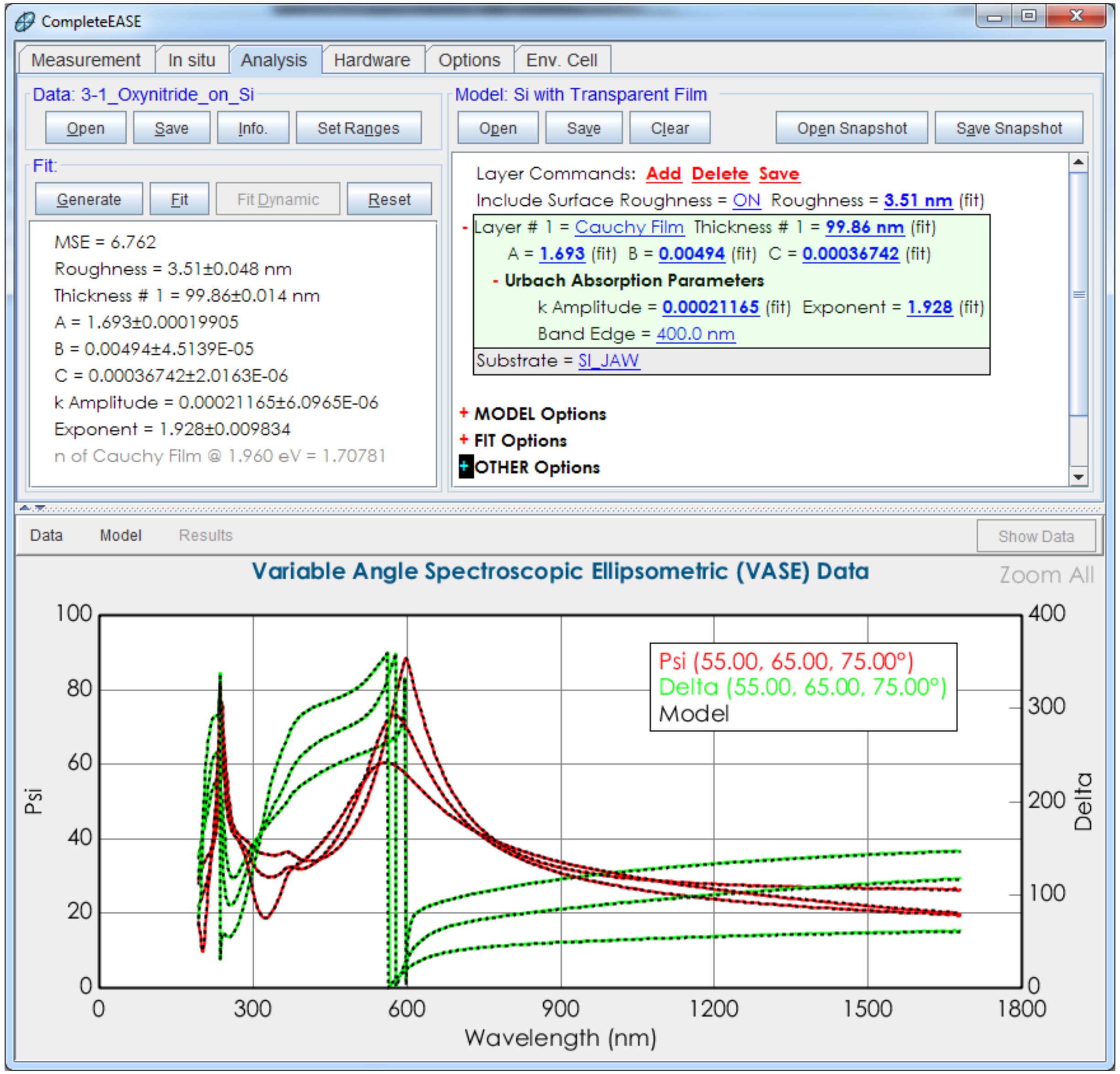
Si with Transparent Film.mod

HINT:
Try Alternate Models

RESULTS



Optical Constants of Cauchy Film vs. nm
n
k
2.10
2.00
1.90
1.80
1.70
1.60
0.15
0.12
0.09
0.06
0.03
0.00
0
300
600
900
1200
1500
1800
Wavelength (nm)



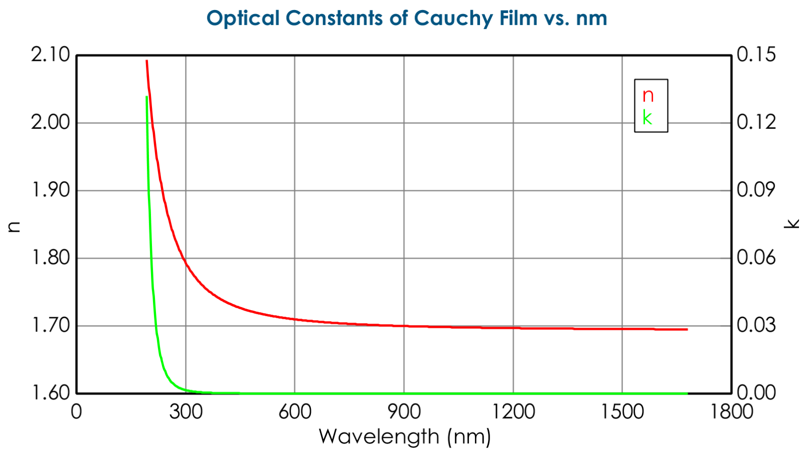
CompleteEASE
Measurement
In situ
Analysis
Hardware
Options
Env. Cell
Data: 3-1_Oxynitride_on_Si
Open
Save
Info.
Set Ranges
Model: Si with Transparent Film
Open
Save
Clear
Open Snapshot
Save Snapshot
Fit:
Generate
Fit
Fit Dynamic
Reset
MSE = 6.762
Roughness = 3.51±0.048 nm
Thickness # 1 = 99.86±0.014 nm
A = 1.693±0.00019905
B = 0.00494±4.5139E-05
C = 0.00036742±2.0163E-06
k Amplitude = 0.00021165±6.0965E-06
Exponent = 1.928±0.009834
n of Cauchy Film @ 1.960 eV = 1.70781
Layer Commands: Add Delete Save
Include Surface Roughness = ON Roughness = 3.51 nm (fit)
Layer # 1 = Cauchy Film Thickness # 1 = 99.86 nm (fit)
A = 1.693 (fit) B = 0.00494 (fit) C = 0.00036742 (fit)
Urbach Absorption Parameters
k Amplitude = 0.00021165 (fit) Exponent = 1.928 (fit)
Band Edge = 400.0 nm
Substrate = SI_JAW
+ MODEL Options
+ FIT Options
+ OTHER Options
Data
Model
Results
Show Data
Variable Angle Spectroscopic Ellipsometric (VASE) Data
Zoom All
Psi (55.00, 65.00, 75.00°)
Delta (55.00, 65.00, 75.00°)
Model
Psi
Delta
100
80
60
40
20
0
400
300
200
100
0
0
300
600
900
1200
1500
1800
Wavelength (nm)

URBACH ABSORPTION PARAMETERS

- k Amplitude
  - Often the only fit parameter needed
  - Controls amplitude of the exponential tail
- Exponent
  - Controls shape of the tail
  - Default value often ok
- Band Edge
  - Specifies point at which k = k Amp
  - Typically set to shortest λ (not critical)
  - Only rescales other parameters
  - Not fittable

- Substrate = Cauchy
  A = 1.450 B = 0.01000 C = 0.0000
  - **Urbach Absorption Parameters**
    k Amplitude = 0.0000 Exponent = 1.500
    Band Edge = 400.0 nm

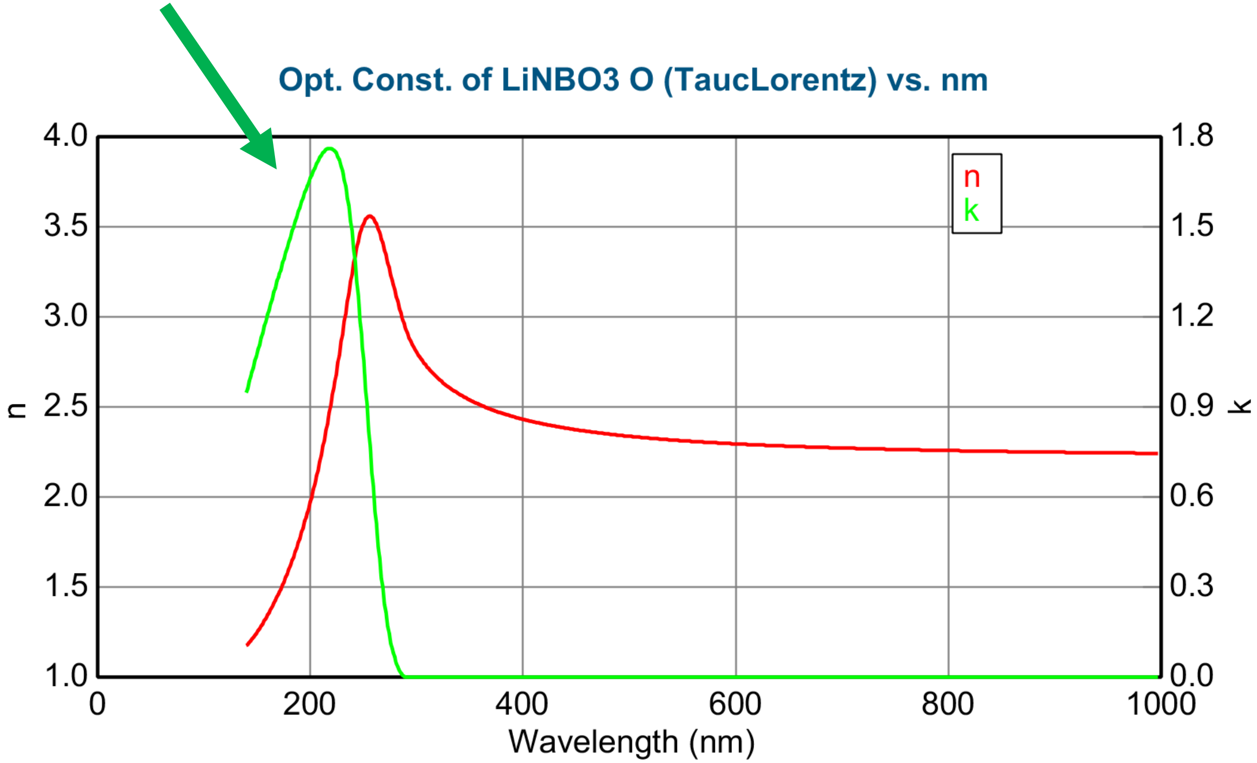
$$n(\lambda) = A + \frac{B}{\lambda^2} + \frac{C}{\lambda^4}$$
$$k = k\_Amplitude \cdot e^{Exponent(E - Band\_Edge)}$$



URBACH ABSORPTION

- Advantages
  - Easy to use
  - Works well for absorption tail
- Disadvantages
  - Cannot be used for complex absorption
  - Not Kramers-Kronig consistent

Would Urbach work here?



MODELING DIFFERENT MATERIALS

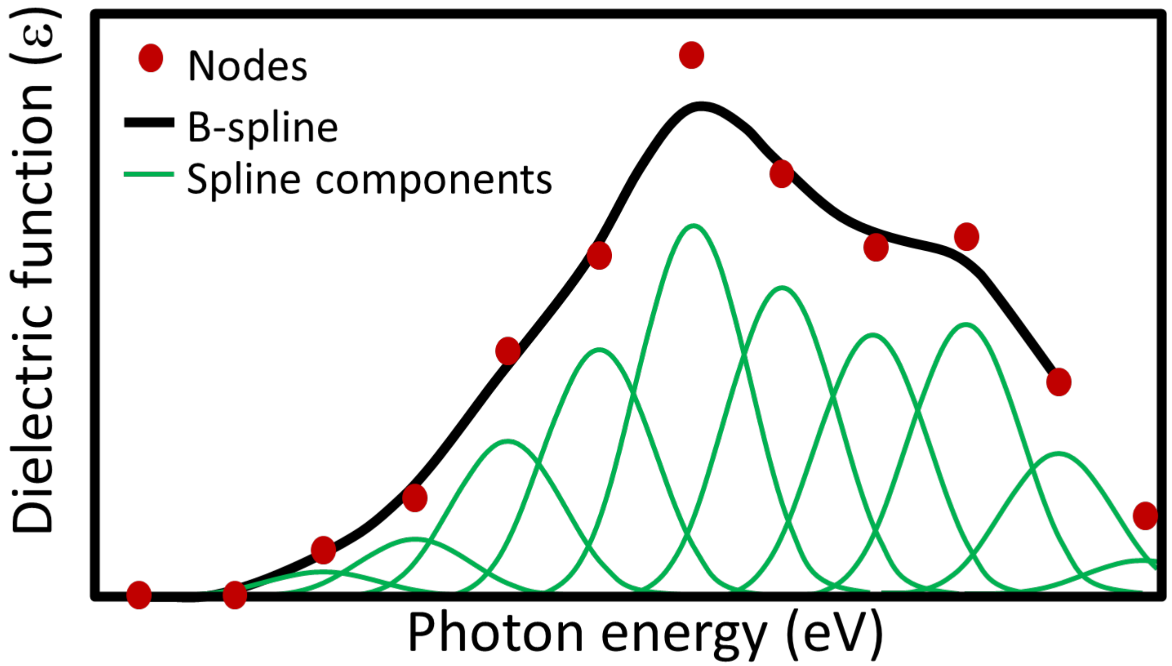
For purpose of SE, we have 3 general categories:

Transparent

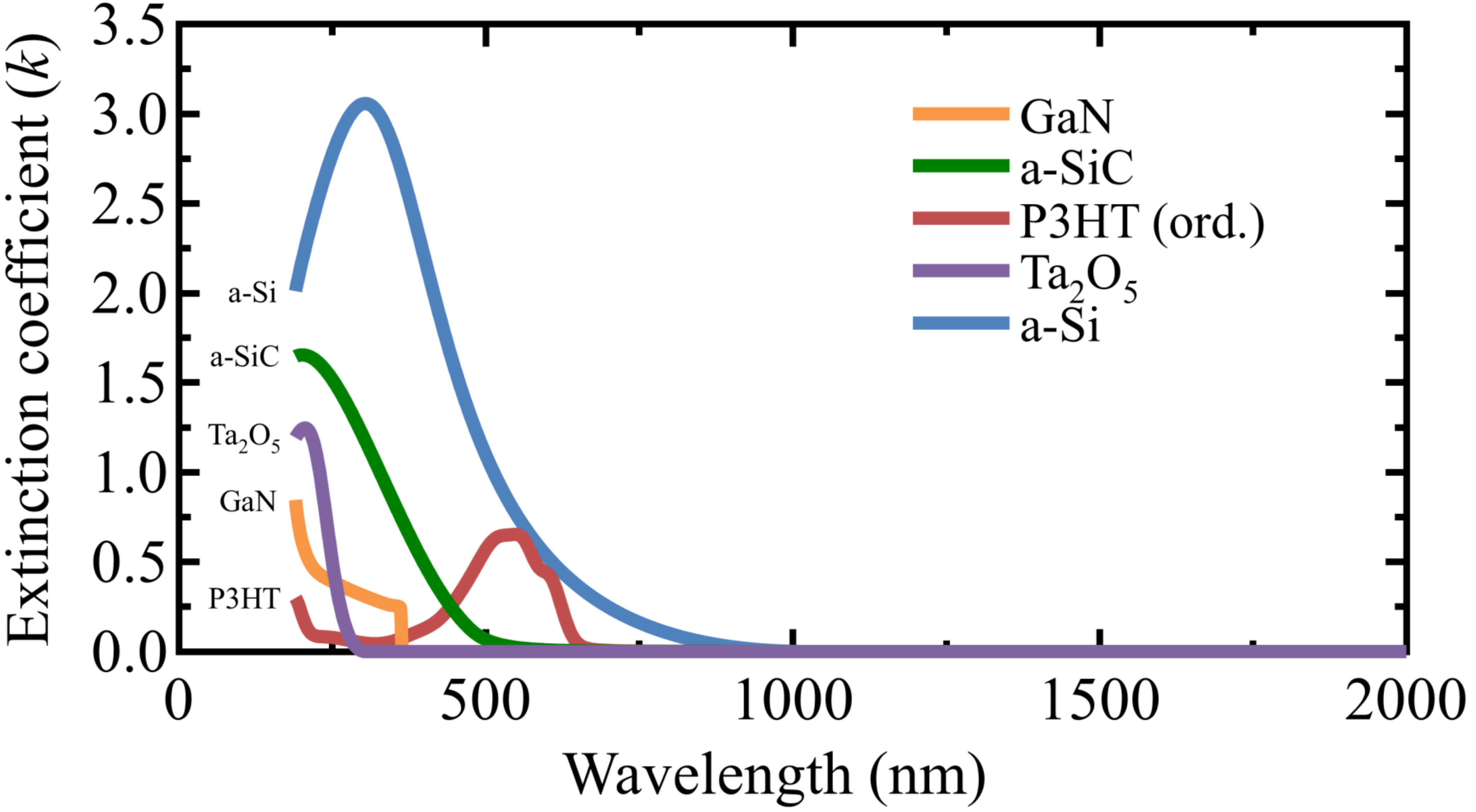
Absorbing Regions

Absorbing

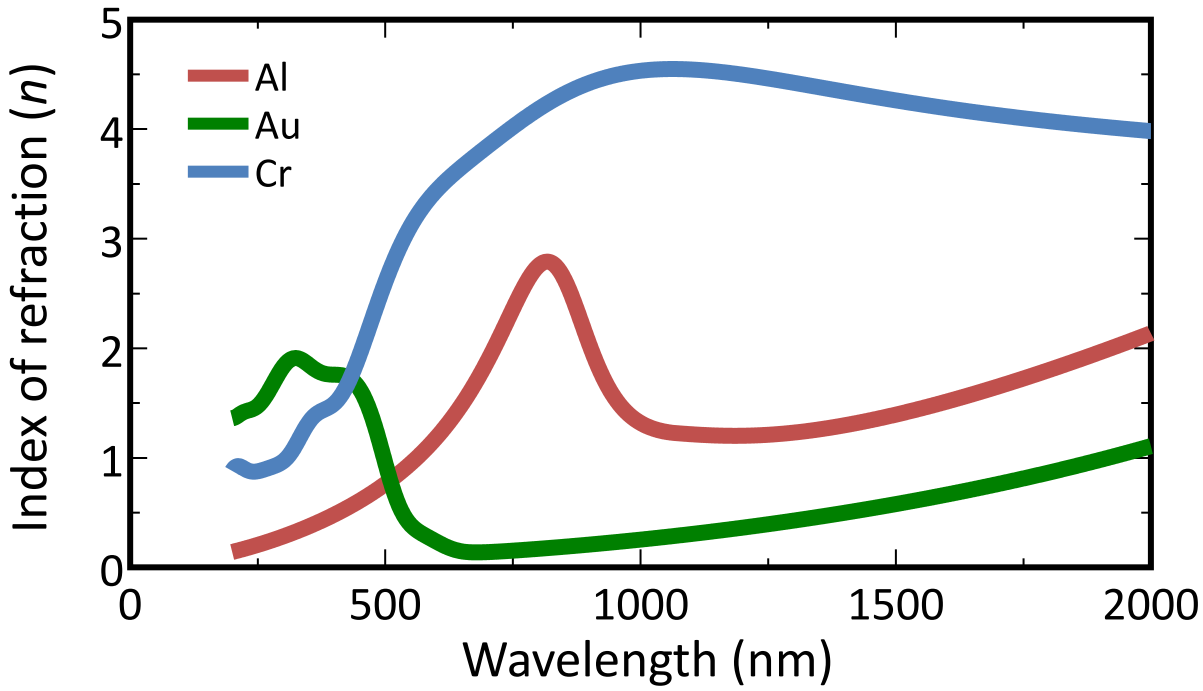
NEW TOOL: B-SPLINE

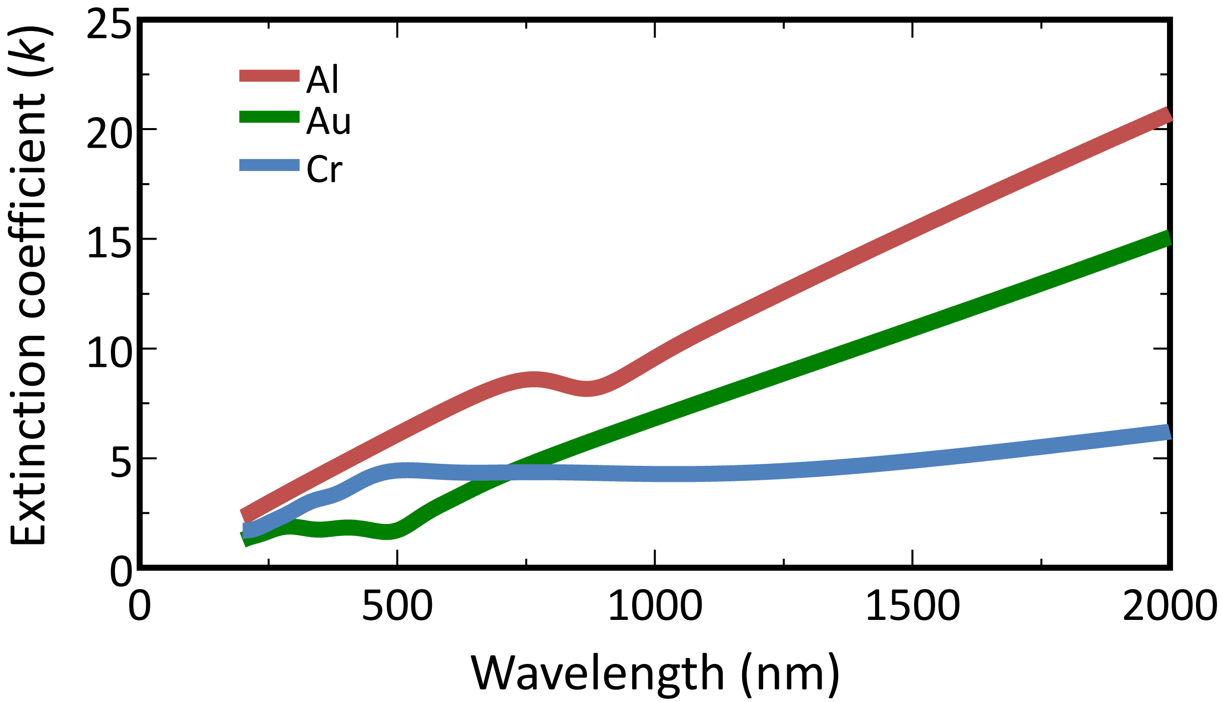


MATERIALS WITH ABSORBING REGIONS

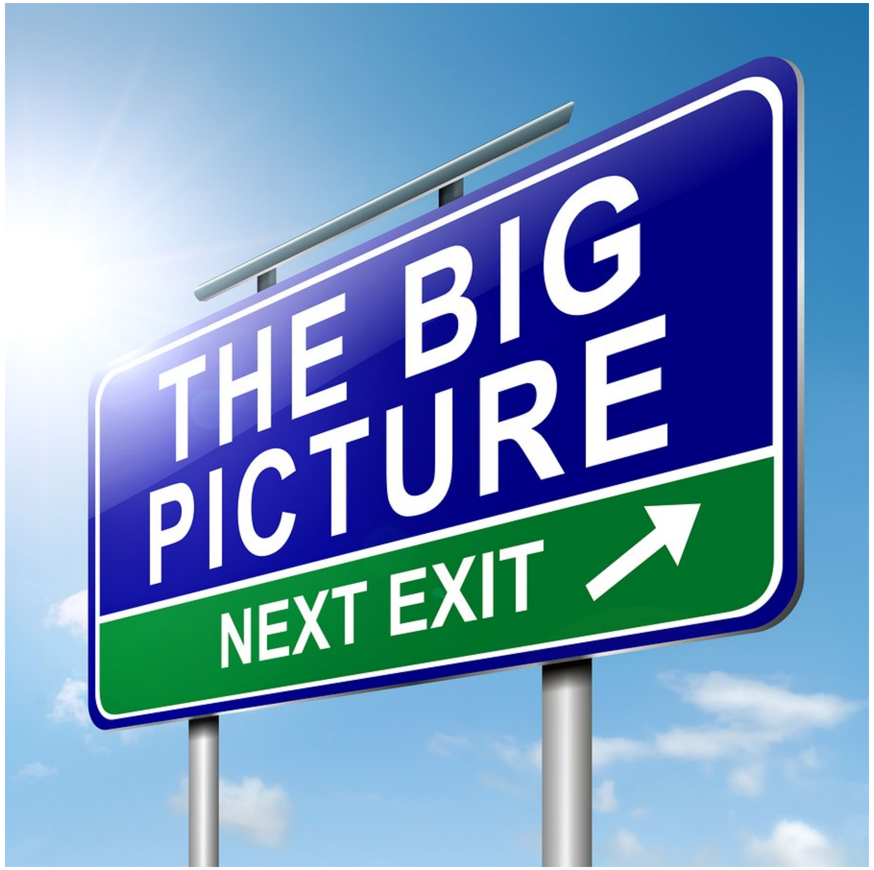


ABSORBING MATERIALS (METALS)





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*).

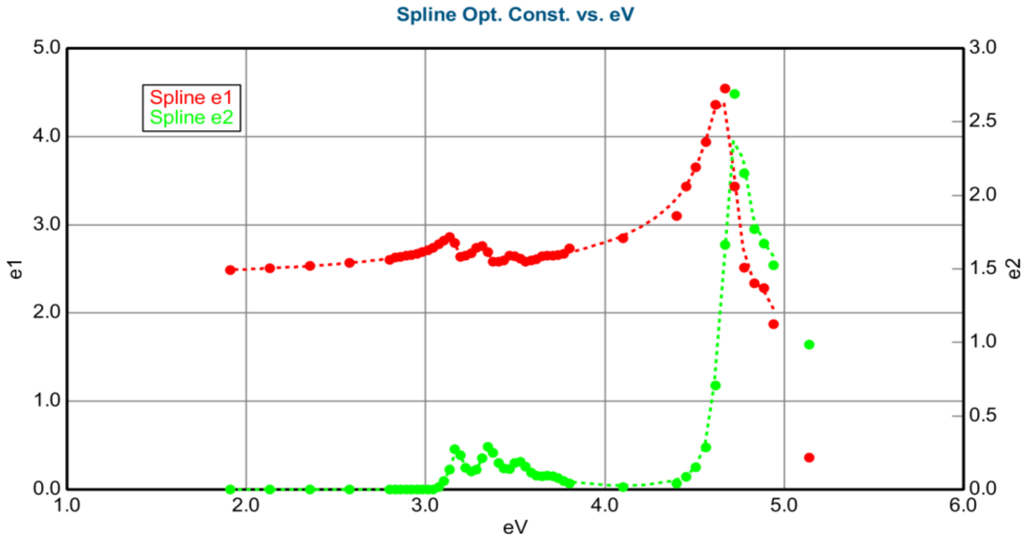
- Benefits:
  - Smooth, continuous functions
  - Can constrain to “physical” shapes

MODELING ABSORBING REGION

B-Spline

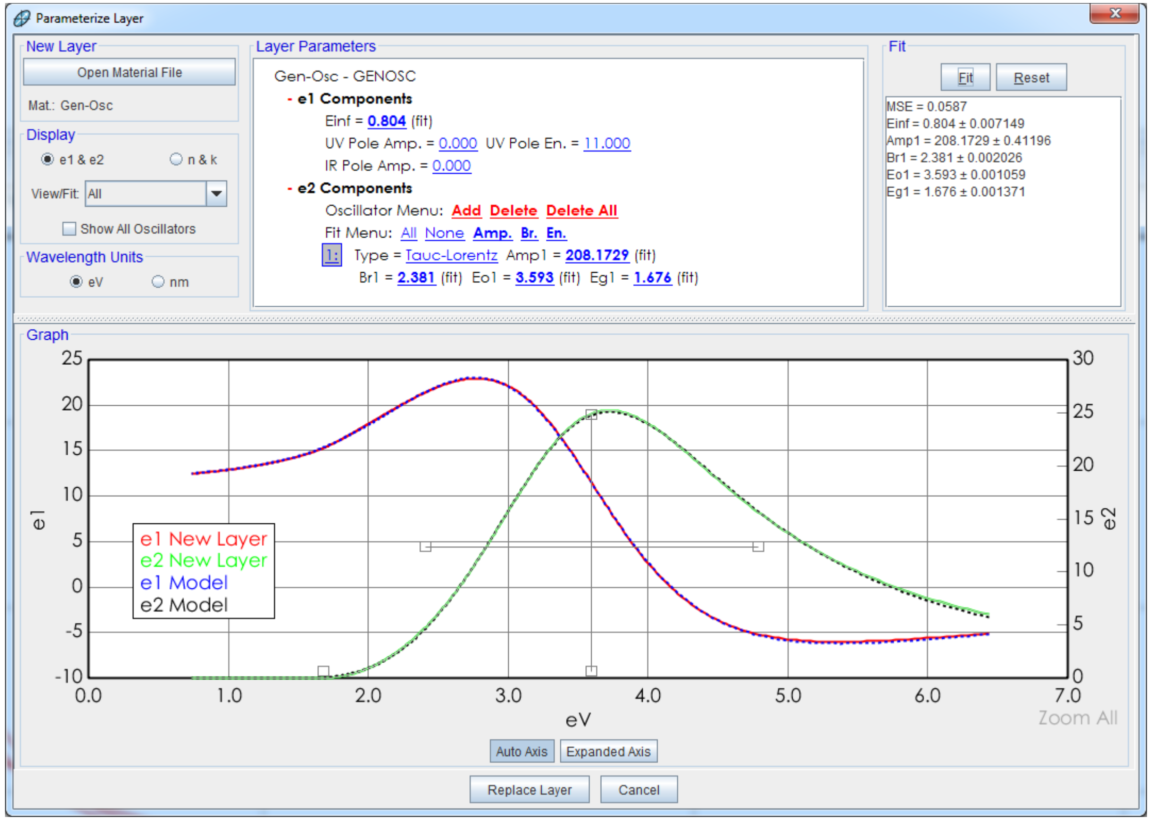
- Interpolation functions to best describe the shape of optical constants

\- Layer # 1 = B-Spline Thickness # 1 = **44.41 nm** (fit)
Resolution (eV) = 0.300 19 Pts. (0.738-6.438 eV) **Draw Node Graph**
Fit Opt. Const. = ON
Use KK Mode = OFF
\+ **Nodes**
\+ **Advanced**



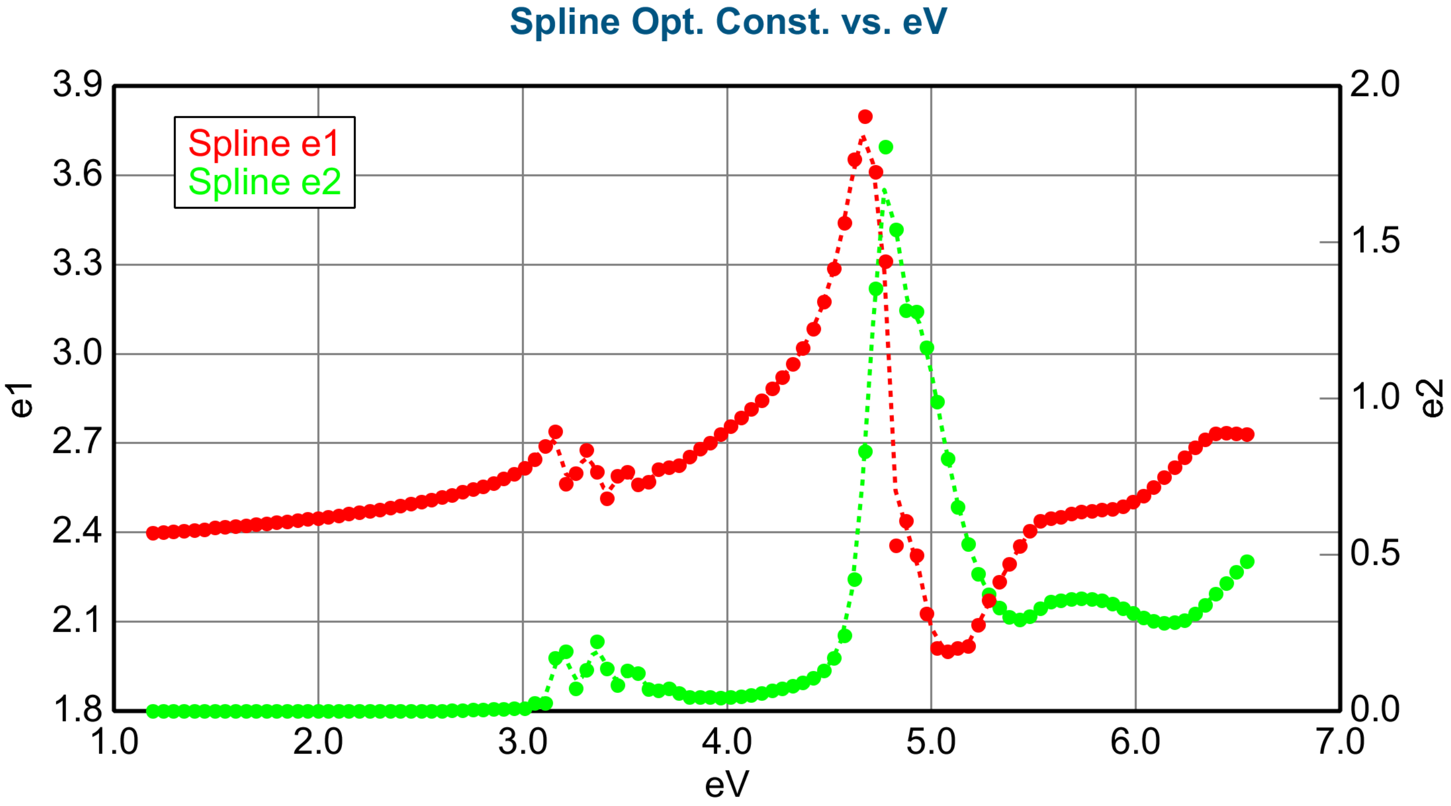
Gen-Osc

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



NEW TOOL: B-SPLINE

Simple spline curve designed to represent your optical properties as a function of wavelength



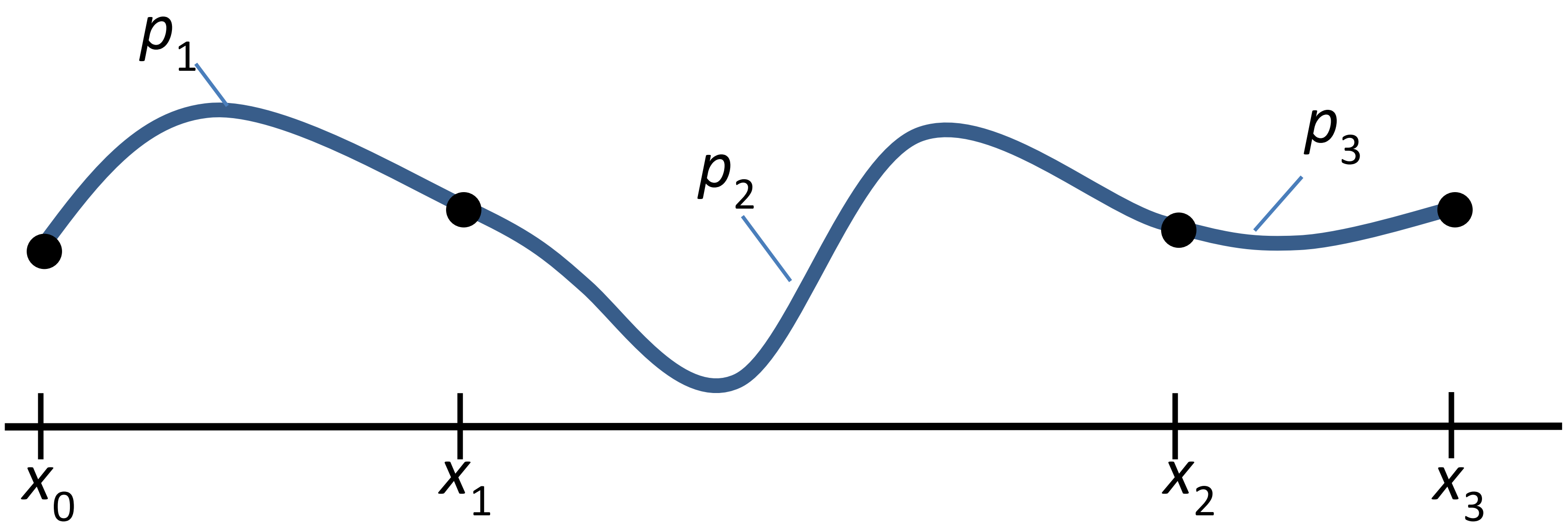
NICE FEATURES OF B-SPLINE

1. Smooth and continuous curve
2. Curve will not go beyond control points. Thus, avoid negative k by forcing control points ≥ 0.
3. When one point moves, it only affects shape of curve near this point – unlike some functions which affect the shape everywhere.
4. Easy to apply Kramers-Kronig Integration

SMOOTH FUNCTIONS

- Polynomials: $$p_m(x) = a_m x^m + a_{m-1} x^{m-1} + \ldots + a_1 x + a_0$$

- Splines use multiple connected polynomials.



WHAT IS B-SPLINE?

- **B**: Basis functions
- **Spline**: Sum of basis functions

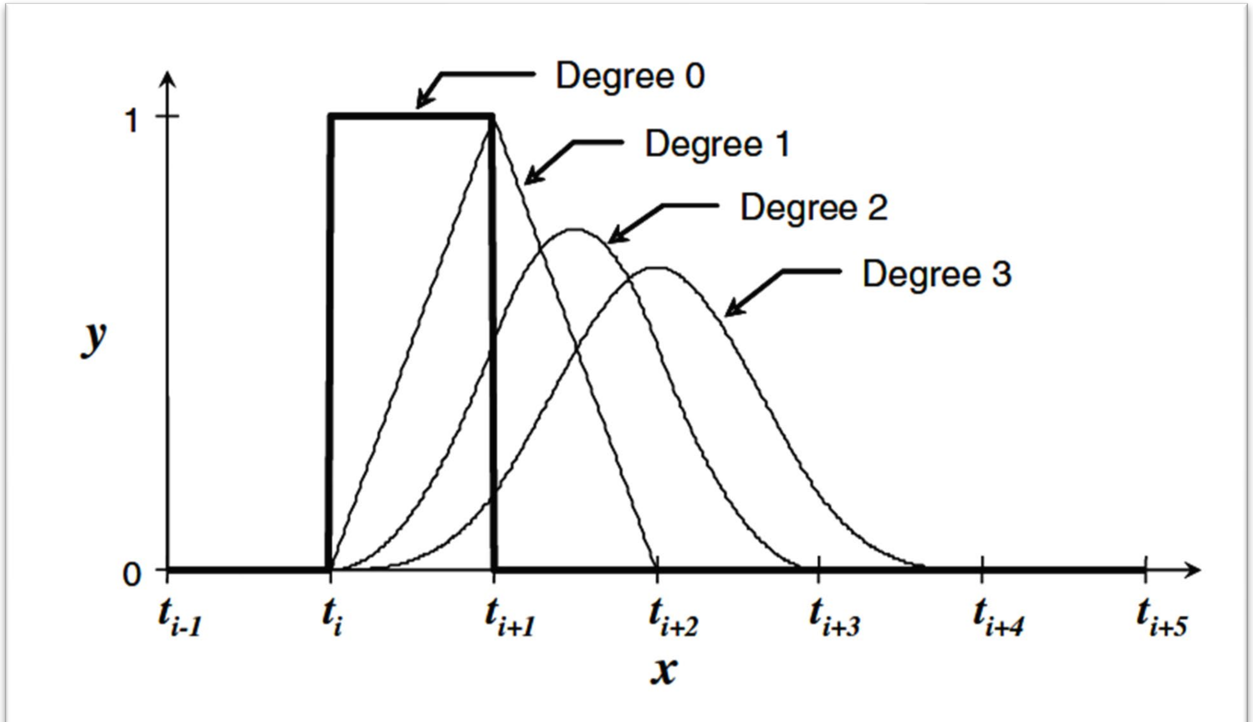
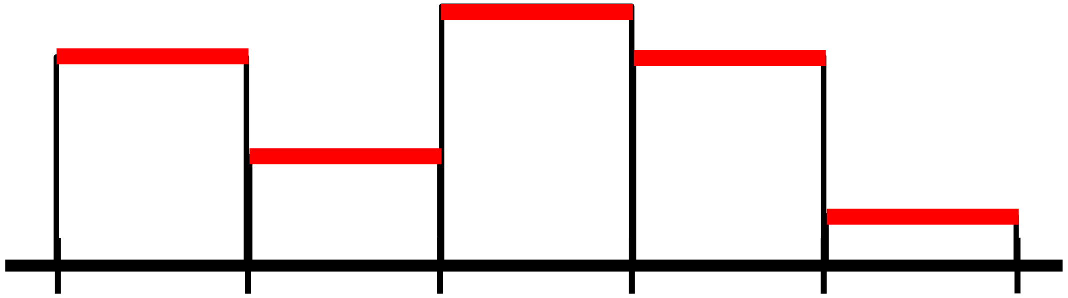
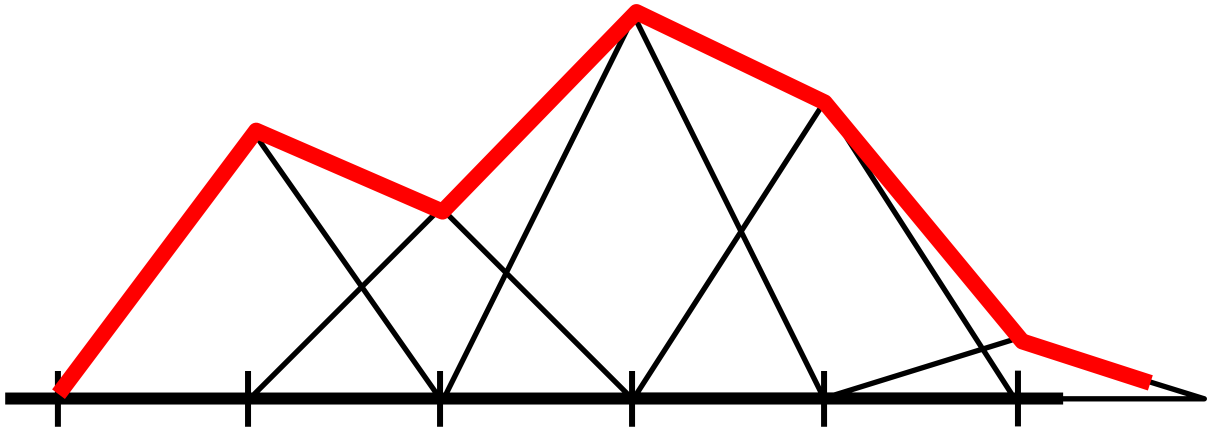


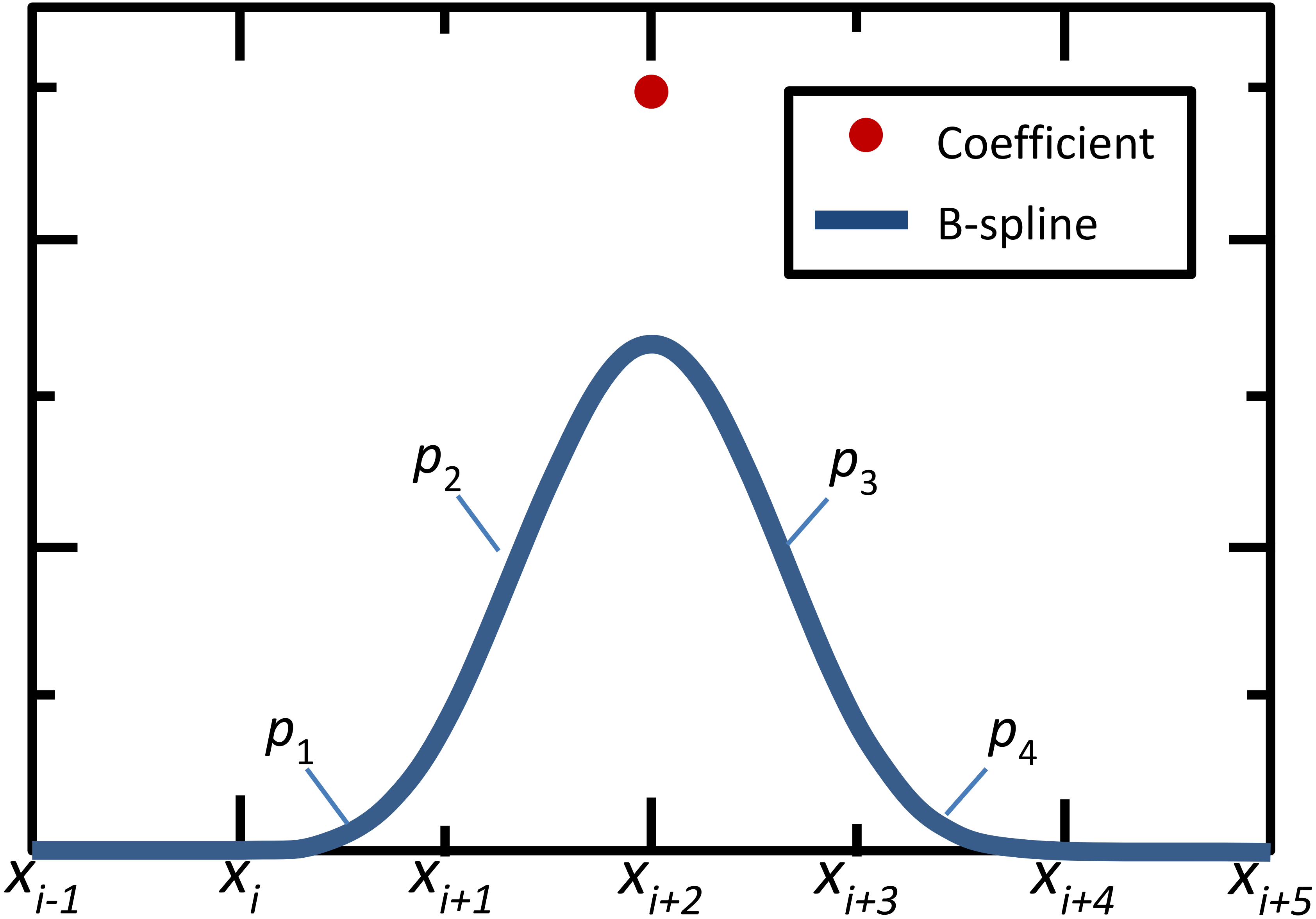
Figure 1 B-spline basis function t_i for degrees 0, 1, 2, and 3.

B. Johs and J.S. Hale, "Dielectric function representation by B-splines", *Phys. Stat. Sol. (a)* 2008.





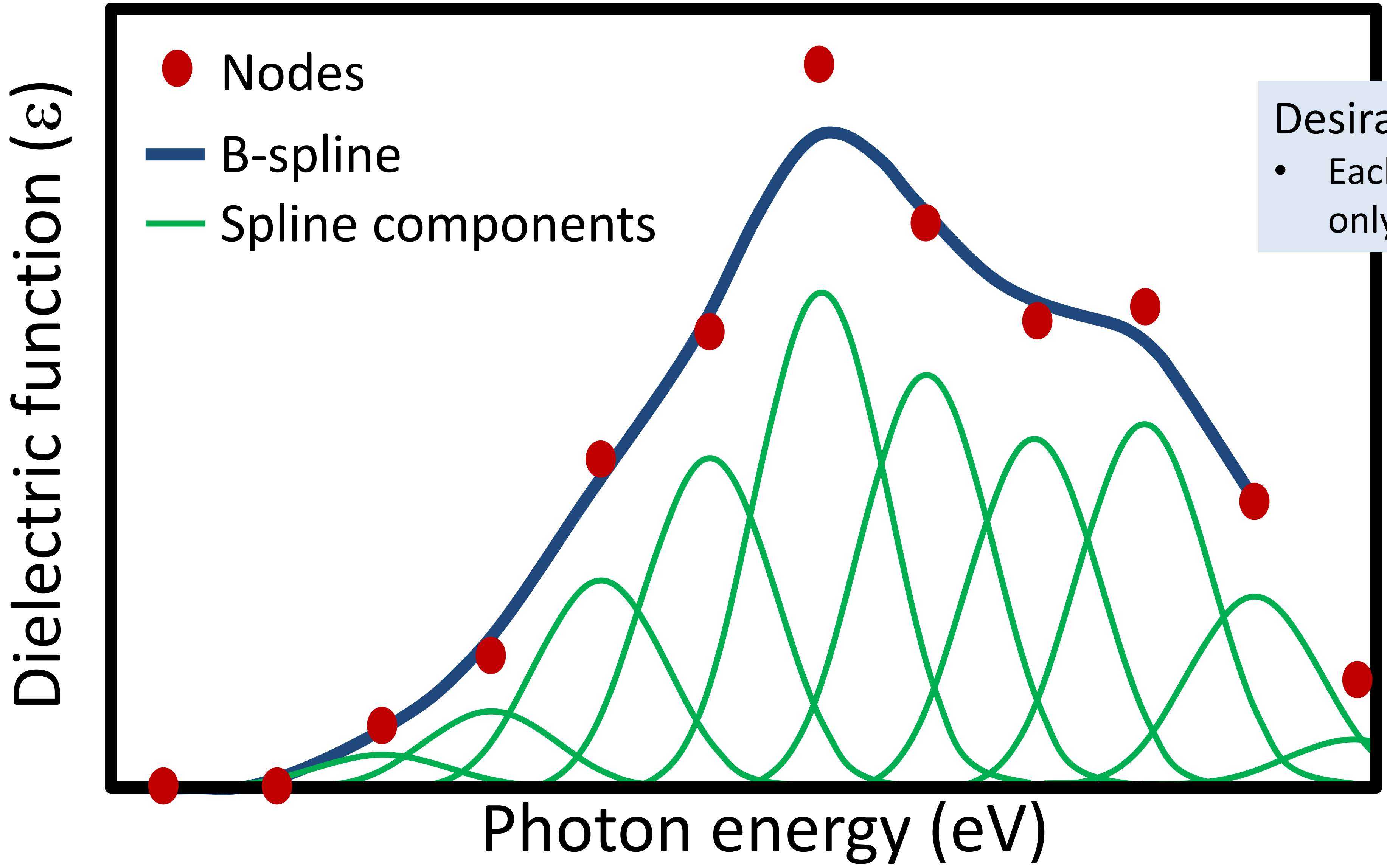
3RD DEGREE BASIS FUNCTION



Desirable Property #1:

- Function, 1st and 2nd derivatives are smooth and continuous.

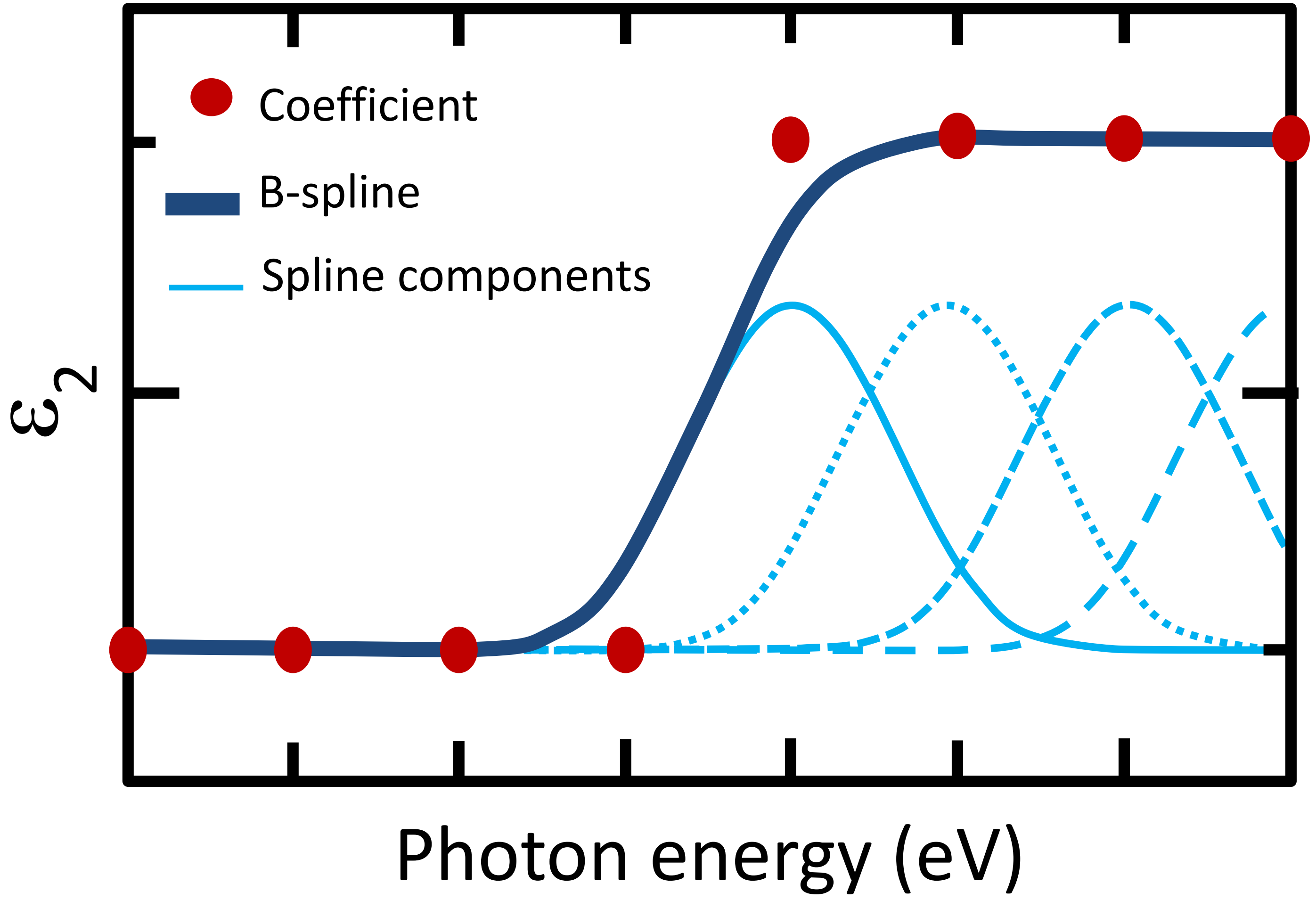
BASIS SPLINE: SUMMED FUNCTION



Desirable Property #2:

- Each basis function affects only "local" shape of curve.

B-SPLINE: CONVEX HULL PROPERTY

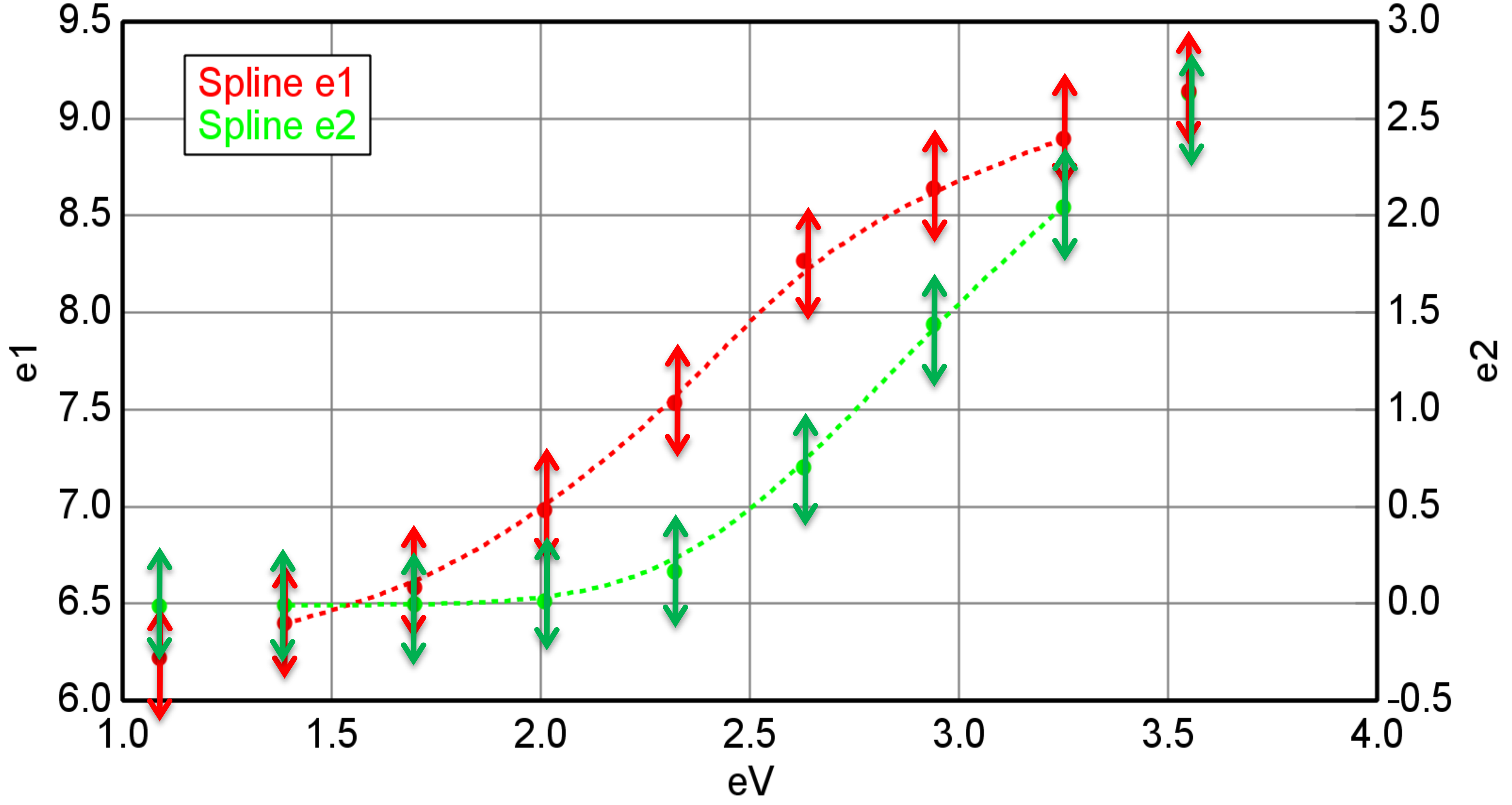


Desirable Property #3:

- Summed function can't exceed highest or lowest node amplitudes.

OPTICAL FUNCTIONS WITH B-SPLINES

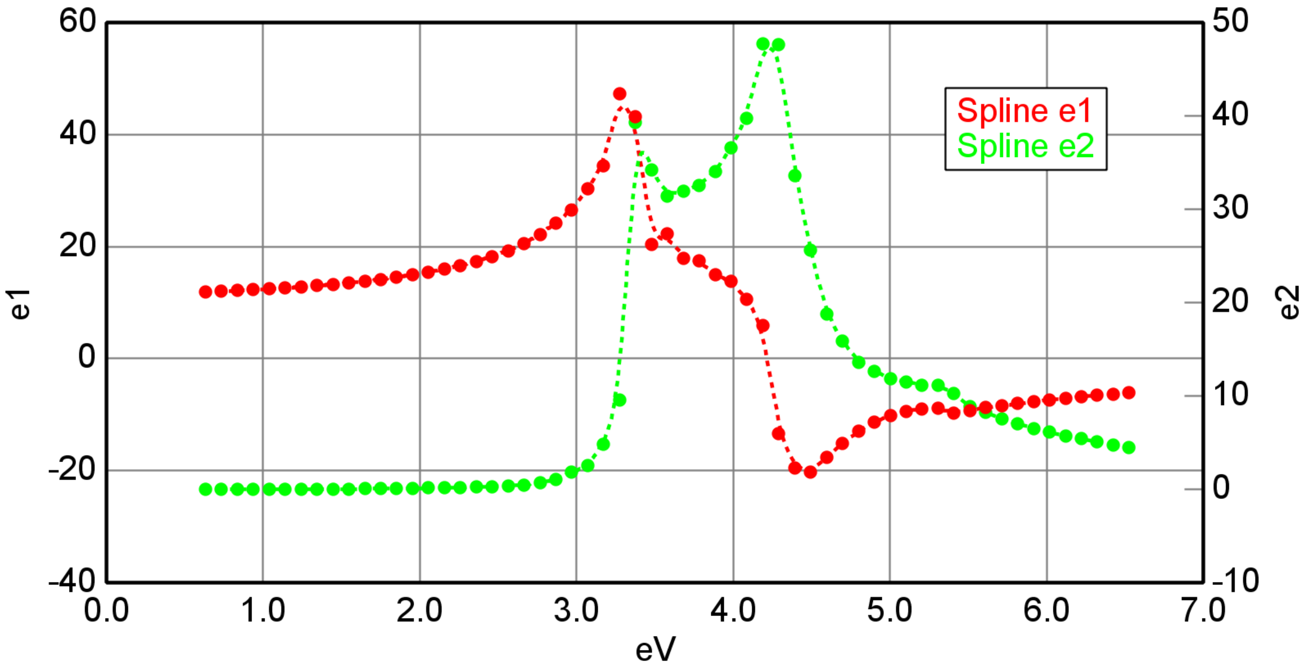
- Two B-splines are independently adjusted: ε_1 and ε_2.



B-SPLINE LAYER

- Substrate = B-Spline
  - Resolution (eV) = 0.300   18 Pts. (1.241-6.453 eV)   Draw Node Graph
  - Fit Opt. Const. = ON
  - Use KK Mode = OFF
  - + **Nodes**
  - + **Advanced**

B-Spline Node Graph for Si with 0.100 eV Resolution

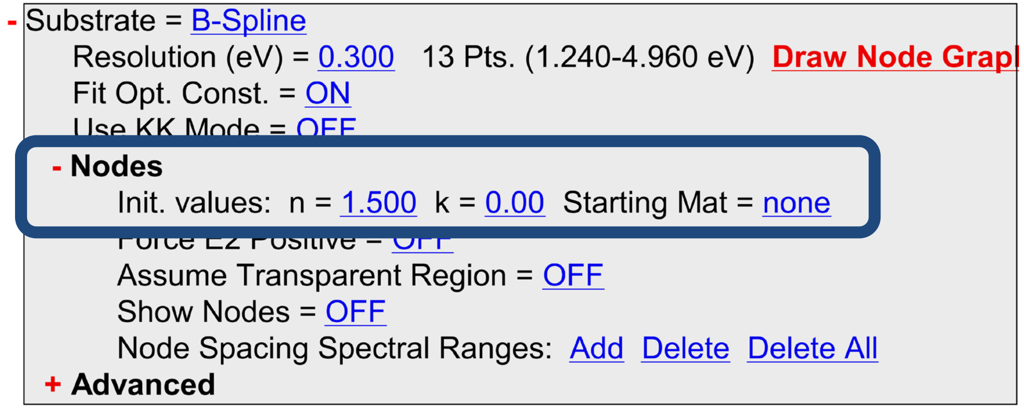


- Found in **Basic** folder.
- Nodes are spaced in eV.
- Draw Node Graph displays position of nodes and resulting dielectric function.

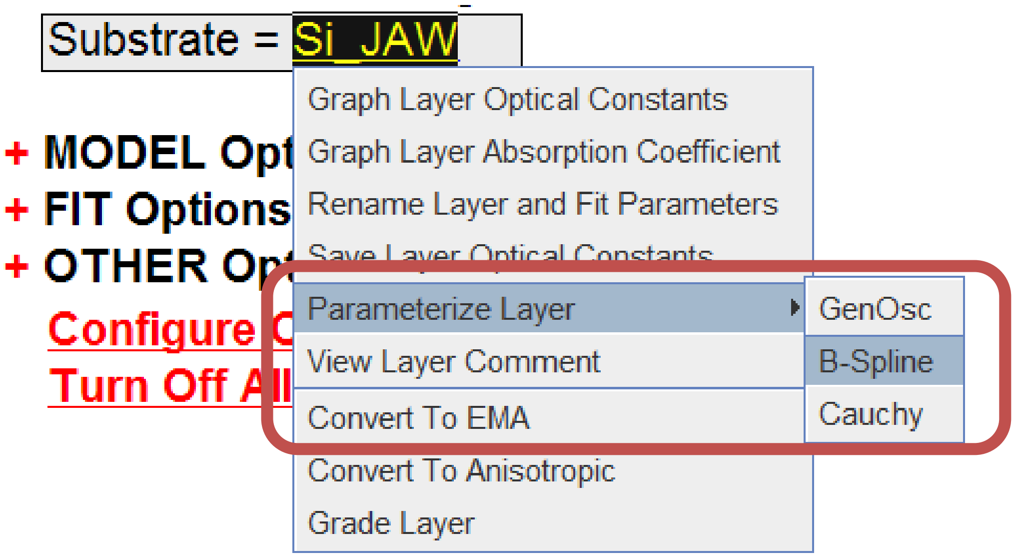
GETTING STARTED WITH A B-SPLINE

- Move the Nodes to a good location for your material:

Add B-Spline Layer:
Set “Init. Values”

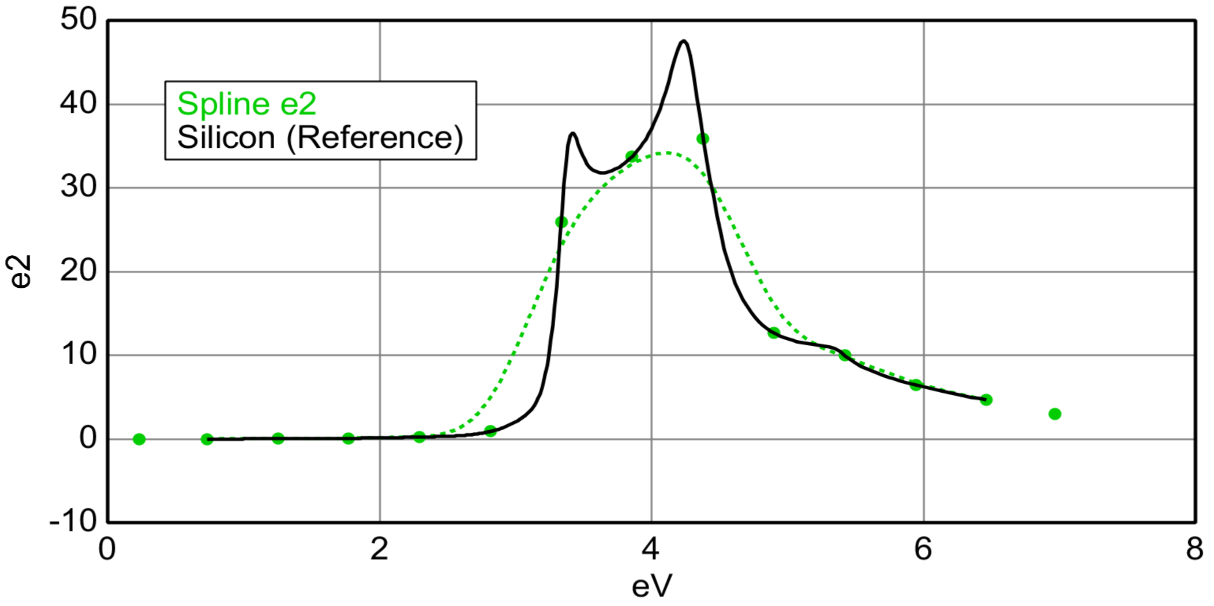


Add Material:
Right-click > Parameterize Layer

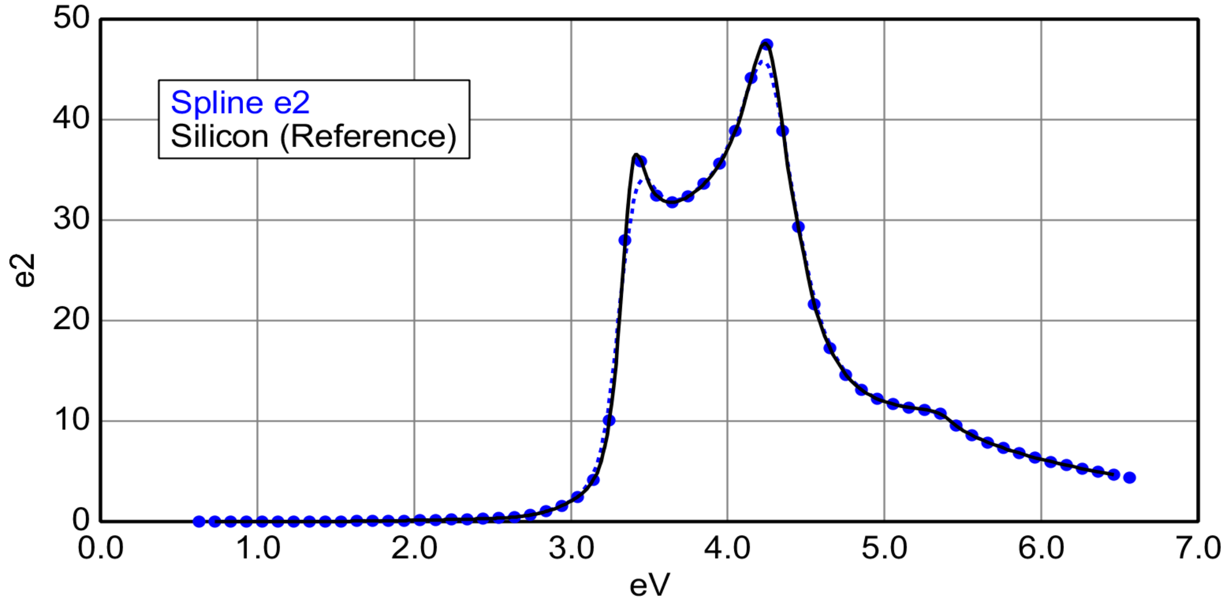


CHOOSING NODE SPACING

0.5 eV Node Spacing



0.1 eV Node Spacing



Node Spacing Goal:

- Decrease to describe optical constant features.
- Increase to reduce total # of “free fit parameters”

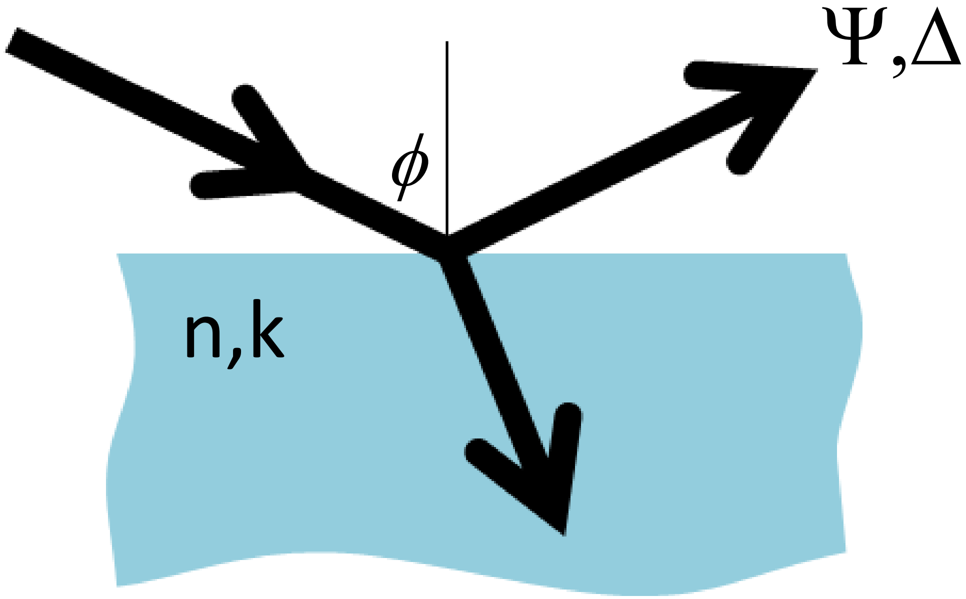
NODE SPACING RECOMMENDATIONS

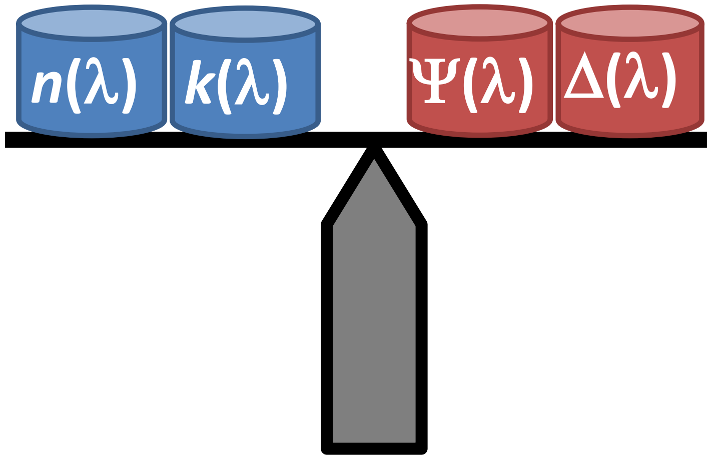
Amorphous Dielectrics and Semiconductors	0.5 eV
Metals	0.3 eV
Organics	0.1 eV
Crystalline Materials	0.05 eV

OPAQUE LAYERS

- Treat metal as "substrate" if no light returns from bottom of layer. Typically 50-150nm thick.

Absorbing





2 Measured Data (Ψ,Δ)
2 Unknowns (*n*,*k*)

OPAQUE METAL FITTING PROCEDURES

Preparing the B-spline

Add B-Spline as Substrate in Model

↓

Expand Nodes: Add Metal as “Starting Mat”

Add Metal as Substrate in Model

↓

Right-Click on Metal “name” Parameterize Layer > B-spline

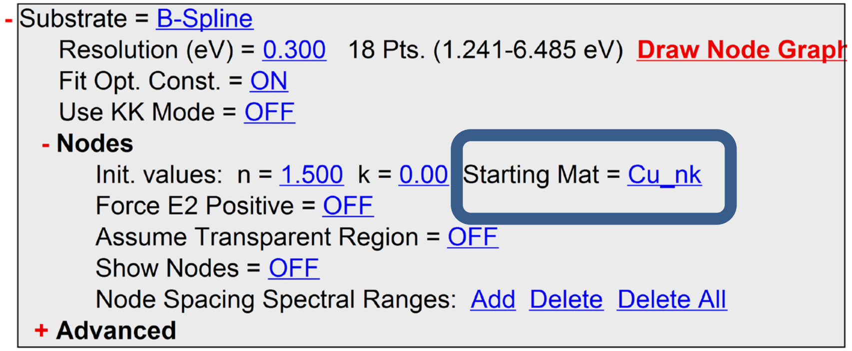
↓

Press Fit

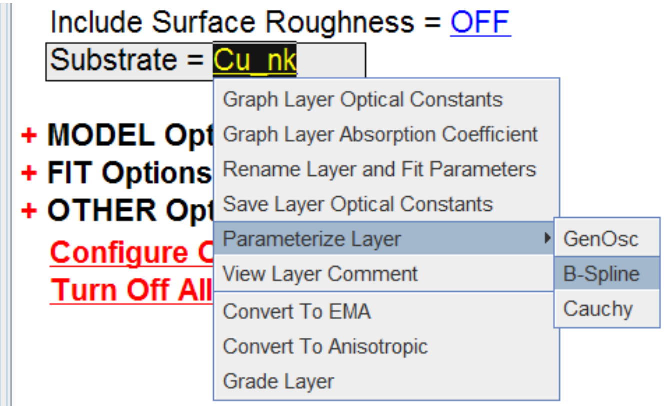
↓

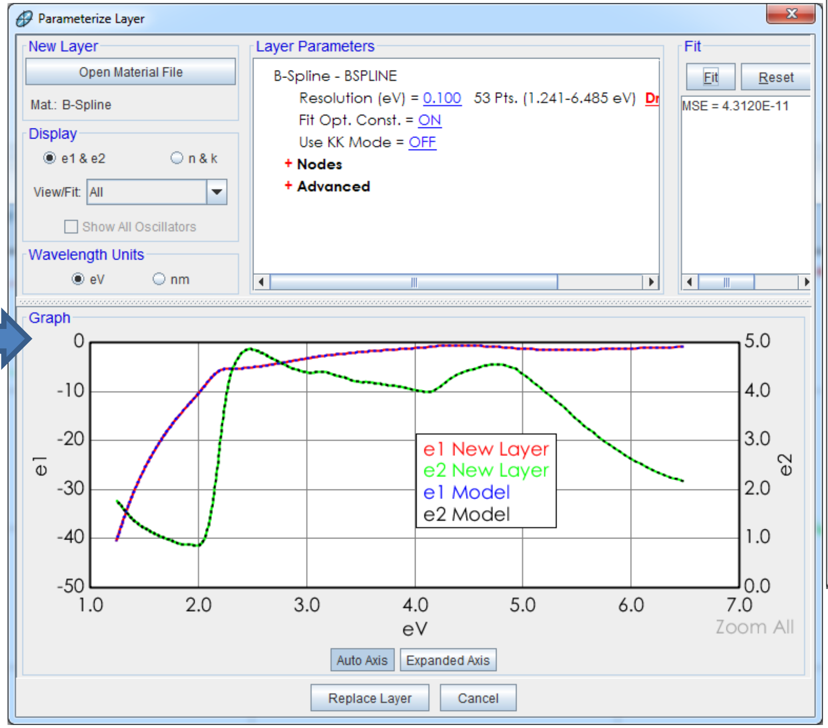
Optimize Node Resolution

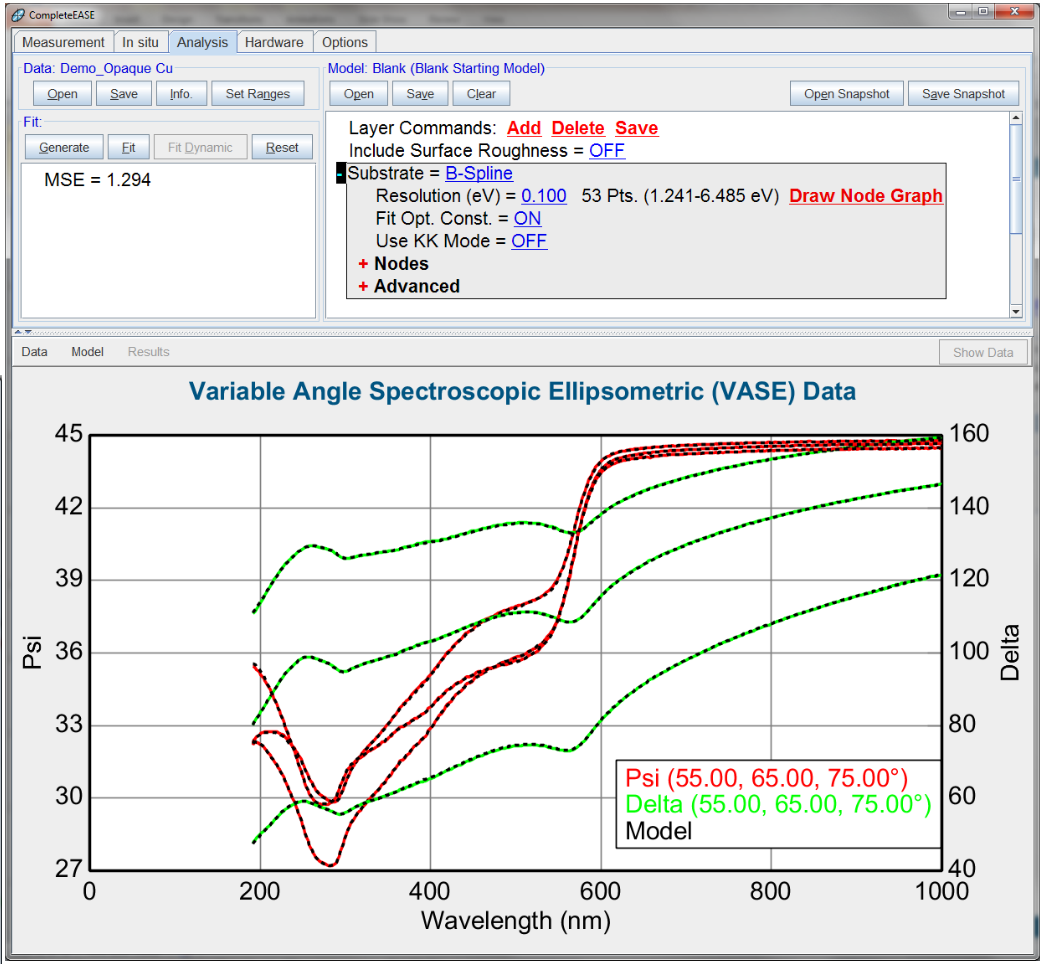
DEMONSTRATION: OPAQUE COPPER



OR

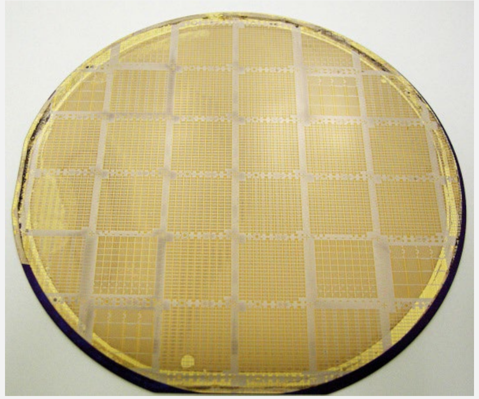






2 3-2_100nm_Ni_on_Si.SE

- Assume Ni is opaque and use B-spline to determine layer optical constants



QUESTIONS:

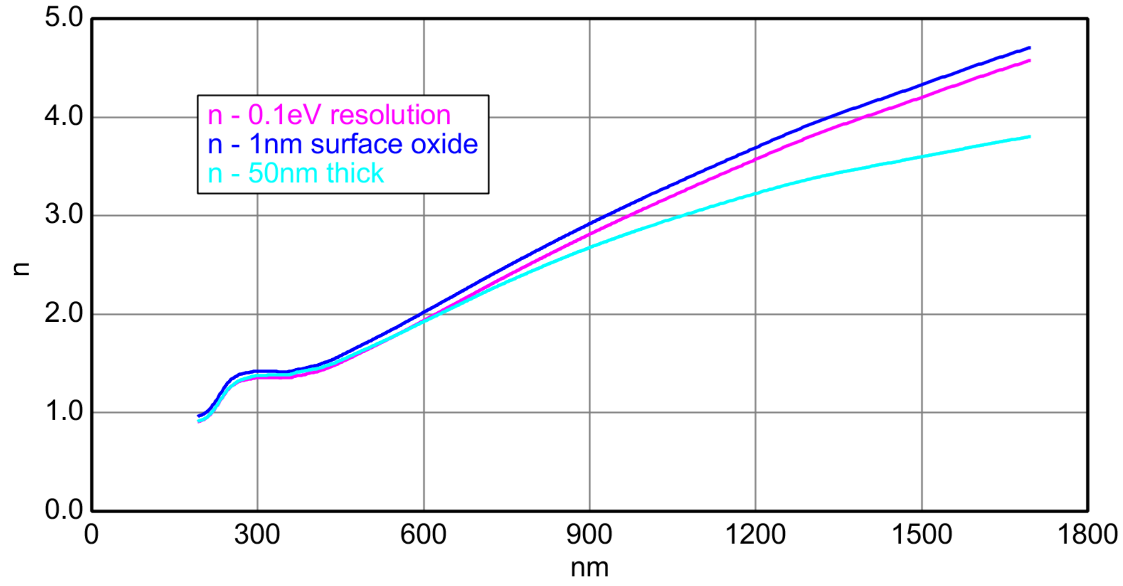
- Compare four node resolutions (1, 0.5, 0.3 and 0.1 eV) – which is preferred?

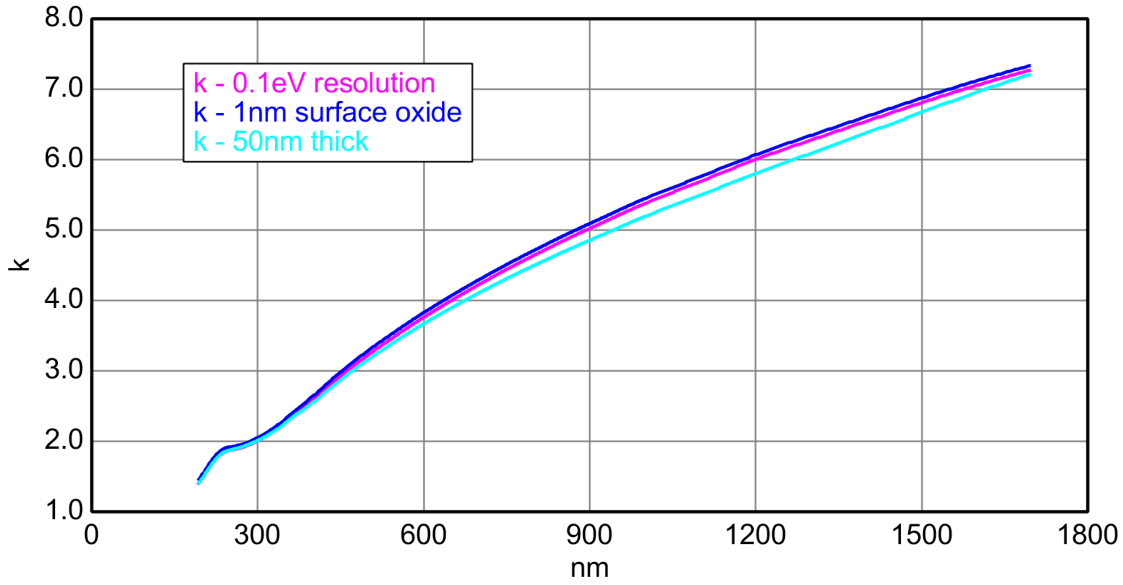
BONUS:

- How are the optical constants affected if:
  - Nickel is actually 50nm thick
  - Surface is oxidized (estimate with 1nm thick SiO_2)

RESULTS

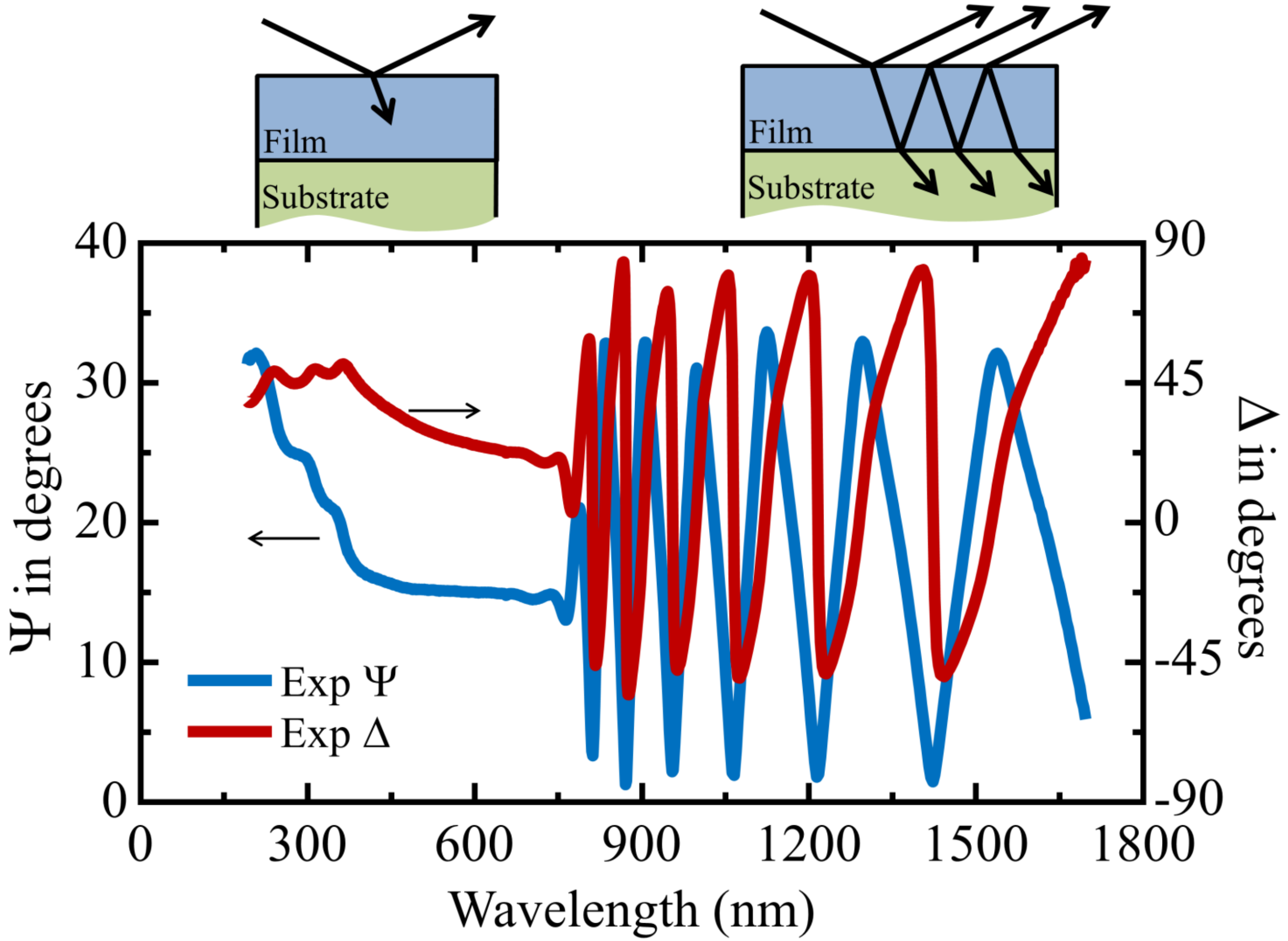
Node Resolution	# Fit Parms	MSE
1.0 eV	12	12.7
0.5 eV	24	2.6
0.3 eV	40	1.6
0.1 eV	116	1.5





FILMS WITH ABSORBING REGION

- Need to determine thickness, *n* and *k*.

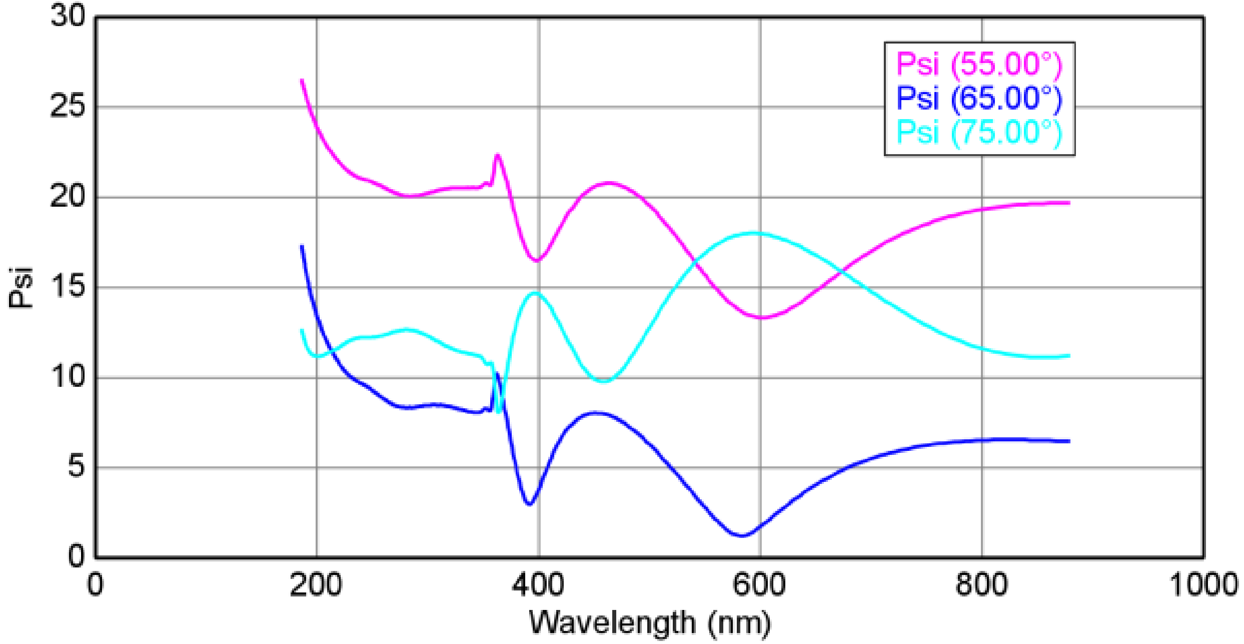


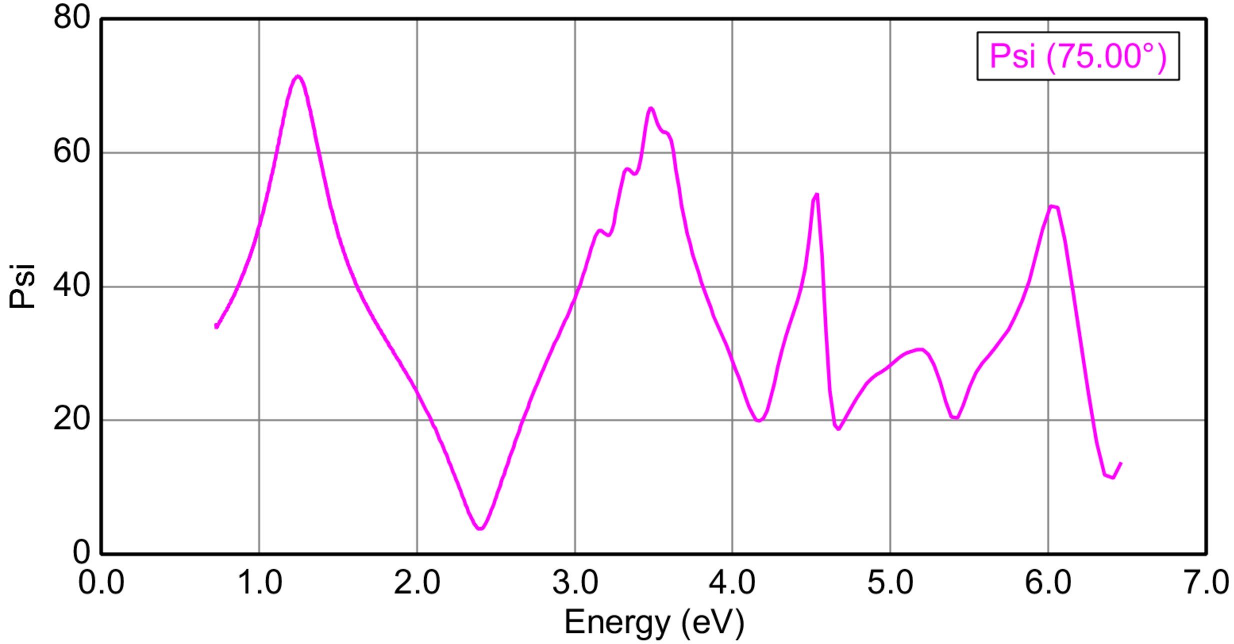
Absorbing Regions

IDENTIFYING THE ABSORBING REGION

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

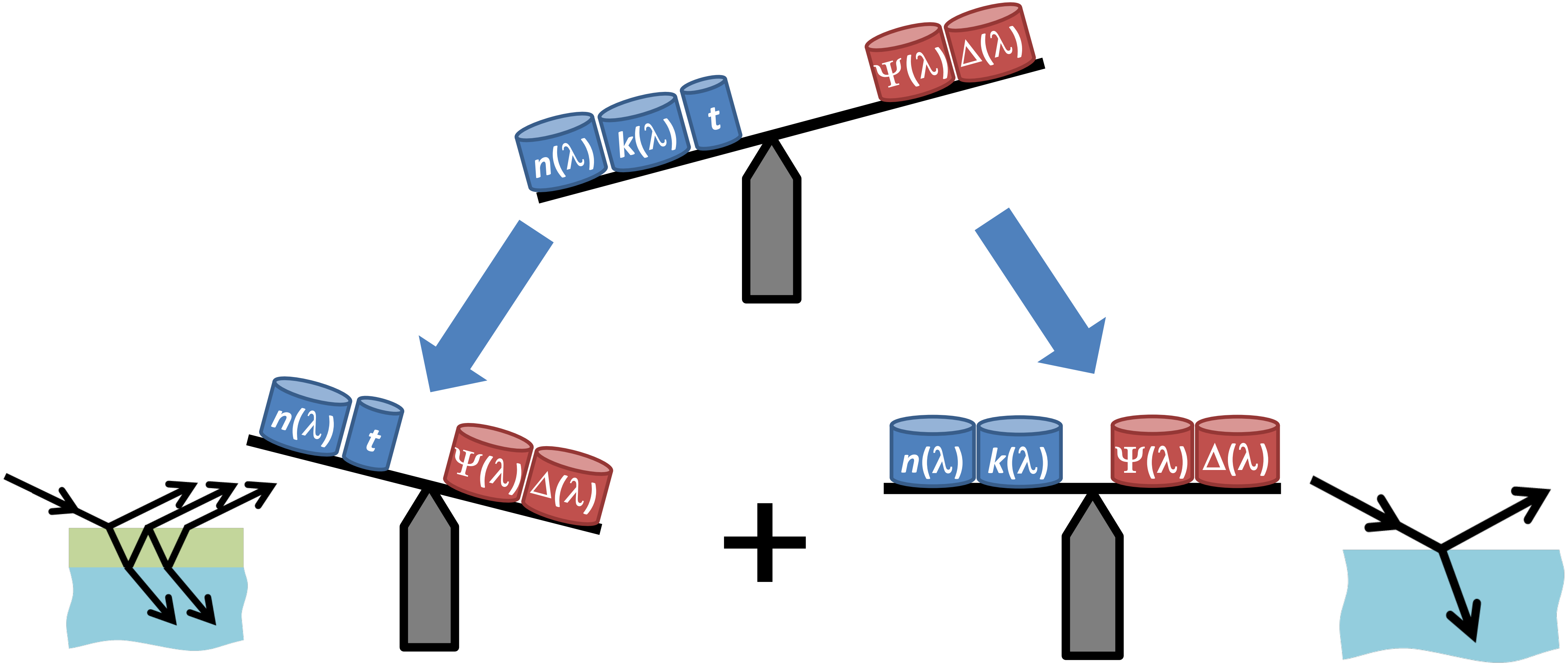
1	2





STRATEGY: FILMS WITH ABSORBING REGION

Separate problem into two steps:



B-SPLINE PROCEDURE (ABSORBING REGION)

1. Fit Transparent Region with Cauchy

⬇

2. Right-Click on Cauchy:
   "Parameterize Layer → B-Spline"

⬇

3. Setup B-Spline, Fit to Reference, Replace Layer

⬇

4. Wavelength Range Expansion Fit

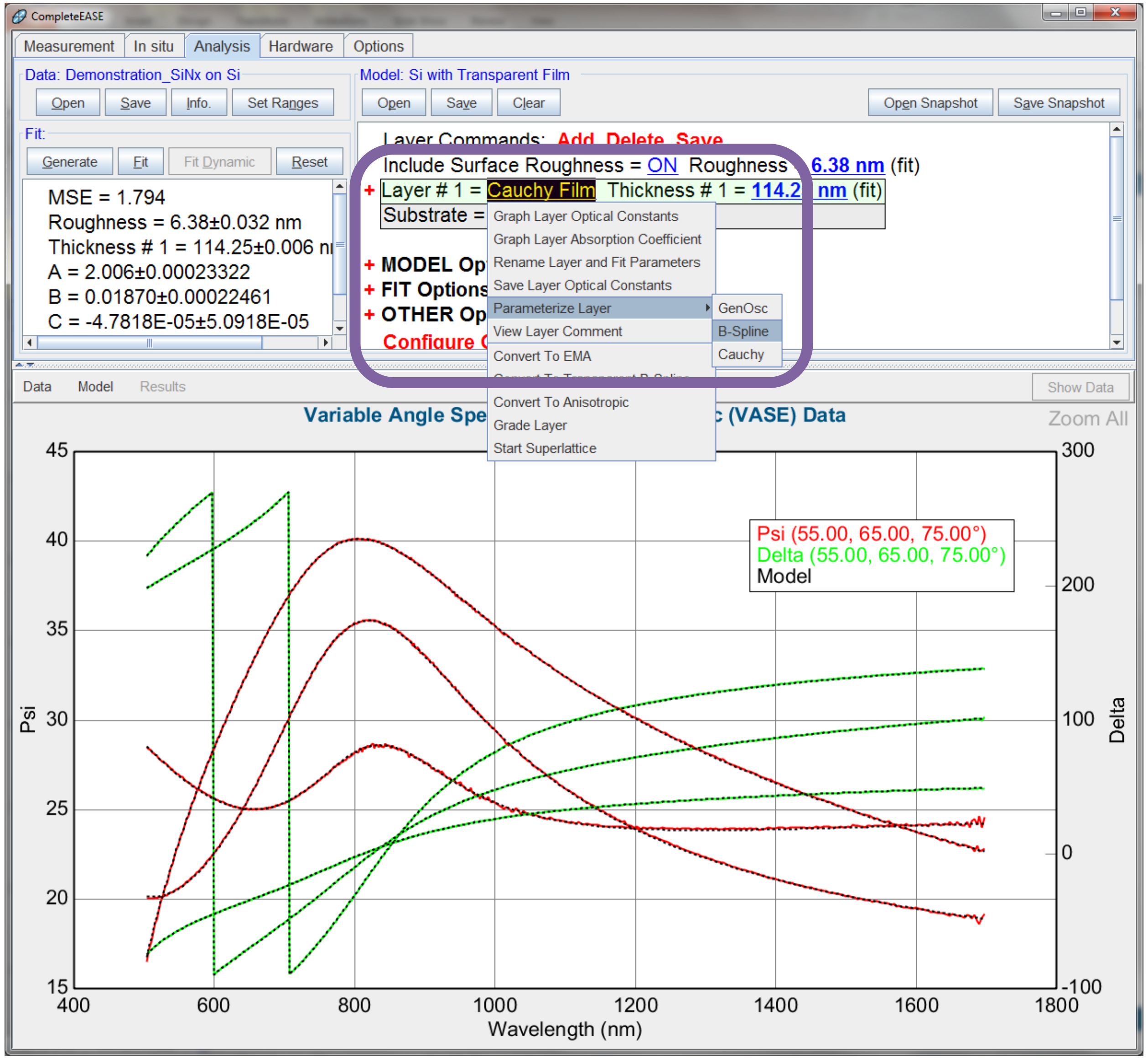
⬇

Optimize Node Resolution, Roughness, Grading,…

DEMONSTRATION: SINX ON SI

1 Fit Transparent Region with Cauchy

2 Right-Click on Cauchy: "Parameterize Layer → B-Spline"



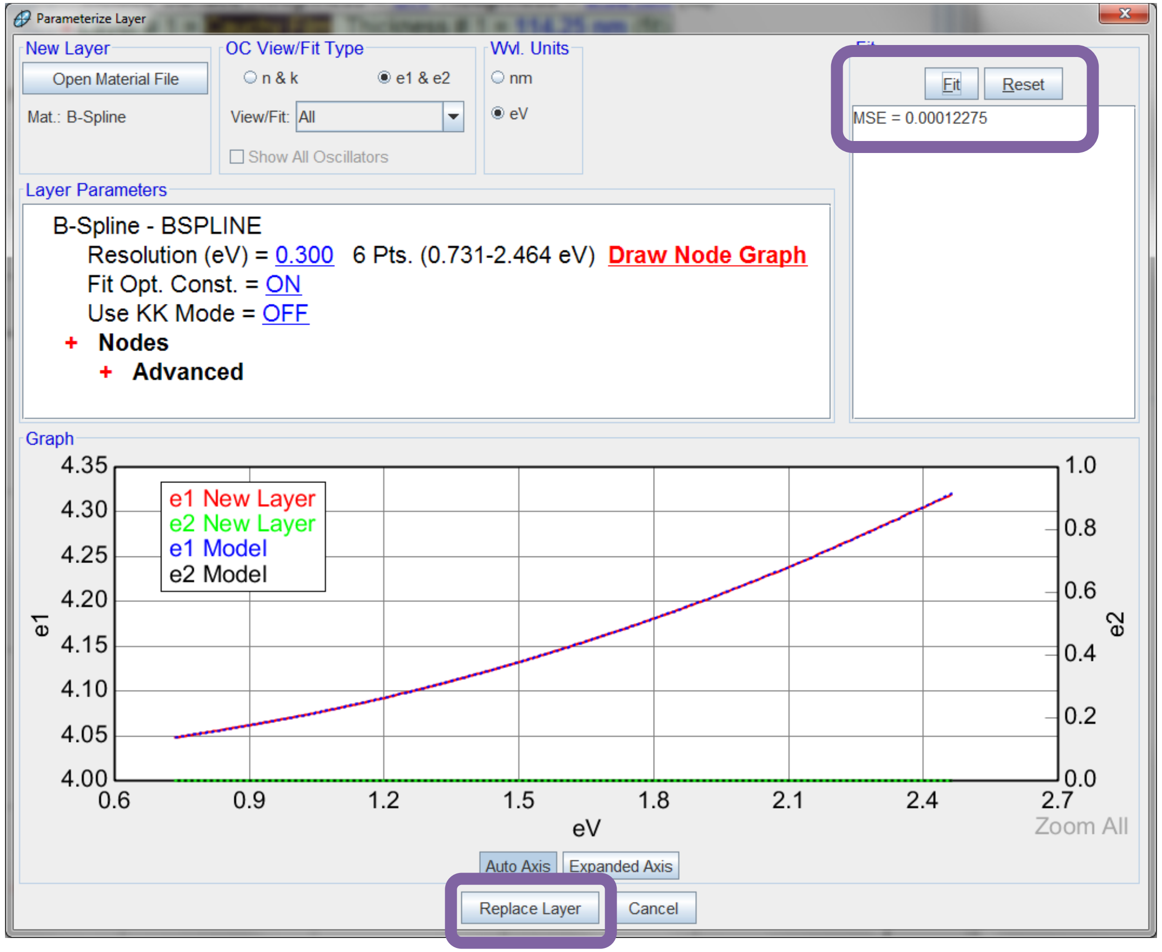
DEMONSTRATION: SIN_x ON SI

Parameterize Layer window is used to match optical constants with new layer

3 **Setup B-Spline, Fit to Reference, Replace Layer**

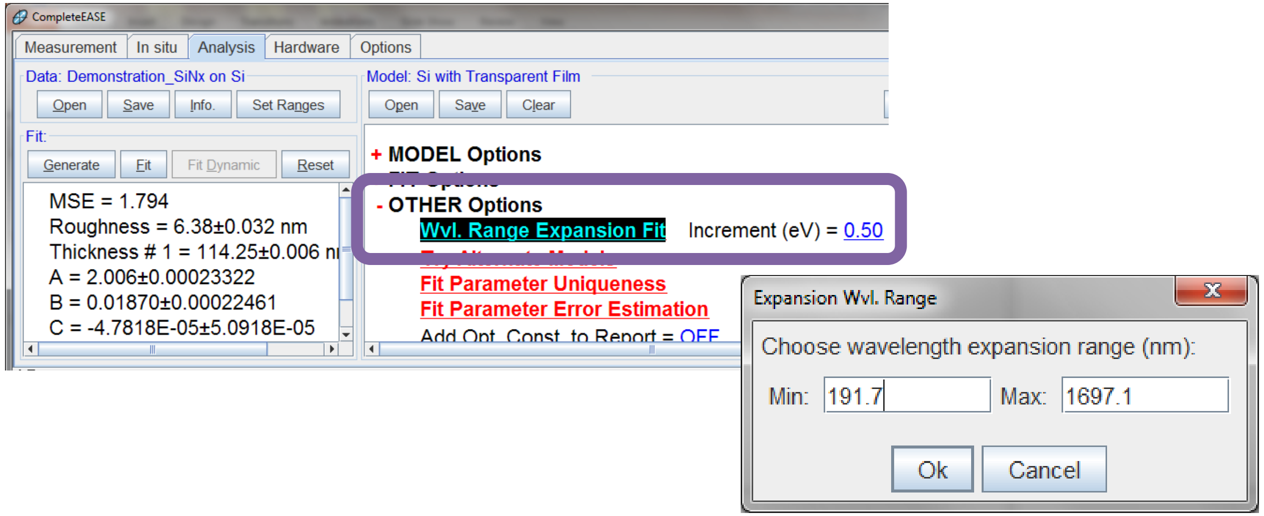
Setting up B-spline:

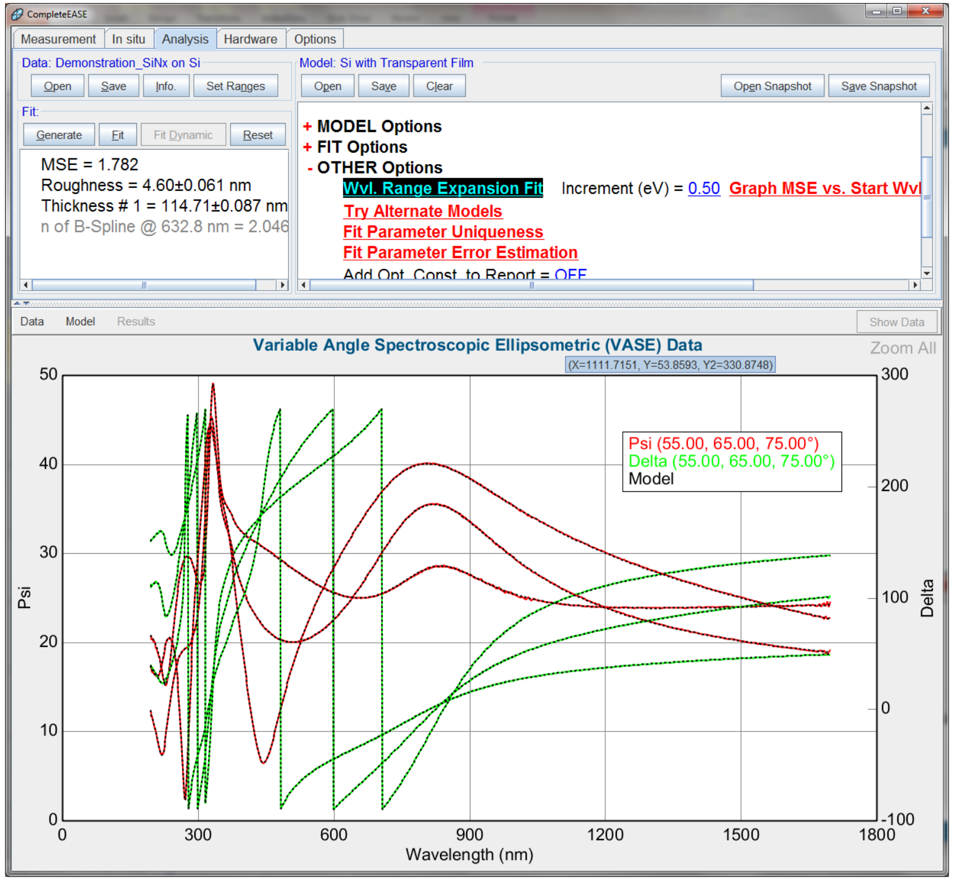
- Choose Node Resolution

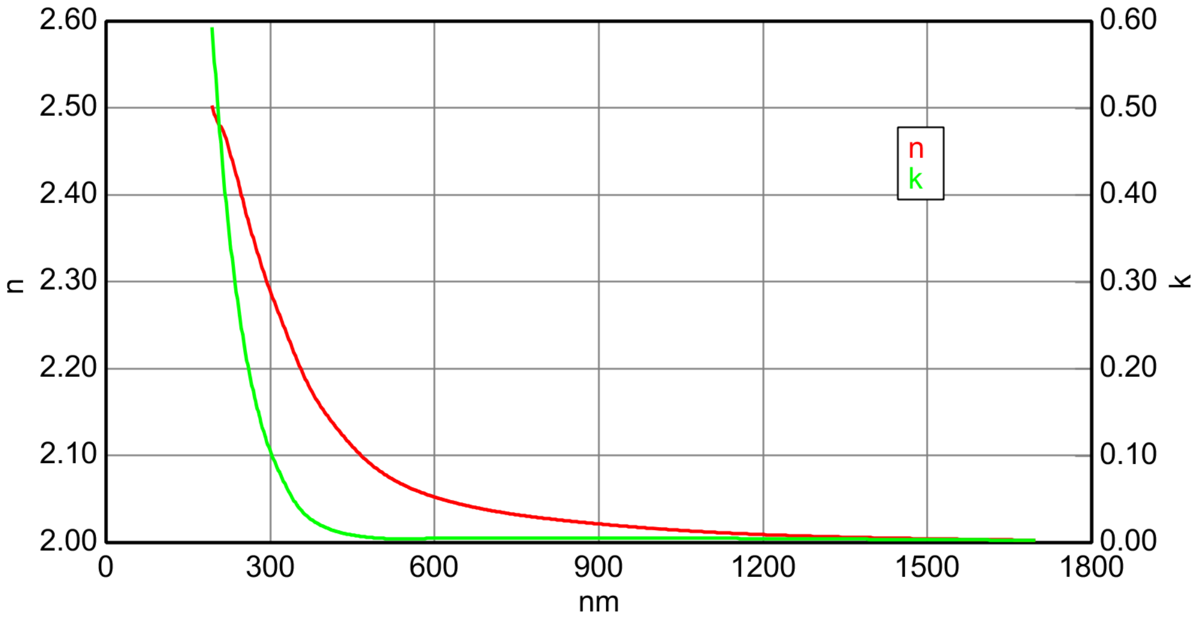


DEMONSTRATION: SIN_X ON SI

4 **Wavelength Range Expansion Fit**

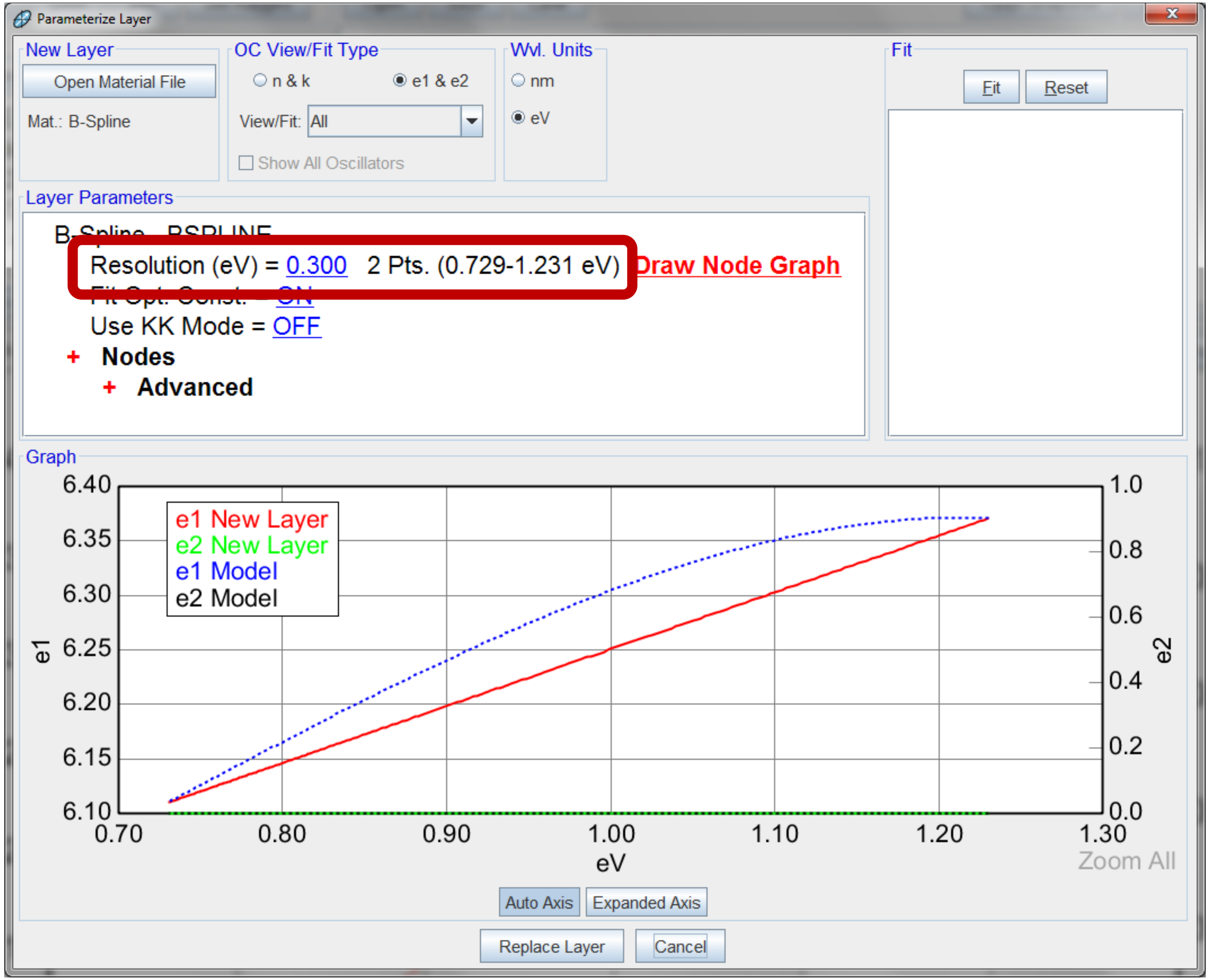






WARNING: NODES TOO WIDELY SPACED

- B-Spline requires minimum of **4 Pts.**
- Otherwise it reverts to simple polynomial.



BREAK!!

3-3_SiC_on_Si.SE

- **Determine SiC optical constants using B-Spline method** (starting with Transparent Cauchy)

QUESTIONS:

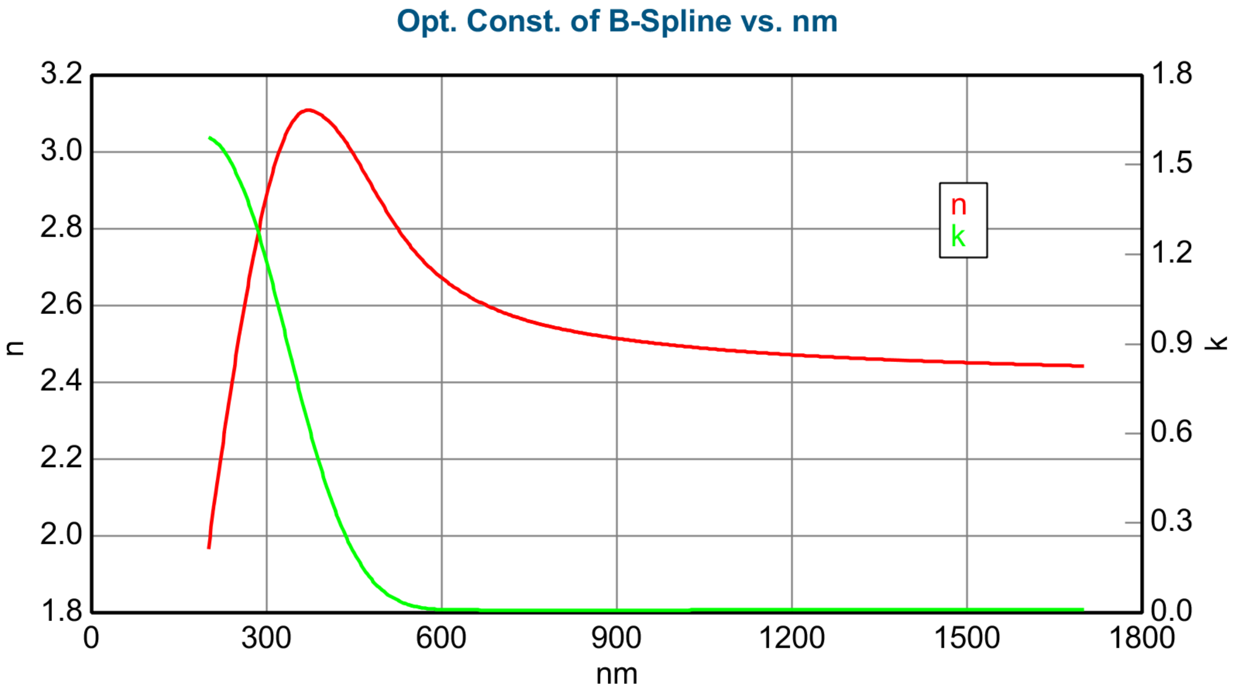
- What is your preferred resolution?
- Is roughness required?

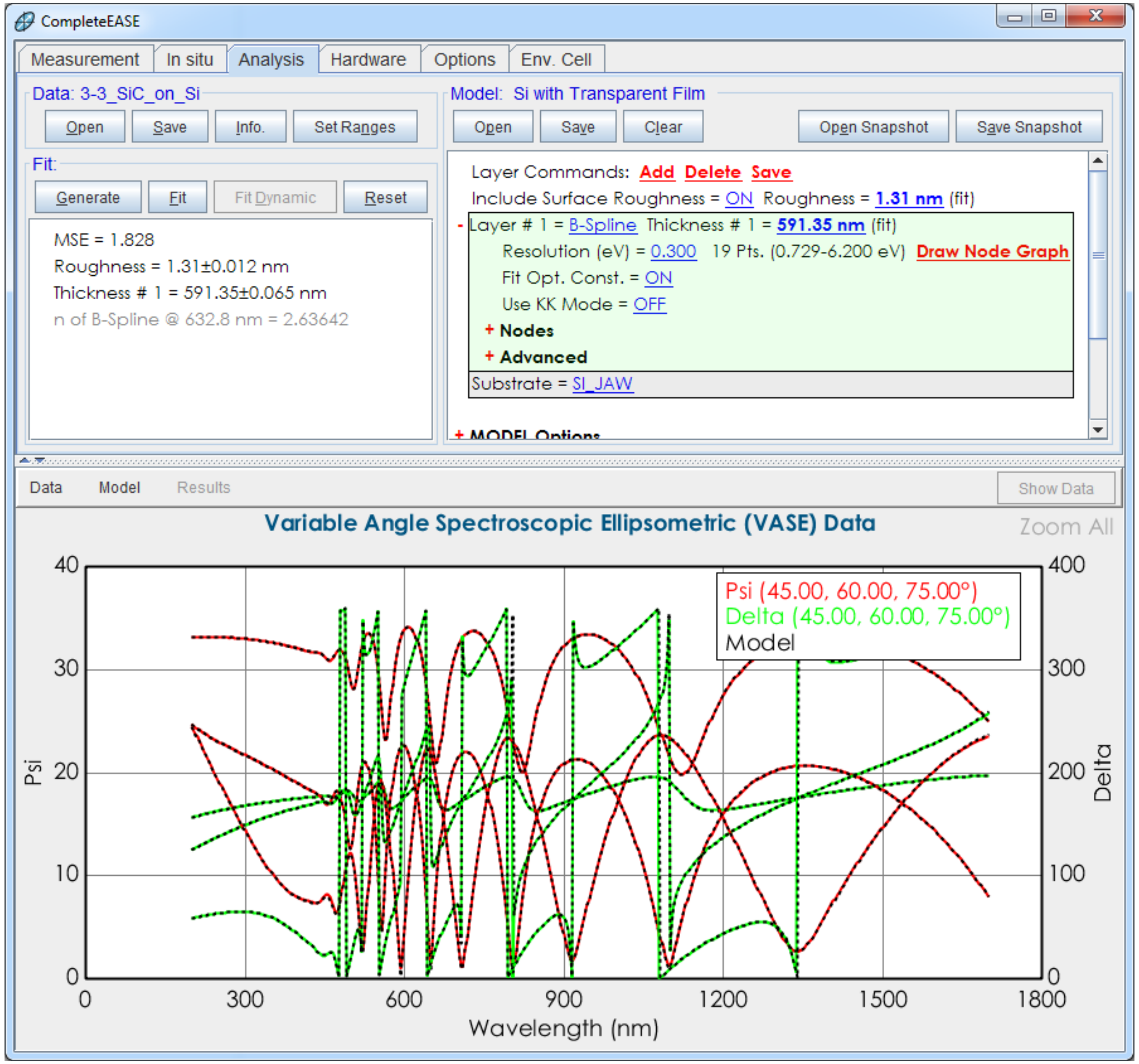
RESULTS

Roughness = **1.31 nm** (fit)

- Layer # 1 = B-Spline Thickness # 1 = **591.35 nm** (fit)
  - Resolution (eV) = 0.300 19 Pts. (0.729-6.200 eV) **Draw Node Graph**
  - Fit Opt. Const. = ON
  - Use KK Mode = OFF
  - **+ Nodes**
  - **+ Advanced**

Substrate = SI_JAW





CAUSALITY AND KRAMERS-KRONIG

- KK relations consider optical properties as "response" at a given time/place due to "cause" at all other times and places.
- Causality: There can't be a response before there is a cause.

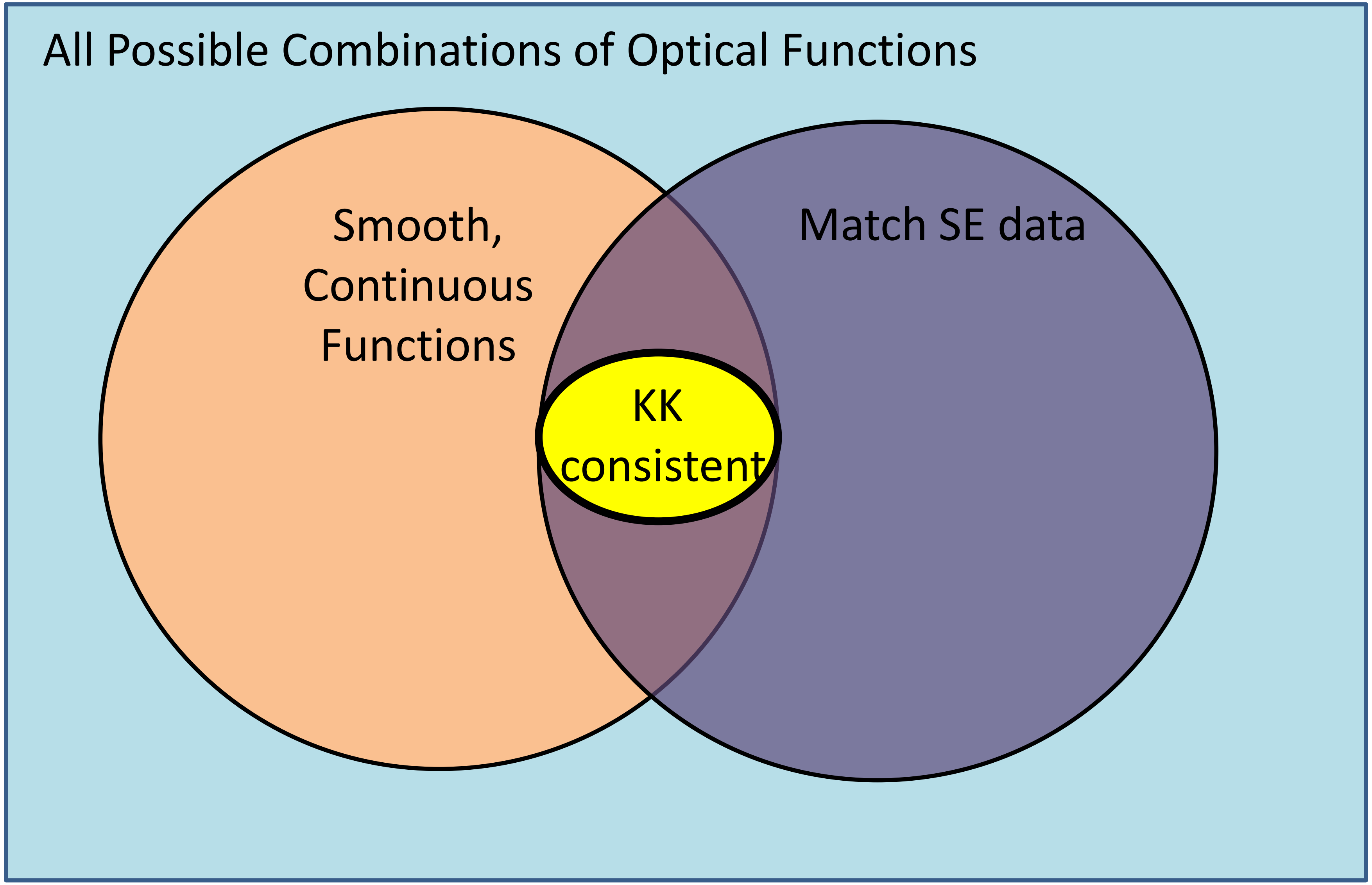
KK relations give a "Physical" tie between the real and imaginary optical functions.

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

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

P is "principal part "

KRAMERS-KRONIG CONSISTENCY

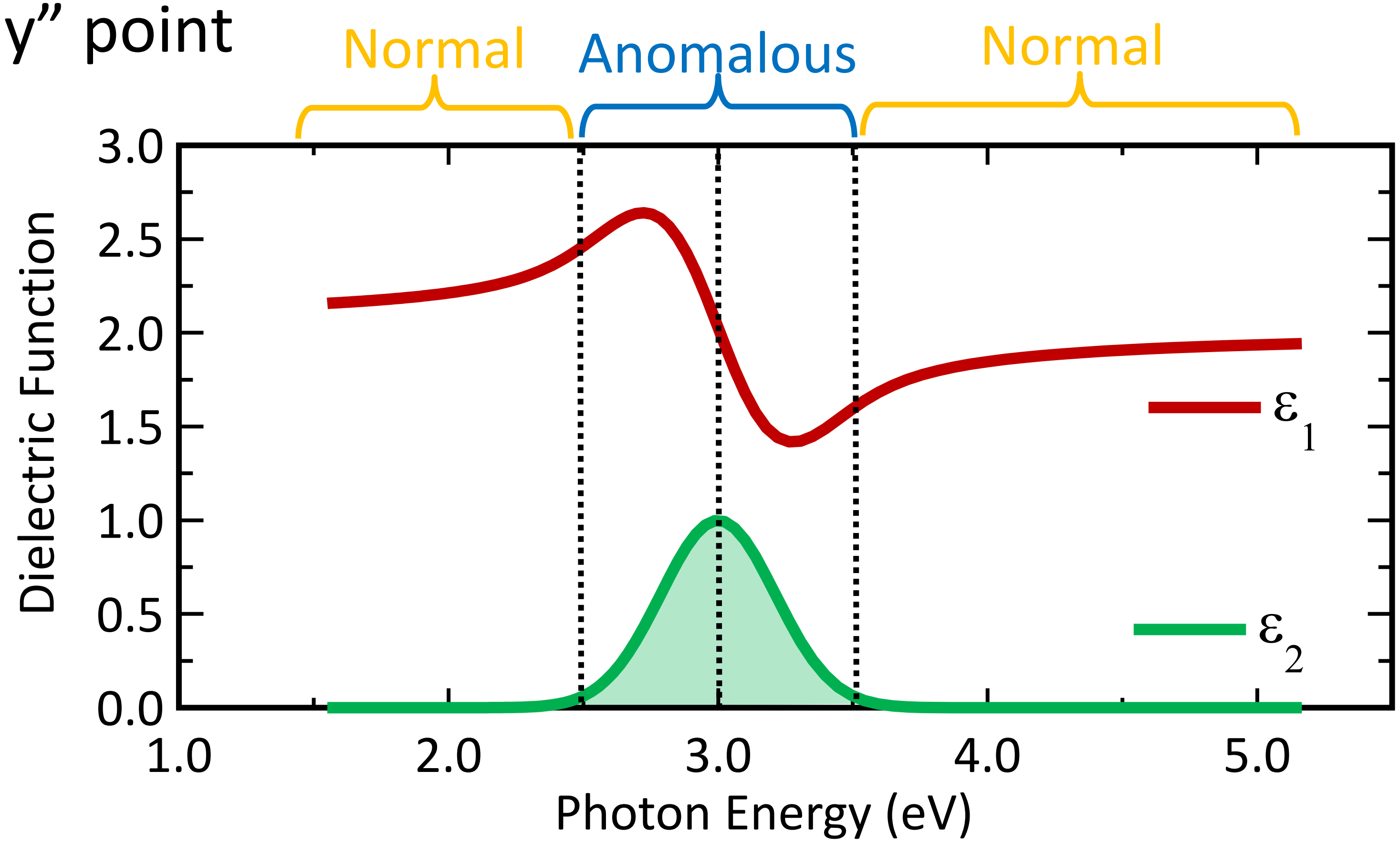


Does not guarantee correct answer, but rules out many incorrect answers

KK IMPLICATIONS ON OPTICAL FUNCTIONS

- Normal / Anomalous regions
- Integration = <u>area</u> under curve.
- Absorption peak is "half-way" point for downward wiggle.

"Bumps Make Wiggles"



USING THE KK EQUATION

- We will describe ε_2 and calculate ε_1 from KK equation:

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

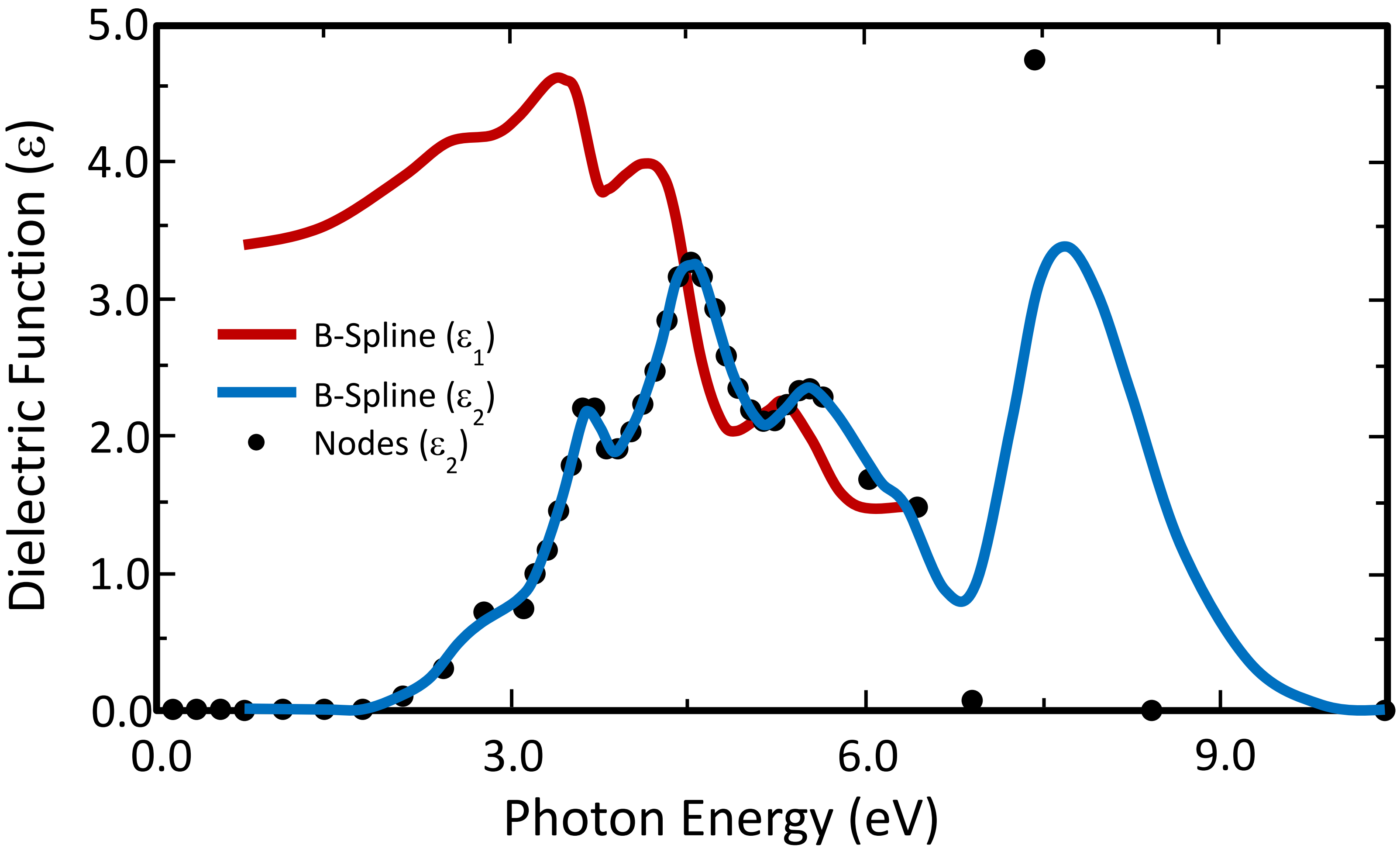
- Bumps create Wiggles
  - Every absorption *bump* in ε_2 is associated with a roll-over *wiggle* in ε_1
  - Larger *bumps* create larger *wiggles*.

- All Frequencies
  - The calculation of ε_1 depends on the values of ε_2 at ALL Frequencies.

KRAMERS-KRONIG B-SPLINE

- Substrate = B-Spline
  - Resolution (eV) = 0.300   19 Pts. (0.729-6.200 eV)   **Draw Node Graph**
  - Fit Opt. Const. = ON
  - Use KK Mode = ON (In Use)
  - **- Kramers-Kronig**
    - E Inf = **1.250** (fit)
    - IR Amp = **0.00** (fit)   IR Br = 0.000
    - Use Default TieOff Behavior = ON
    - View Tie Off Positions = OFF
  - **+ Nodes**
  - **+ Advanced**

KRAMERS-KRONIG B-SPLINE



- B-Spline function for ε_2
- KK integral used for ε_1

To account for ALL frequencies:

- **Einf** (constant offset)
- **IR Amp** and **IR Br** (low-eV contribution)
- **Tie-Offs** (absorption outside measured range)

3-3_SiC_on_Si.SE (REVISIT)

- **Determine SiC optical constants using B-Spline method** (this time use KK mode)

QUESTIONS:

- Does surface roughness help?
- Does grading help?
- Does anisotropy help?
- Did you try any other alternate models?

MORE B-SPLINE FEATURES: NODES

Roughness = **1.33 nm** (fit)

- Layer # 1 = B-Spline Thickness # 1 = **591.51 nm** (fit)
  - Resolution (eV) = 0.150 39 Pts. (0.731-6.451 eV) **Draw Node Graph**
  - Fit Opt. Const. = ON
  - Use KK Mode = OFF
  - **Nodes**
    - Init. values: n = 1.500 k = 0.00 Starting Mat = Cauchy Film
    - Force E2 Positive = OFF
    - Assume Transparent Region = OFF
    - Show Nodes = OFF
    - Node Spacing Spectral Ranges: Add Delete Delete All
  - + **Advanced**

Substrate = SI_JAW

Assume Transparent Region = ON
Assume Band Gap = ON Band Gap (eV) = 1.200

Assume Transparent Region = ON
Assume Band Gap = OFF Transparent Region = 500.0 nm - 10000.0 nm

CONVERT TO TRANSPARENT B-SPLINE

Fit Transparent Region using Cauchy Procedure

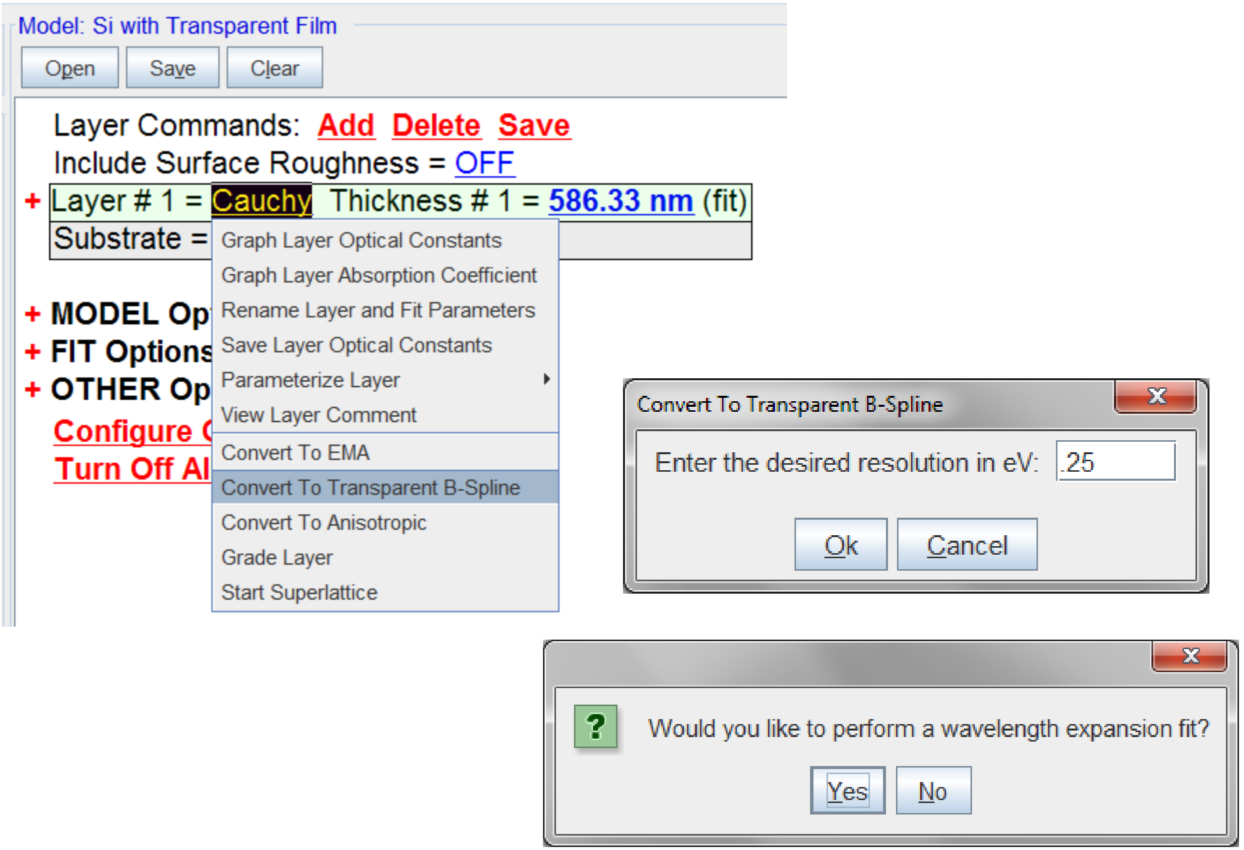
⬇

Right-Click on Cauchy → "Convert to Transparent B-Spline"

- Enter Node Resolution
- Wavelength-Expansion Fit

⬇

Optimize Node Resolution, Roughness, Grading,…



- Forces e2 positive, uses KK mode, sets Cauchy range to be transparent

BREAKDOWN OF 'CONVERT TO TRANSPARENT B-SPLINE'

Changes layer type to B-Spline using desired resolution in eV

↓

Sets Cauchy wavelength range to be transparent range

↓

Turns on KK mode

↓

Forces e2 positive

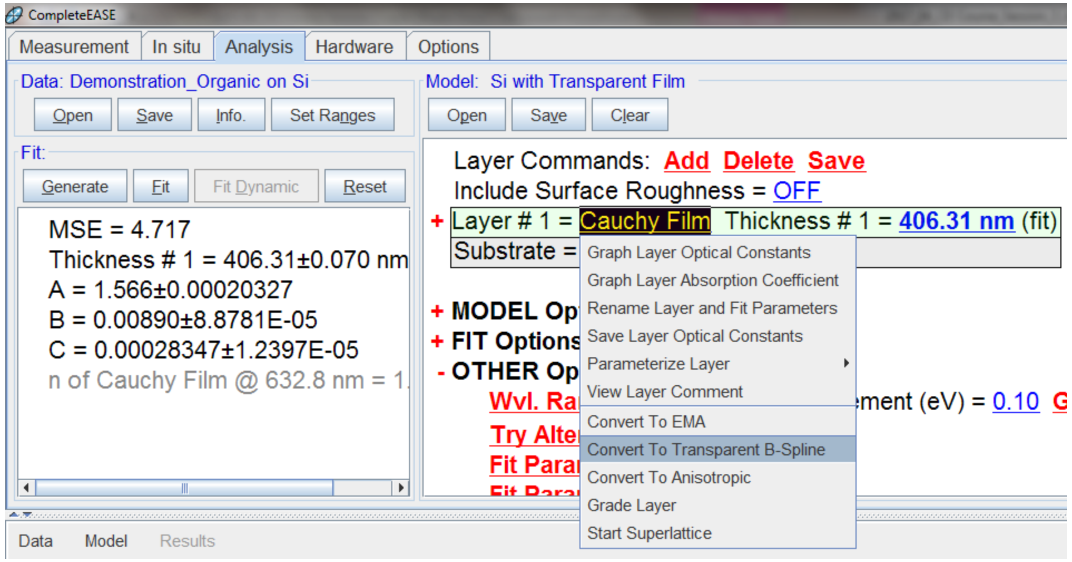
↓

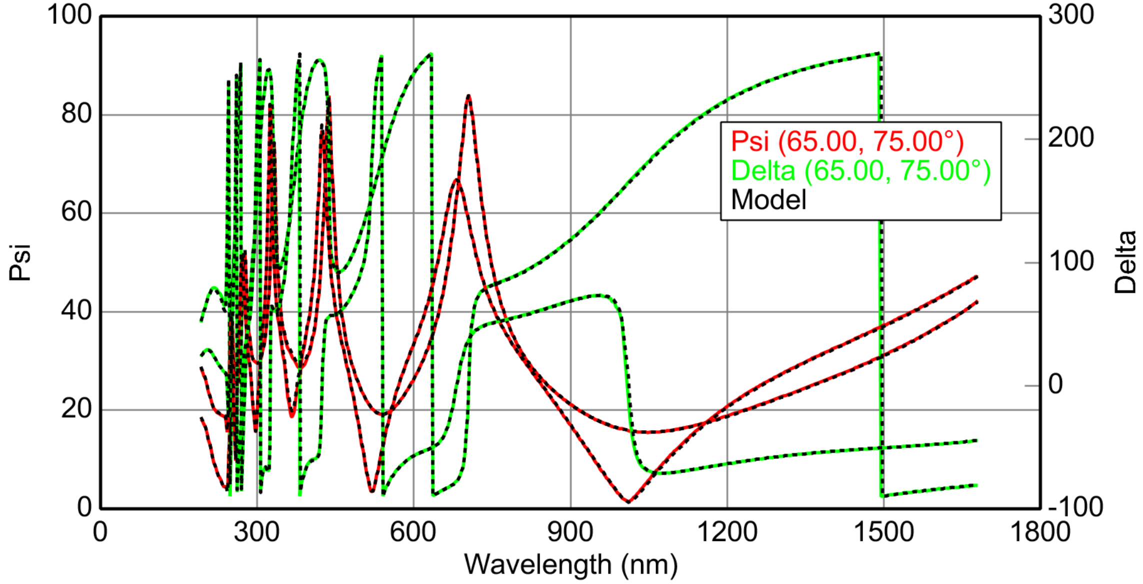
Performs Wavelength Range Expansion Fit

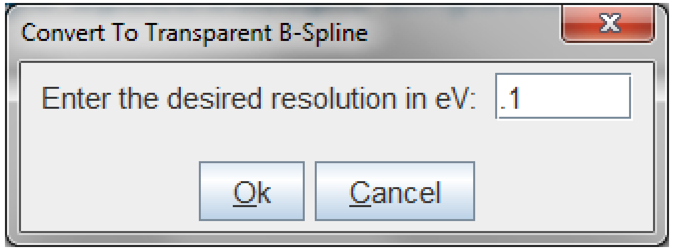
↓

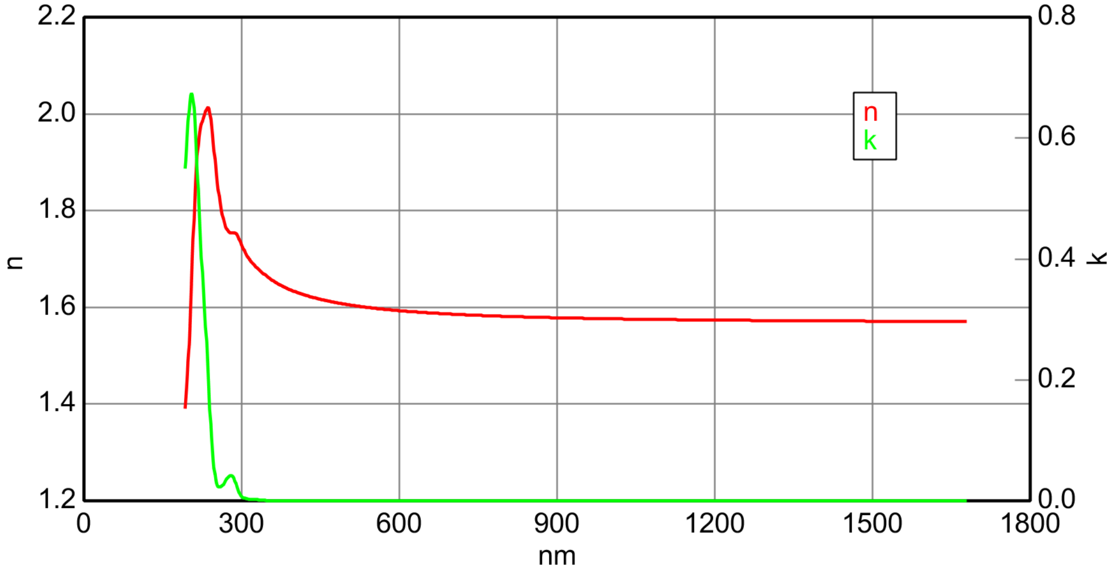
Reevaluates tie-off on the UV side

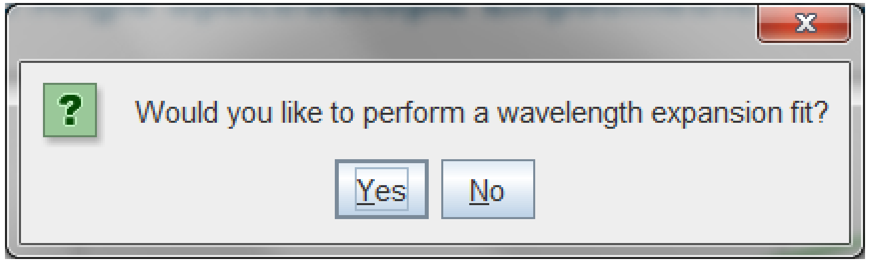
DEMONSTRATION: ORGANIC ON SI











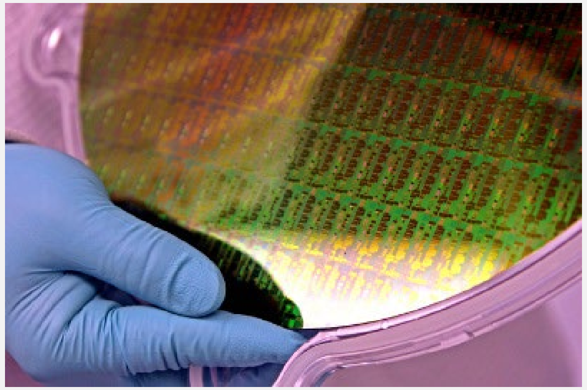
SIMPLIFIED B-SPLINE PROCEDURE

Si with Transparent Film → Transparent B-spline

1. **Fit Transparent Region with built-in Si with Transparent Film Model**
2. **Right-Click on Cauchy Film → Convert To Transparent B-Spline**
3. **Enter resolution in eV**
4. **Click Yes to perform Wavelength Range Expansion Fit**
5. **Optimize Node Resolution, Roughness, Grading,…**

3-4_Photoresist_on_Si.SE

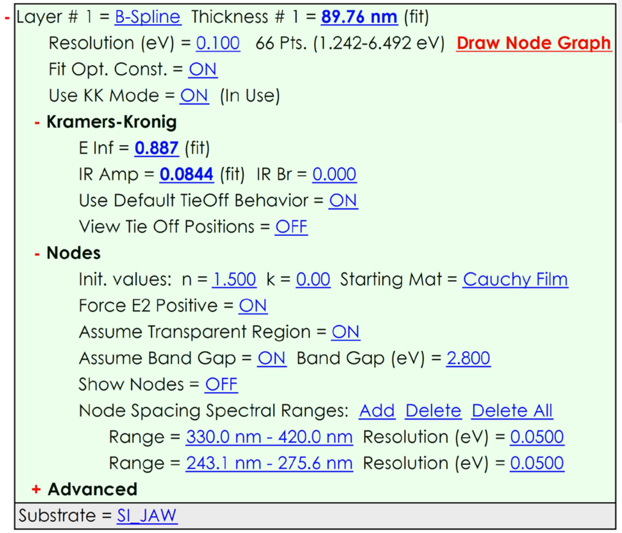
- **Determine optical constants using B-Spline method** (starting with Transparent Cauchy)



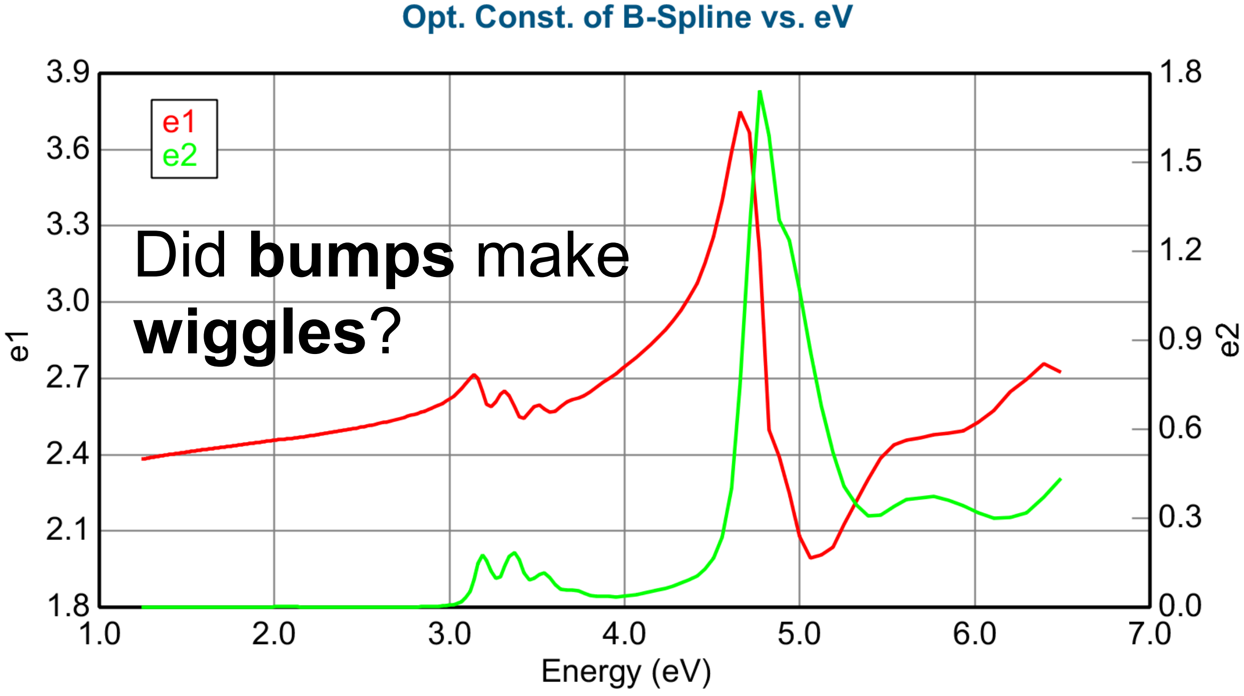
QUESTIONS:

- What is preferred node resolution?
- Transparent region?

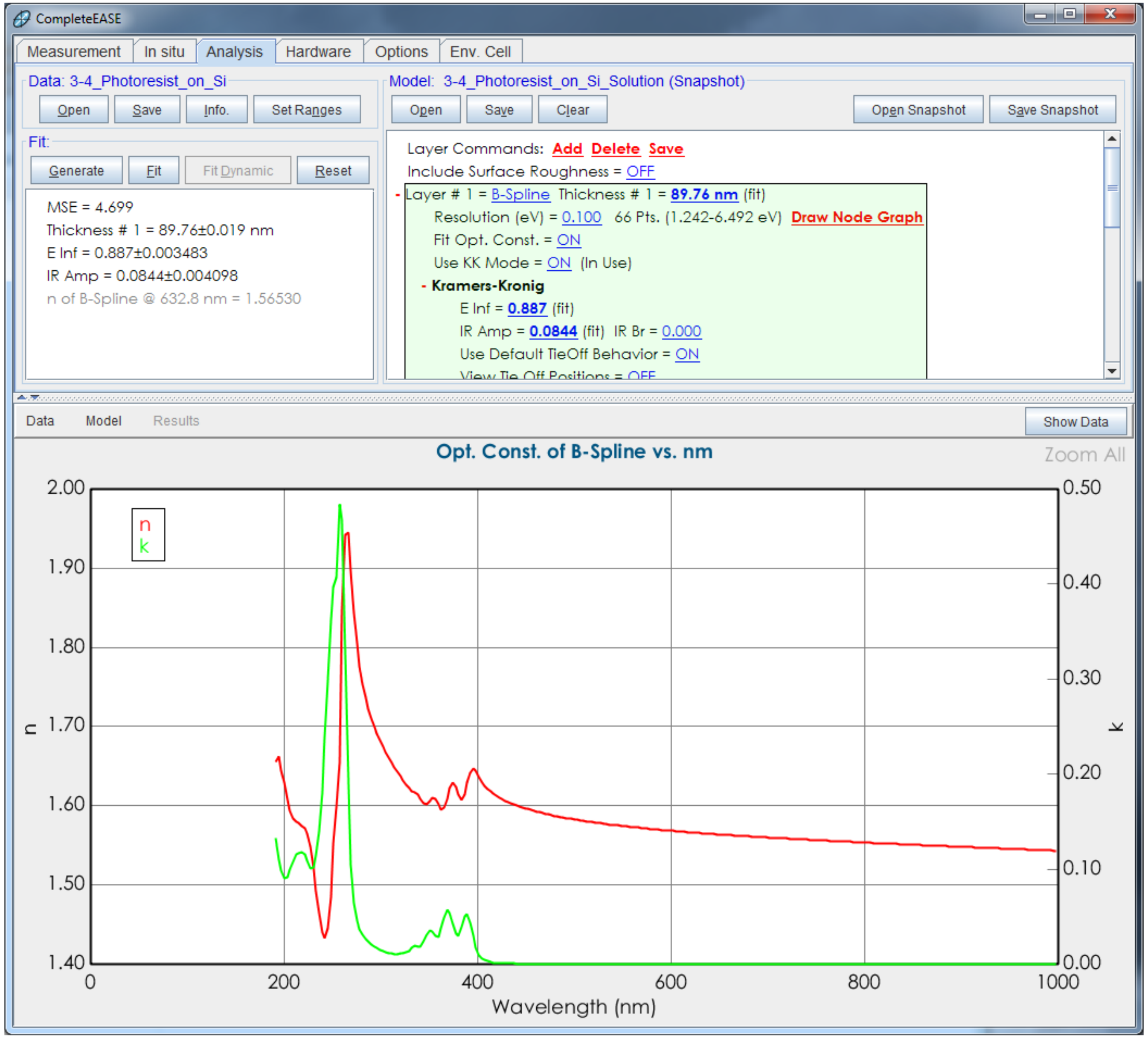
RESULTS



Layer # 1 = B-Spline Thickness # 1 = 89.76 nm (fit)
Resolution (eV) = 0.100 66 Pts. (1.242-6.492 eV) Draw Node Graph
Fit Opt. Const. = ON
Use KK Mode = ON (In Use)
- Kramers-Kronig
E Inf = 0.887 (fit)
IR Amp = 0.0844 (fit) IR Br = 0.000
Use Default TieOff Behavior = ON
View Tie Off Positions = OFF
- Nodes
Init. values: n = 1.500 k = 0.00 Starting Mat = Cauchy Film
Force E2 Positive = ON
Assume Transparent Region = ON
Assume Band Gap = ON Band Gap (eV) = 2.800
Show Nodes = OFF
Node Spacing Spectral Ranges: Add Delete Delete All
Range = 330.0 nm - 420.0 nm Resolution (eV) = 0.0500
Range = 243.1 nm - 275.6 nm Resolution (eV) = 0.0500
+ Advanced
Substrate = SI_JAW

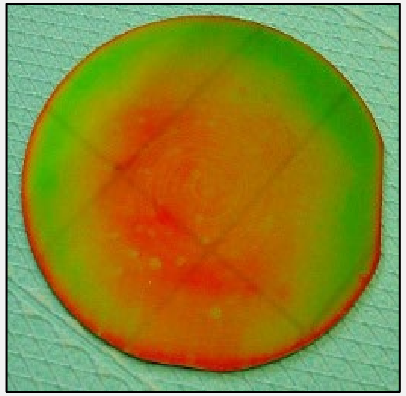


Opt. Const. of B-Spline vs. eV
e1
e2
Did bumps make wiggles?
Energy (eV)
1.0
2.0
3.0
4.0
5.0
6.0
7.0
1.8
2.1
2.4
2.7
3.0
3.3
3.6
3.9
0.0
0.3
0.6
0.9
1.2
1.5
1.8



CompleteEASE
Measurement
In situ
Analysis
Hardware
Options
Env. Cell
Data: 3-4_Photoresist_on_Si
Open
Save
Info.
Set Ranges
Model: 3-4_Photoresist_on_Si_Solution (Snapshot)
Open
Save
Clear
Open Snapshot
Save Snapshot
Fit:
Generate
Fit
Fit Dynamic
Reset
MSE = 4.699
Thickness # 1 = 89.76±0.019 nm
E Inf = 0.887±0.003483
IR Amp = 0.0844±0.004098
n of B-Spline @ 632.8 nm = 1.56530
Layer Commands: Add Delete Save
Include Surface Roughness = OFF
Layer # 1 = B-Spline Thickness # 1 = 89.76 nm (fit)
Resolution (eV) = 0.100 66 Pts. (1.242-6.492 eV) Draw Node Graph
Fit Opt. Const. = ON
Use KK Mode = ON (In Use)
- Kramers-Kronig
E Inf = 0.887 (fit)
IR Amp = 0.0844 (fit) IR Br = 0.000
Use Default TieOff Behavior = ON
Data
Model
Results
Show Data
Opt. Const. of B-Spline vs. nm
Zoom All
n
k
Wavelength (nm)
0
200
400
600
800
1000
1.40
1.50
1.60
1.70
1.80
1.90
2.00
0.00
0.10
0.20
0.30
0.40
0.50

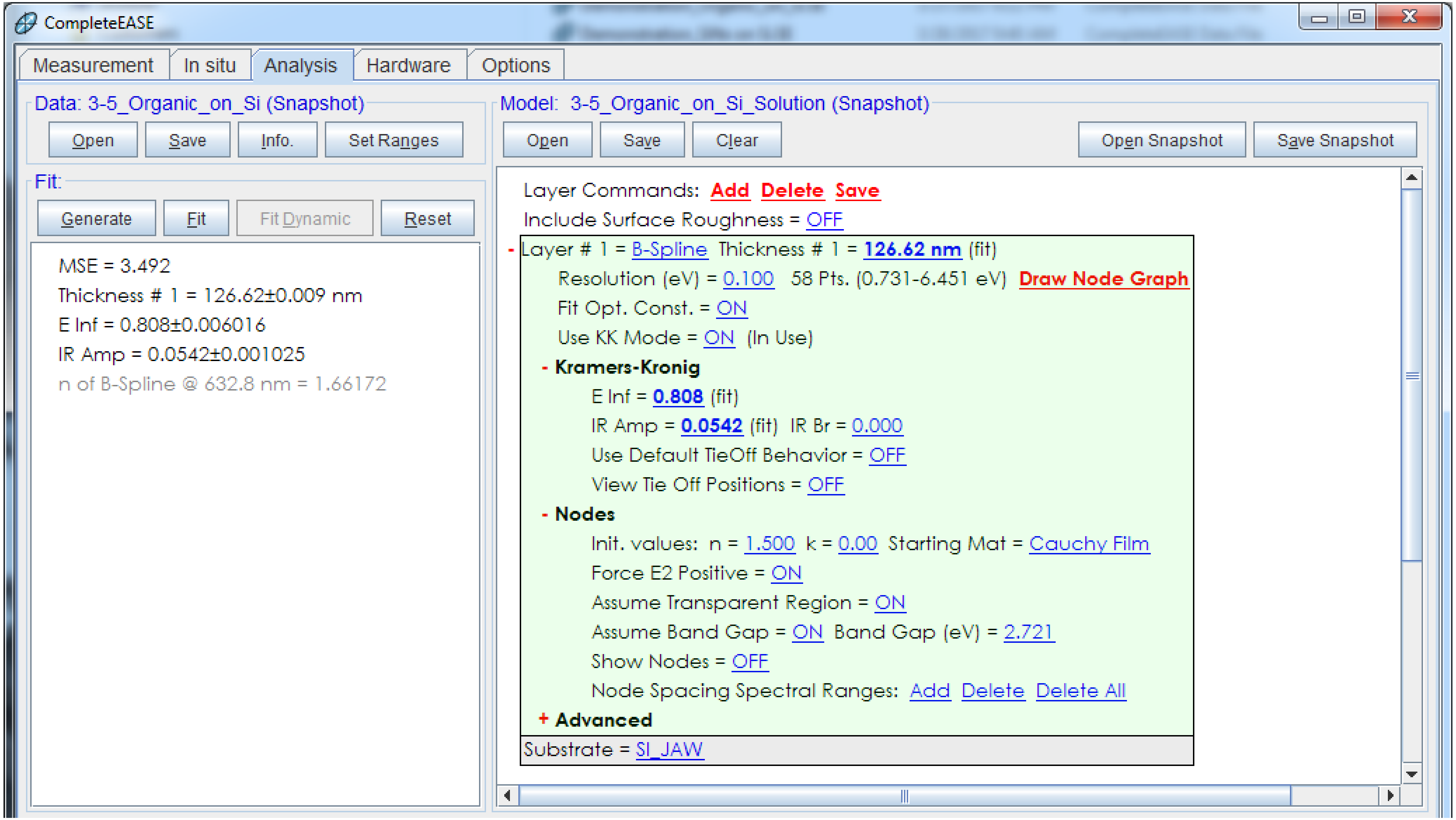
- **Determine optical constants using the Simplified B-Spline Procedure**



QUESTIONS:

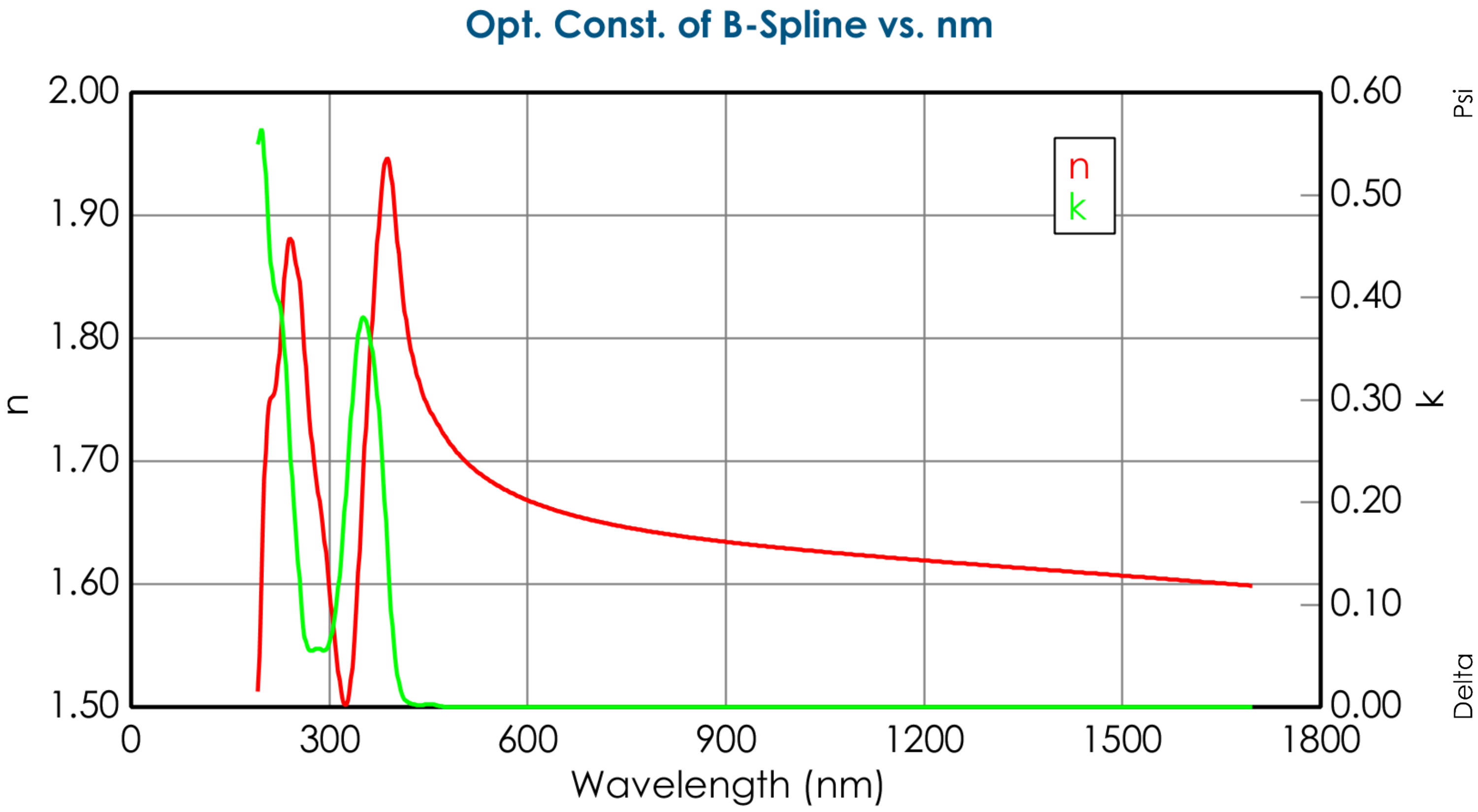
- What is preferred node resolution?

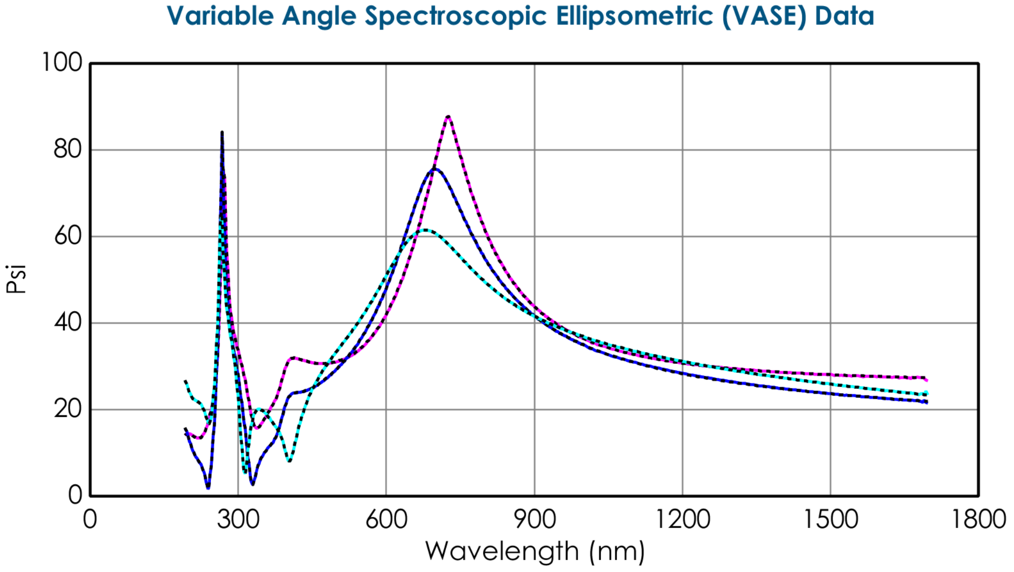
RESULTS

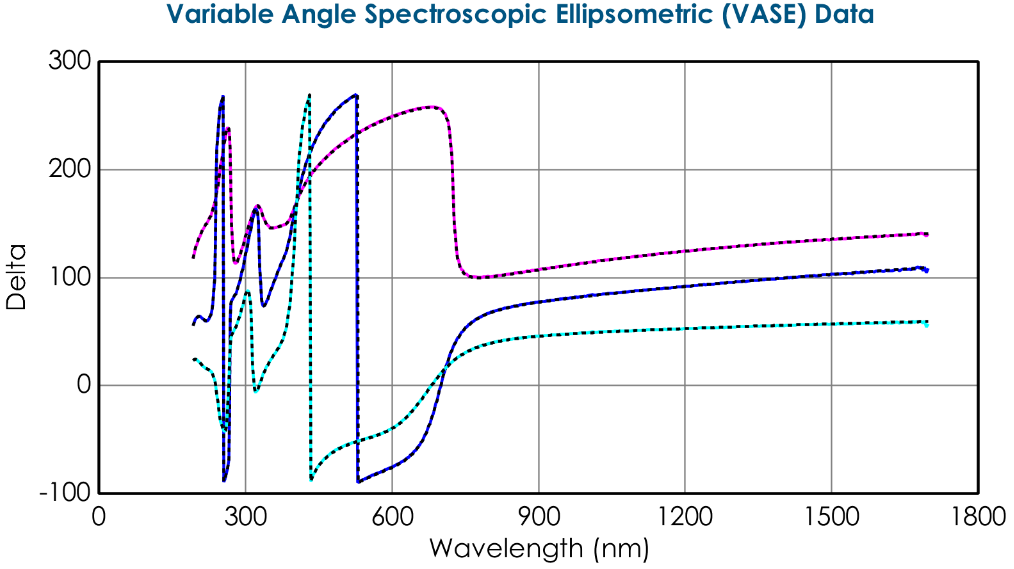


CompleteEASE
Measurement
In situ
Analysis
Hardware
Options
Data: 3-5_Organic_on_Si (Snapshot)
Open
Save
Info.
Set Ranges
Fit:
Generate
Fit
Fit Dynamic
Reset
MSE = 3.492
Thickness # 1 = 126.62±0.009 nm
E Inf = 0.808±0.006016
IR Amp = 0.0542±0.001025
n of B-Spline @ 632.8 nm = 1.66172
Model: 3-5_Organic_on_Si_Solution (Snapshot)
Open
Save
Clear
Open Snapshot
Save Snapshot
Layer Commands: Add Delete Save
Include Surface Roughness = OFF
- Layer # 1 = B-Spline Thickness # 1 = 126.62 nm (fit)
Resolution (eV) = 0.100 58 Pts. (0.731-6.451 eV) Draw Node Graph
Fit Opt. Const. = ON
Use KK Mode = ON (In Use)
- Kramers-Kronig
E Inf = 0.808 (fit)
IR Amp = 0.0542 (fit) IR Br = 0.000
Use Default TieOff Behavior = OFF
View Tie Off Positions = OFF
- Nodes
Init. values: n = 1.500 k = 0.00 Starting Mat = Cauchy Film
Force E2 Positive = ON
Assume Transparent Region = ON
Assume Band Gap = ON Band Gap (eV) = 2.721
Show Nodes = OFF
Node Spacing Spectral Ranges: Add Delete Delete All
+ Advanced
Substrate = SI_JAW

RESULTS – CONTINUED







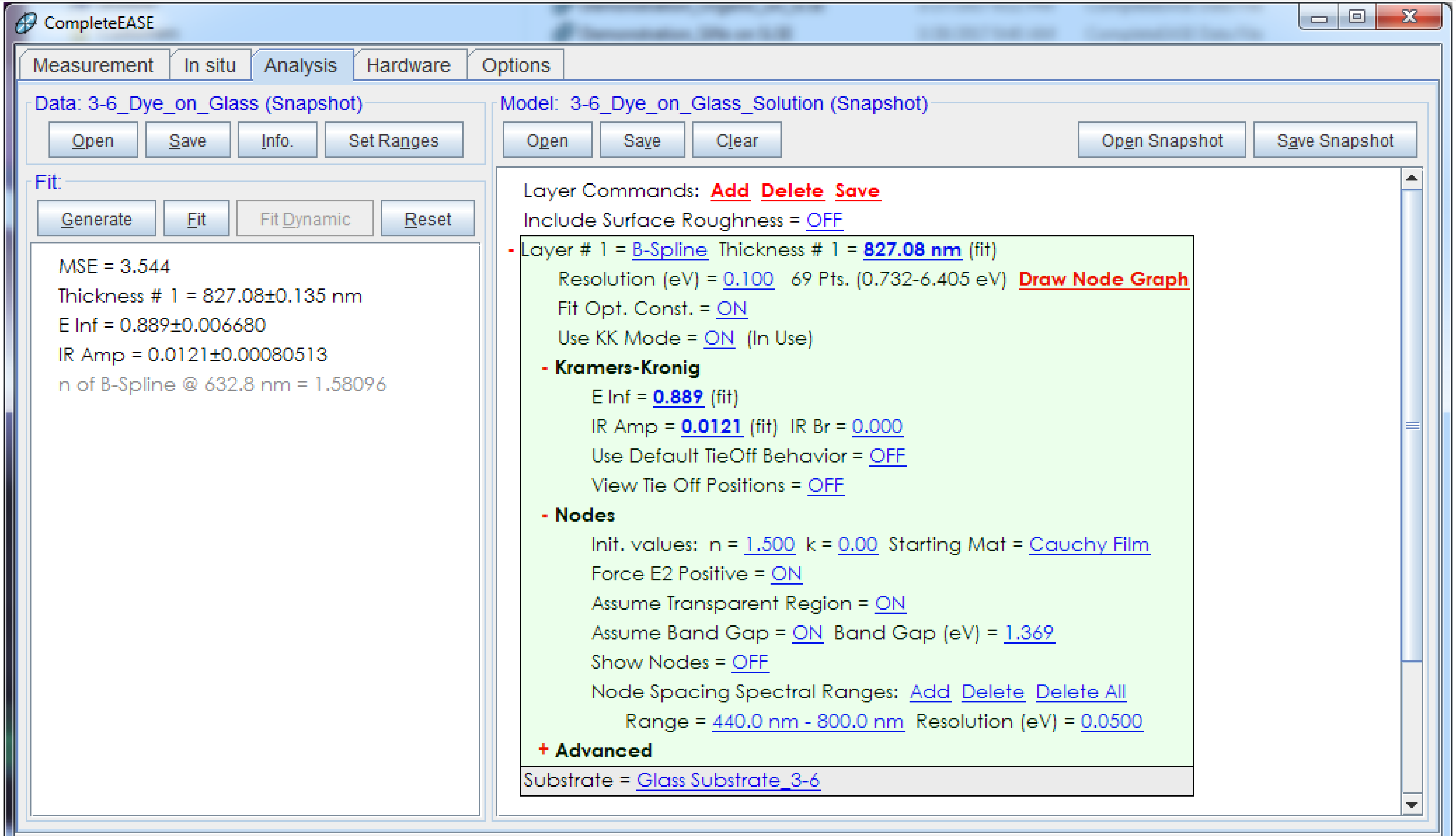
6 3-6_Dye_on_Glass.SE

- Determine optical constants using Simplified B-Spline method
- Use "Glass_Substrate_3-6.mat"

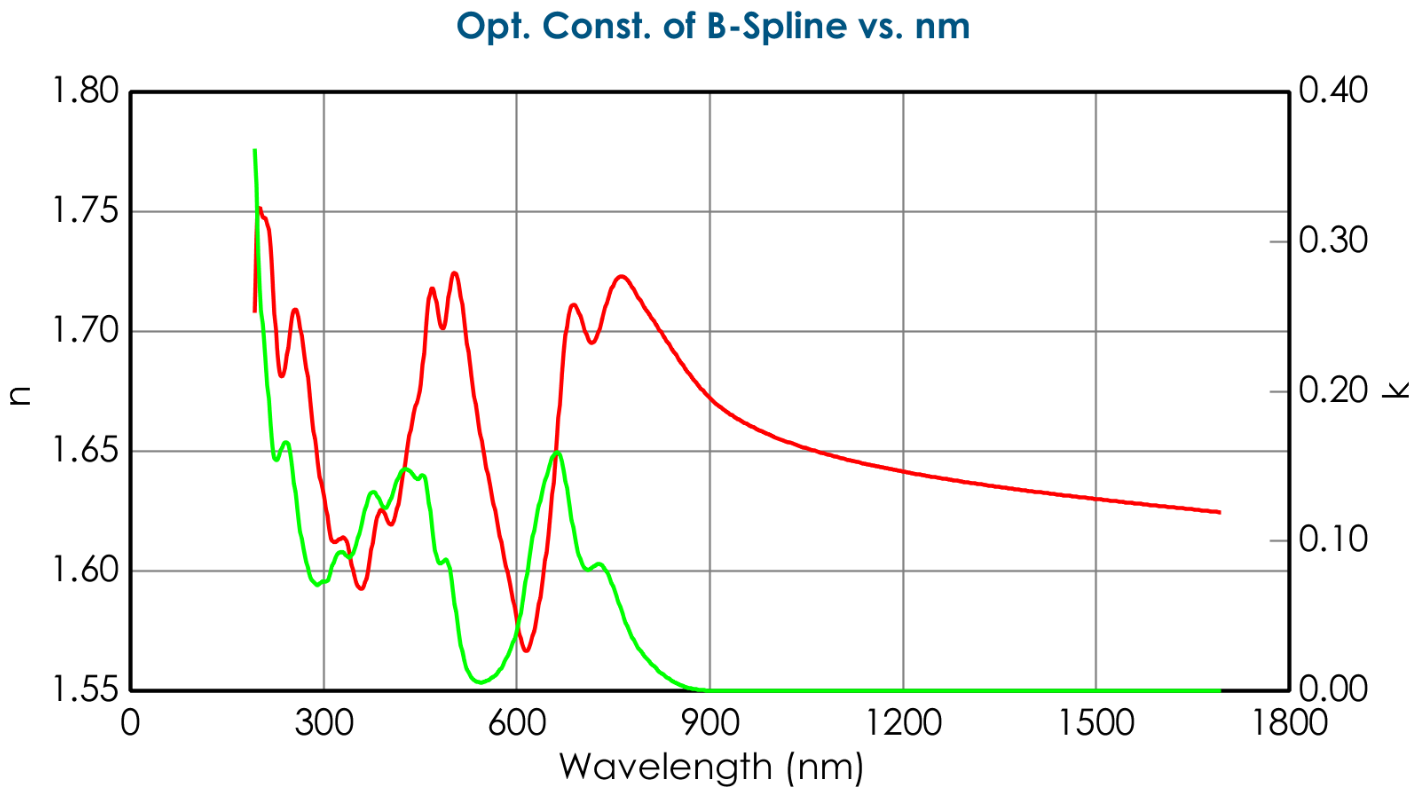
QUESTIONS:

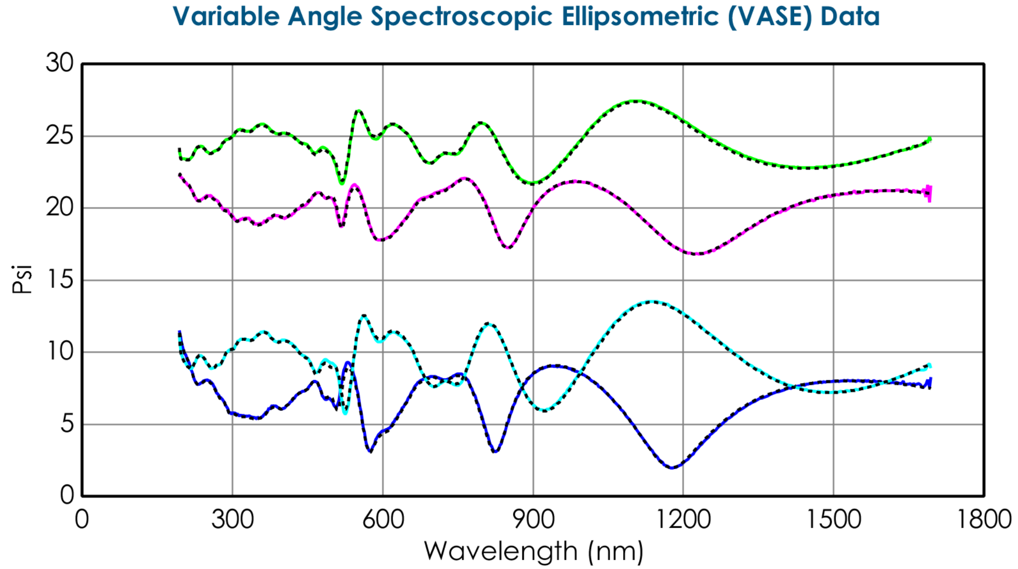
- What is preferred node resolution?
- Is your result correct?

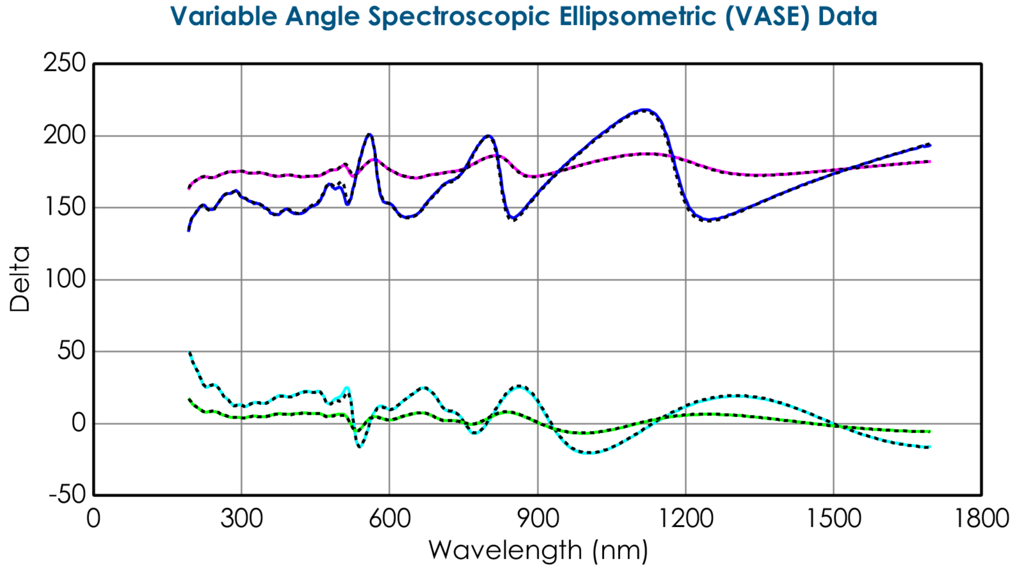
RESULTS


CompleteEASE
Measurement
In situ
Analysis
Hardware
Options
Data: 3-6_Dye_on_Glass (Snapshot)
Open
Save
Info.
Set Ranges
Fit:
Generate
Fit
Fit Dynamic
Reset
MSE = 3.544
Thickness # 1 = 827.08±0.135 nm
E Inf = 0.889±0.006680
IR Amp = 0.0121±0.00080513
n of B-Spline @ 632.8 nm = 1.58096
Model: 3-6_Dye_on_Glass_Solution (Snapshot)
Open
Save
Clear
Open Snapshot
Save Snapshot
Layer Commands: Add Delete Save
Include Surface Roughness = OFF
- Layer # 1 = B-Spline Thickness # 1 = 827.08 nm (fit)
Resolution (eV) = 0.100 69 Pts. (0.732-6.405 eV) Draw Node Graph
Fit Opt. Const. = ON
Use KK Mode = ON (In Use)
- Kramers-Kronig
E Inf = 0.889 (fit)
IR Amp = 0.0121 (fit) IR Br = 0.000
Use Default TieOff Behavior = OFF
View Tie Off Positions = OFF
- Nodes
Init. values: n = 1.500 k = 0.00 Starting Mat = Cauchy Film
Force E2 Positive = ON
Assume Transparent Region = ON
Assume Band Gap = ON Band Gap (eV) = 1.369
Show Nodes = OFF
Node Spacing Spectral Ranges: Add Delete Delete All
Range = 440.0 nm - 800.0 nm Resolution (eV) = 0.0500
+ Advanced
Substrate = Glass Substrate_3-6

RESULTS – CONTINUED







SESSION 3 SUMMARY

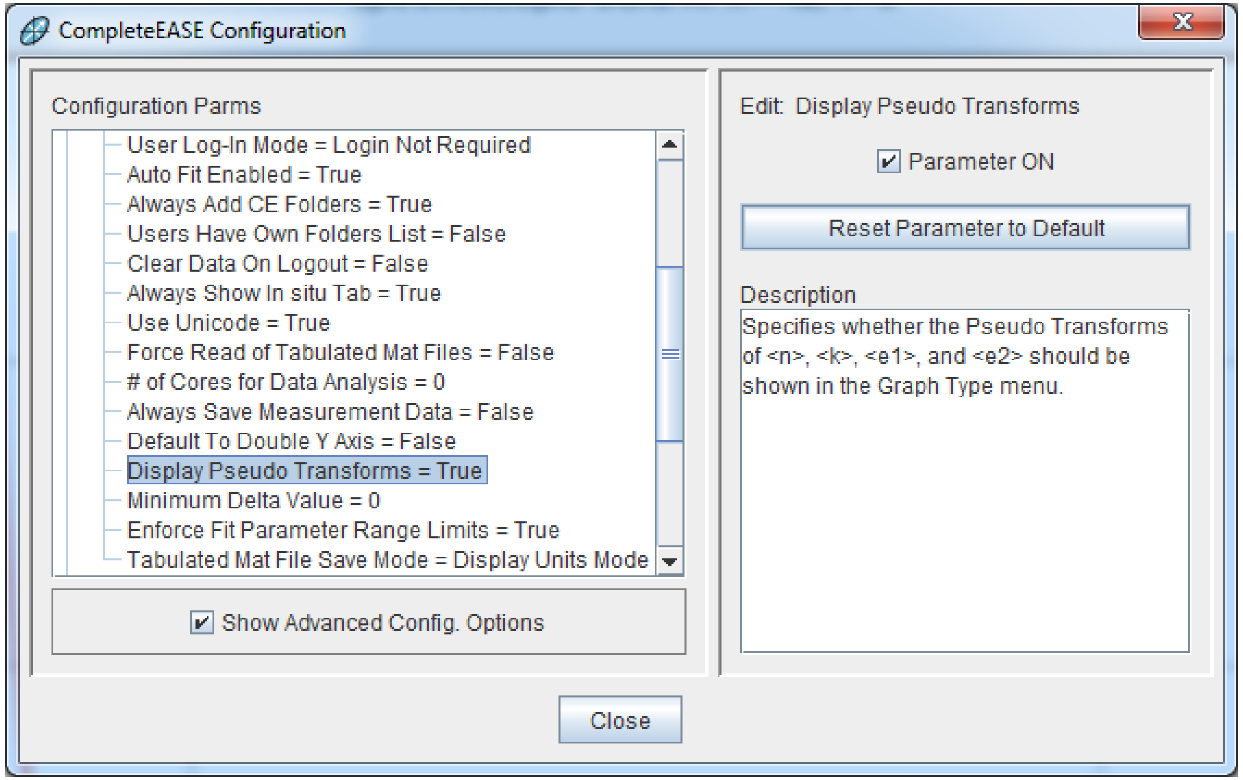
- Use B-spline Layer for:
  - Metal Films
  - UV Absorbing Films
- KK B-Spline helps ensure "physical" results
- Cauchy Fit → "Convert to KK B-spline"

THANK YOU AND ENJOY YOUR LUNCH!

ADDITIONAL SLIDES BEYOND THIS POINT

ENABLING <PSEUDO> TRANSFORMS

- In CompleteEASE 6.42 and newer, the menu option for <Pseudo> Transforms is hidden by default.
- Go to CompleteEASE Configuration > General then change Display Pseudo Transforms = True (*Show advanced must be checked)



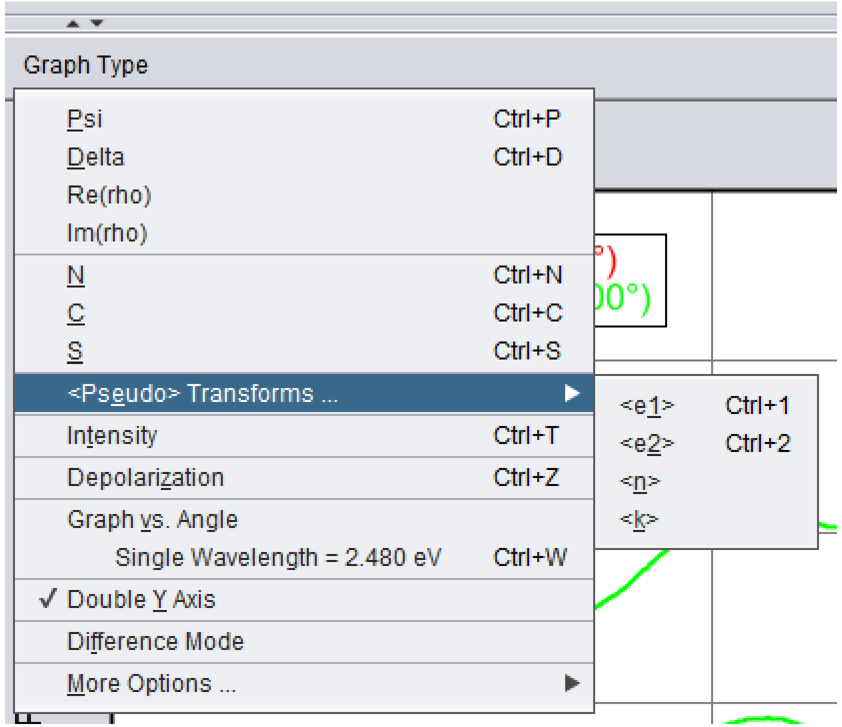
METHOD: DIRECT CONVERSION

- For single reflection from surface, data can be directly "inverted" to get n,k.

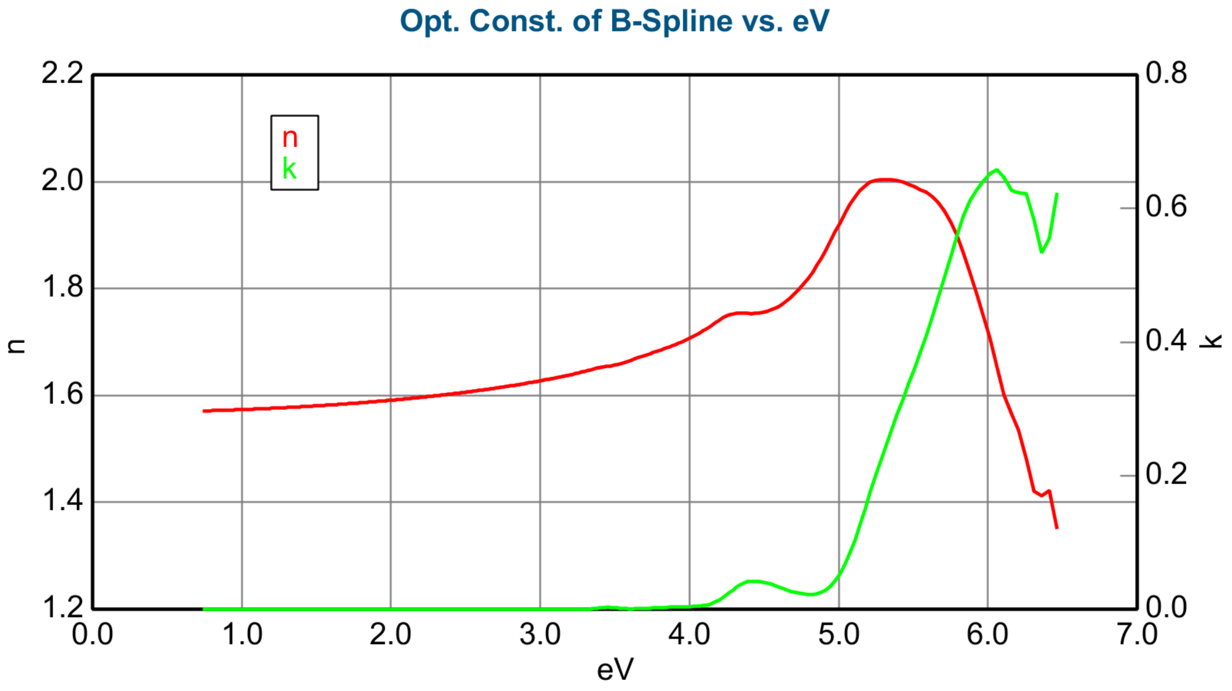
Pseudo Optical Constants
<n>&<k>, <e1>&<e2>

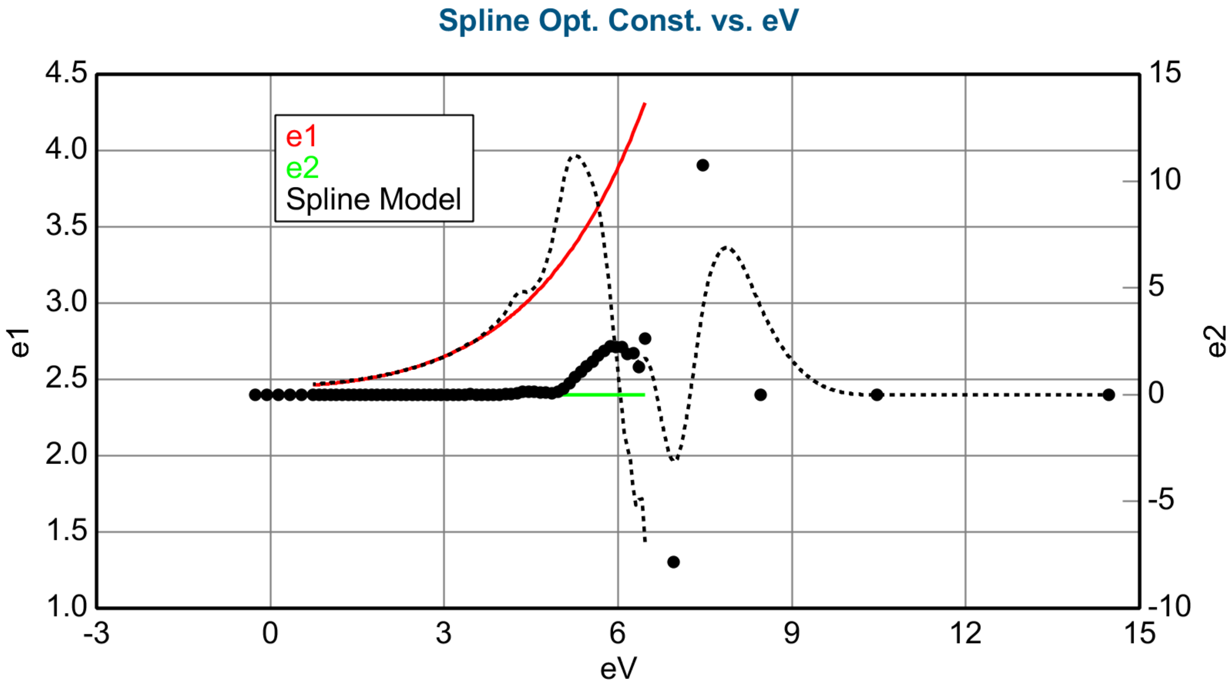
$$\langle \tilde{n} \rangle^2 = \sin^2(\phi) \cdot \left[1 + \tan^2(\phi) \cdot \left(\frac{1-\rho}{1+\rho} \right)^2 \right]$$

$$where, \quad \rho = \tan(\Psi) e^{i\Delta} = \frac{\tilde{r}_p}{\tilde{r}_s}$$



- Open “Demonstration_Organic on Si.SESnap





ADVANCED: FITTING TIE OFF NODES (2)

- Expand “Kramers-Kronig” section of B-Spline:
  - Use Default Tie Off Behavior = OFF
  - View Tie Off Positions = ON
  - Fit “Tie Off n+1” amount (Default = 0.5eV)

- Layer # 1 = B-Spline Thickness # 1 = **406.22 nm** (fit)
  Resolution (eV) = 0.100 58 Pts. (0.738-6.464 eV) **Draw Node Graph**
  Fit Opt. Const. = ON
  Use KK Mode = ON (In Use)
  - **Kramers-Kronig**
    E Inf = **0.627** (fit)
    IR Amp = 0.00 IR Br = 0.000
    Use Default TieOff Behavior = OFF
    View Tie Off Positions = ON
    Tie Off 0 {TieOff(1)-E} = 0.2000
    Tie Off 1 {TieOff(2)-E} = 0.2000
    Tie Off 2 {TieOff(3)-E} = 0.2000 spline_e2(0.138) = 0.000
    Tie Off 3 {TieOff(4)-E} = 0.2000 spline_e2(0.338) = 0.000
    Tie Off 4 (min-E) = 0.2000 spline_e2(0.538) = 0.000
    Tie Off n+1 (max+E) = **0.5000** (fit) spline_e2(6.964) = **-7.8209** (fit)
    Tie Off n+2 {TieOff(n+1)+E} = 0.5000 spline_e2(7.464) = **10.7291** (fit)
    Tie Off n+3 {TieOff(n+2)+E} = 1.0000 spline_e2(8.464) = 0.000
    Tie Off n+4 {TieOff(n+3)+E} = 2.0000
    Tie Off n+5 {TieOff(n+4)+E} = 4.0000
  + **Nodes**
  + **Advanced**

Substrate = SI_JAW

ADVANCED: FITTING TIE OFF NODES (3)

- Results after fitting Tie Off Position.

Fit adjusts value from 0.5 to 4