J.A. Woollam

Ellipsometry Solutions

Semi-absorbing Films using the General Oscillator Layer

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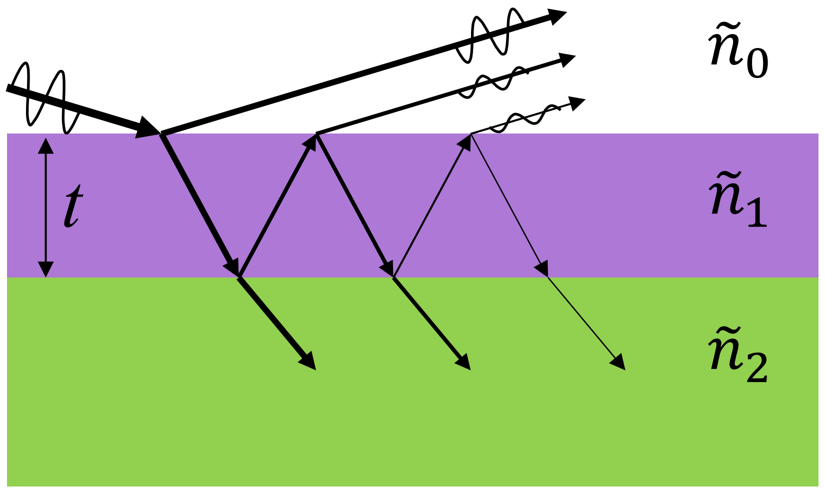
Course Outline

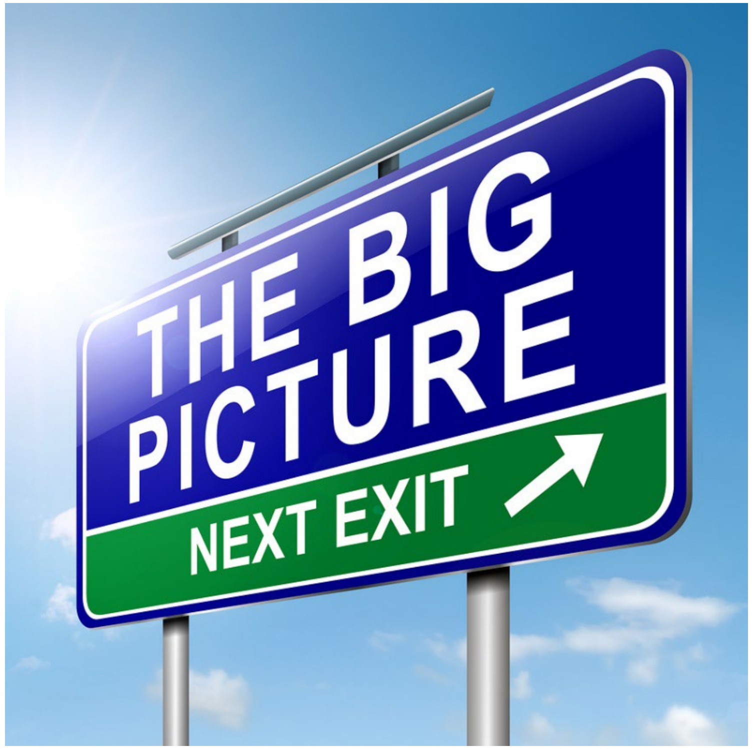
- Session 1: Theory, Substrates (Si and Glass)
- Session 2: Transparent Films
- Session 3: Absorbing & Semi-Absorbing Films (B-Spline)
- **Session 4: Semi-Absorbing Films (Gen-Osc)**
- Session 5: Thin Absorbing Films and Multilayers
- Session 6: Advanced Topics



Session 4 Outline

- General Oscillator Layer
- Fitting materials with absorption using Gen-Osc
  - Pre-built Gen-Osc layers
  - Creating your own Gen-Osc
  - Cauchy → B-Spline → Gen-Osc
- Gen-Osc Diagnosis

Using the Gen-Osc Layer

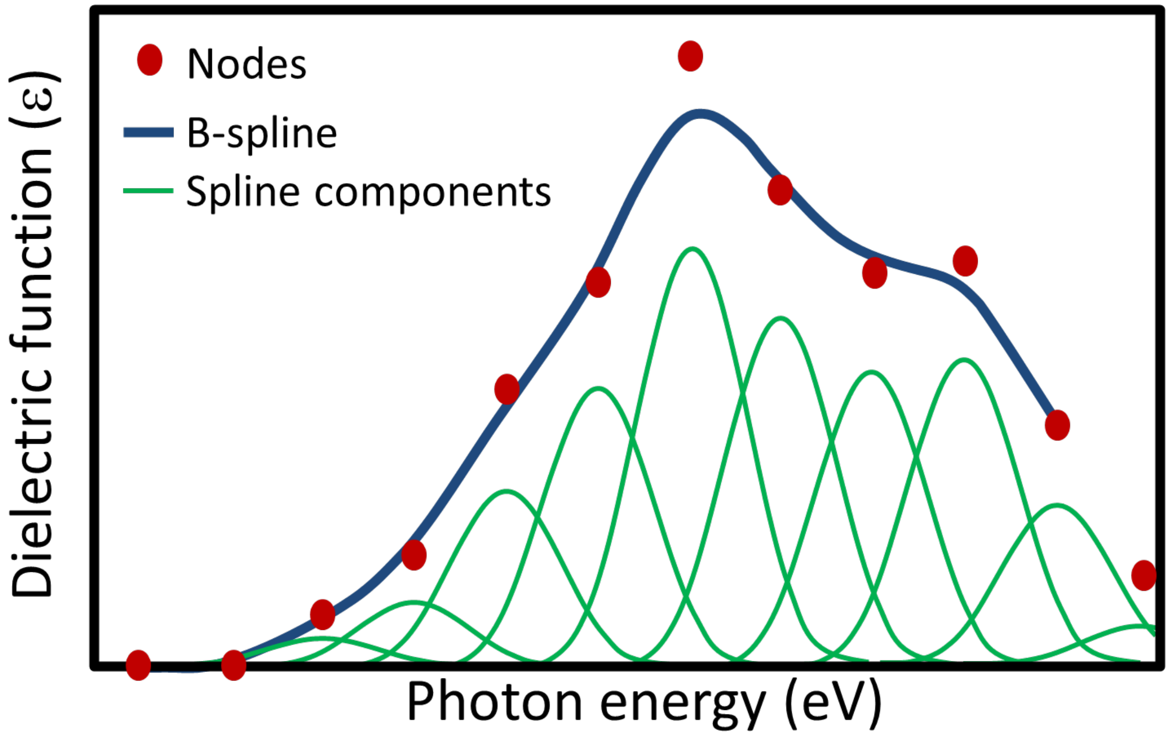


- Gen-Osc contains equations to describe material optical constants
- It is useful for any material (transparent or absorbing)
- It is often more robust than the B-spline

Modeling Absorbing Region

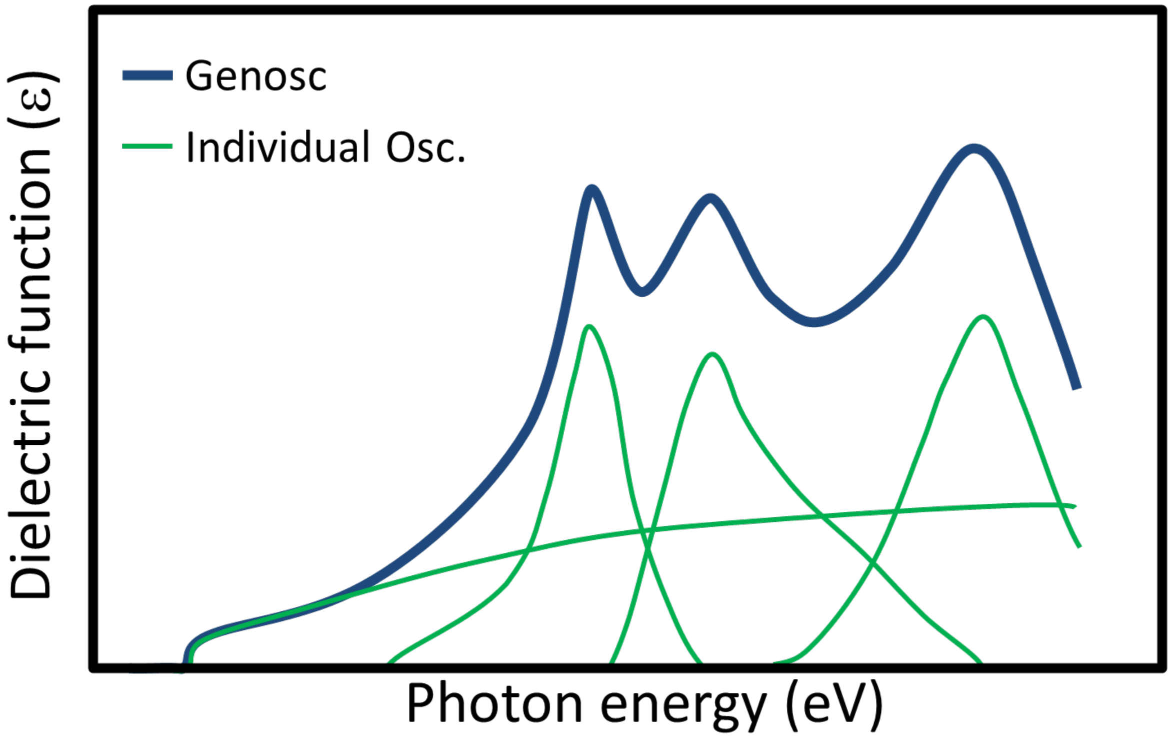
B-Spline

- Overlapping “hills” at preset spacing



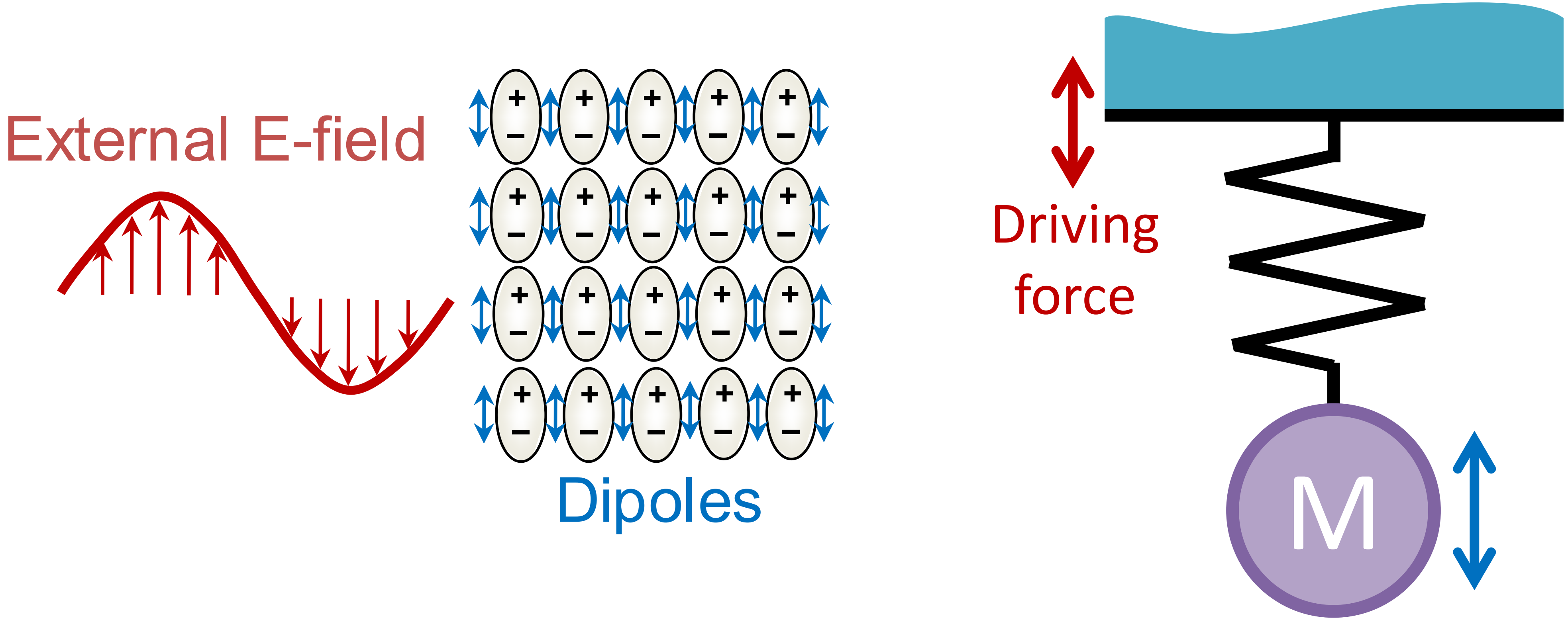
Gen-Osc

- Choice of “hills” with selective shapes

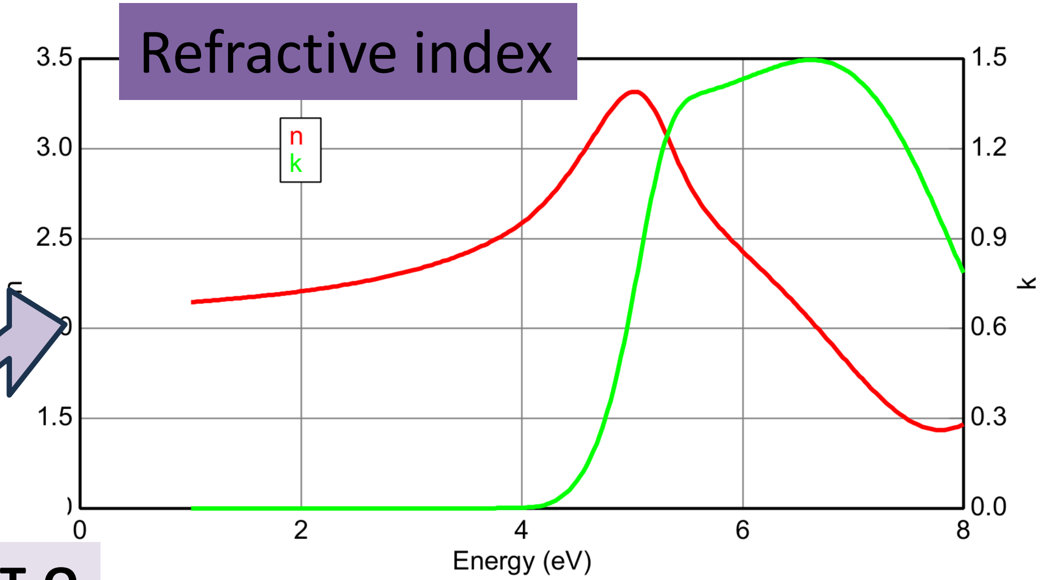


Oscillator Model for Optical Functions

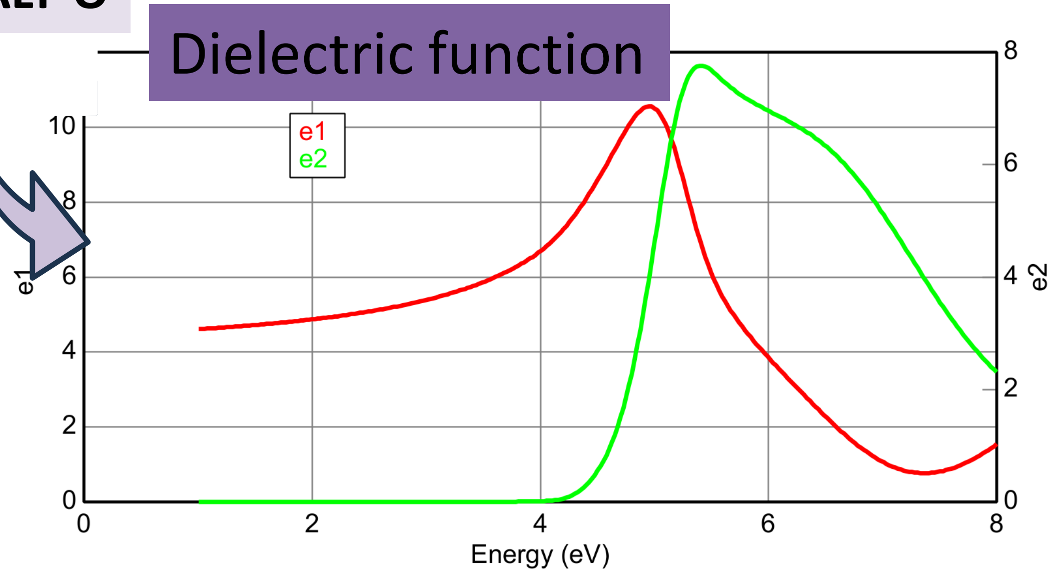
- Interaction between light and materials (optical vibration) can be described by same classical equation of motion as mass on a spring (mechanical vibration)

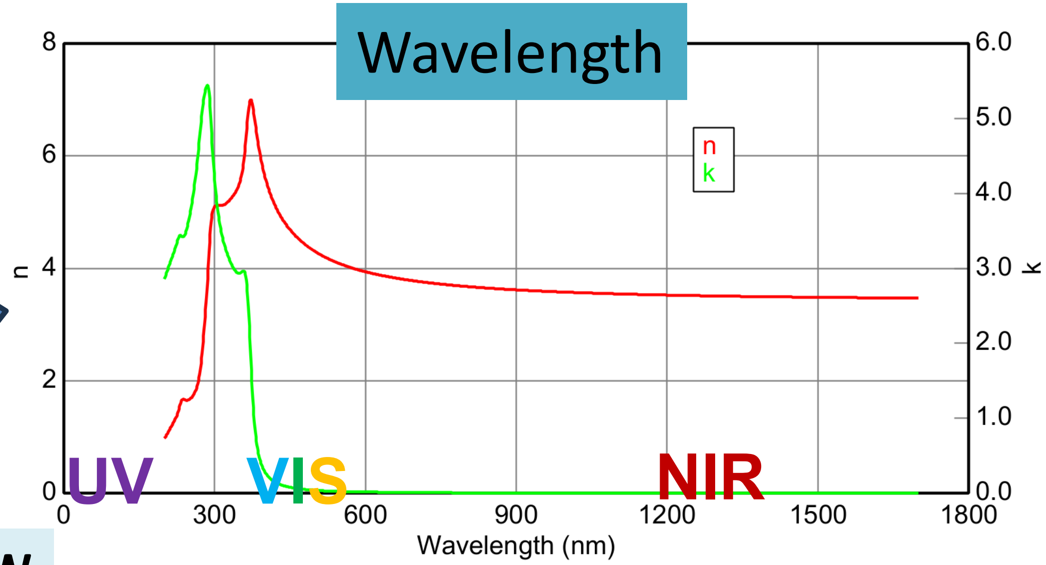


Using Different Units



CTRL-ALT-O





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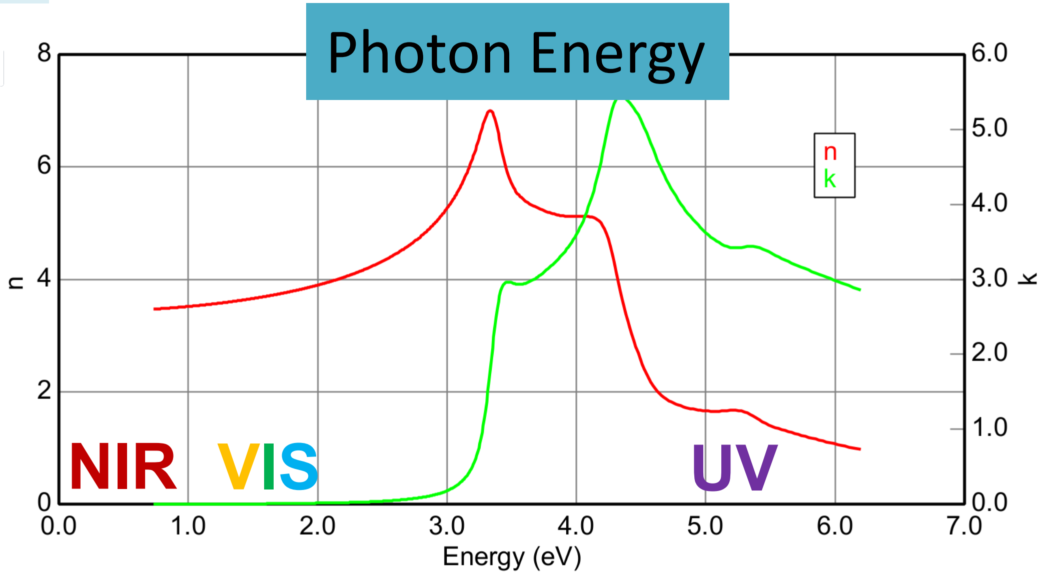
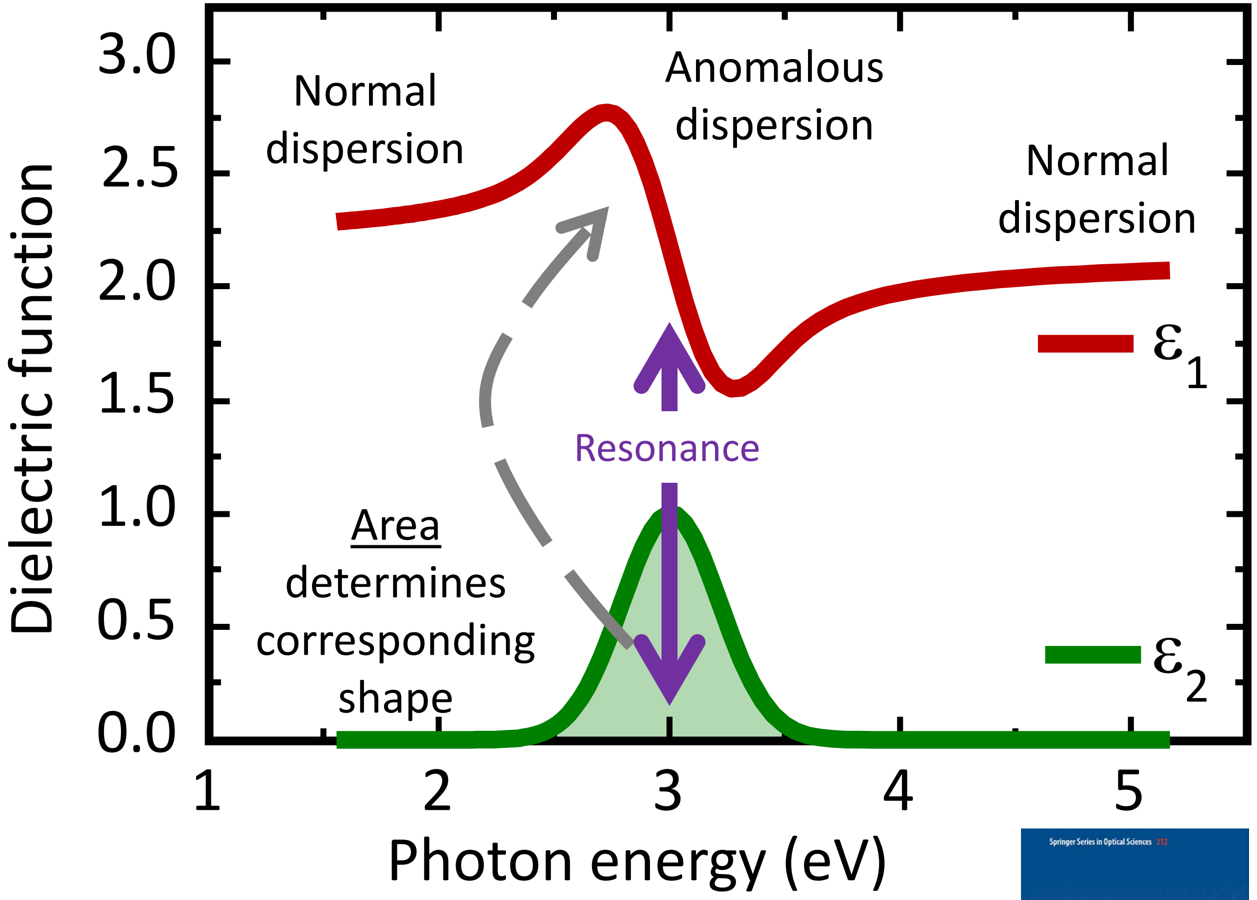
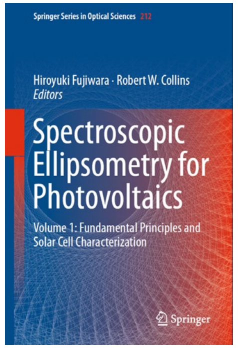


Kramers Kronig Consistency

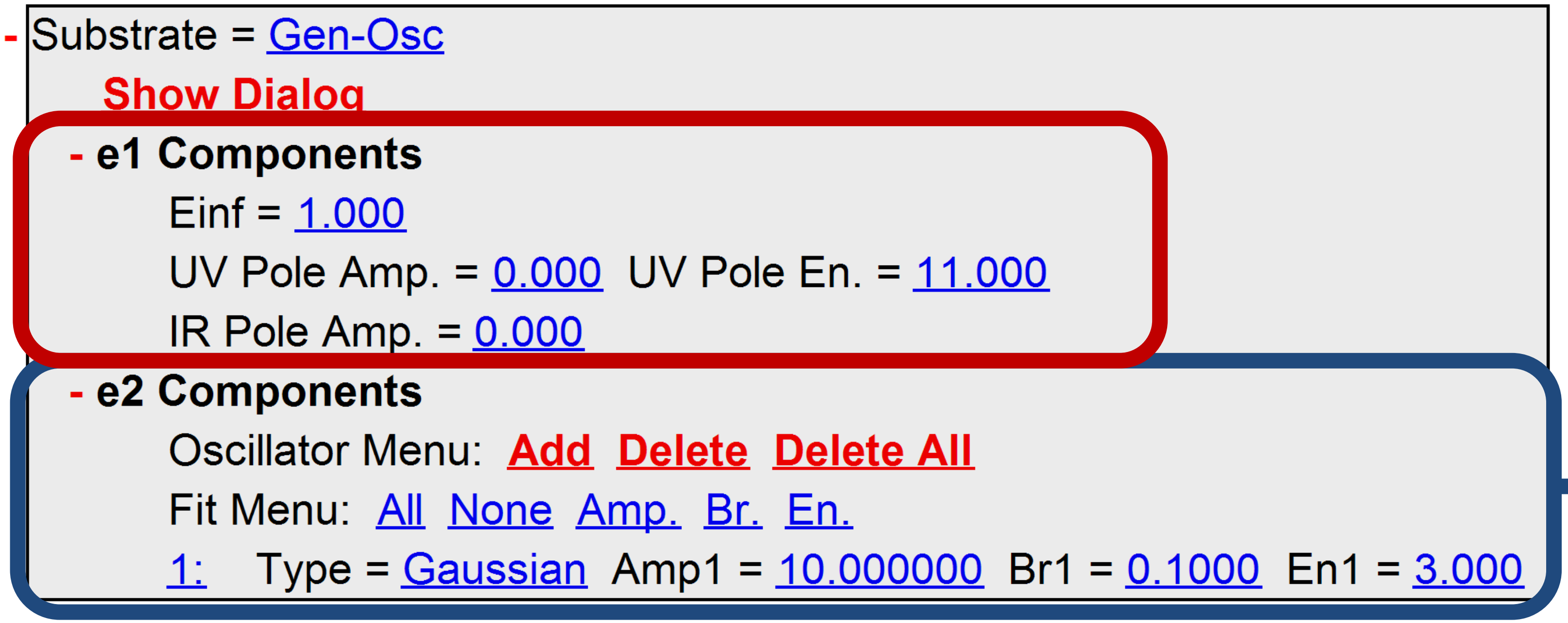
- The dipole response is like a mechanical oscillator
- Real and imaginary components are "connected" via Kramers-Kronig (KK) equations.

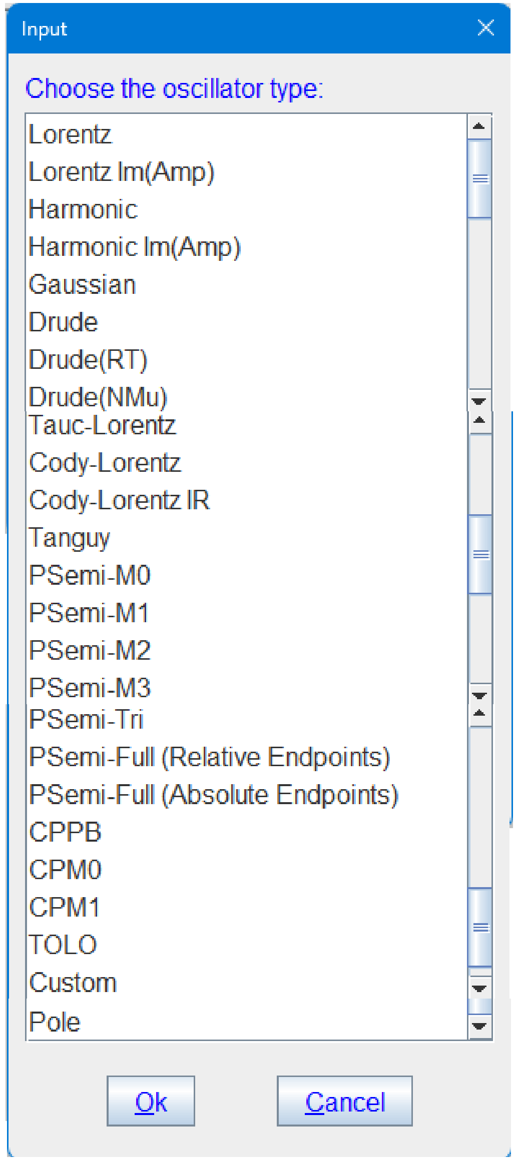
$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{\omega' \varepsilon_2(\omega')}{\omega'^2 - \omega^2} d\omega'$$





Gen-Osc Layer in CompleteEASE





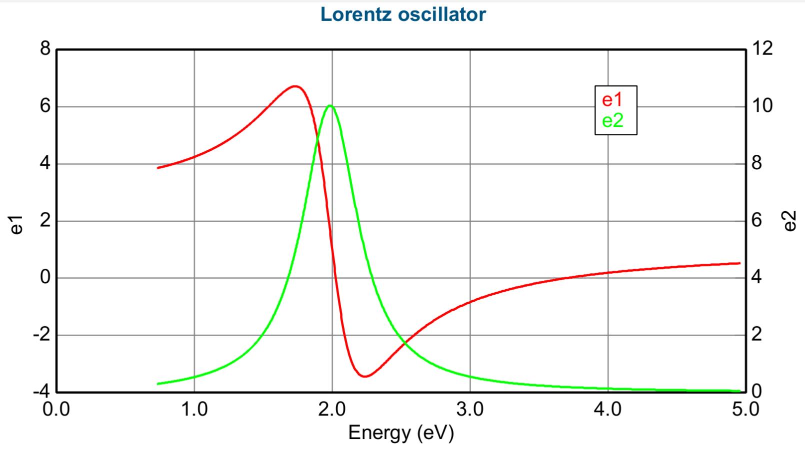
e1 - Einf & Poles:

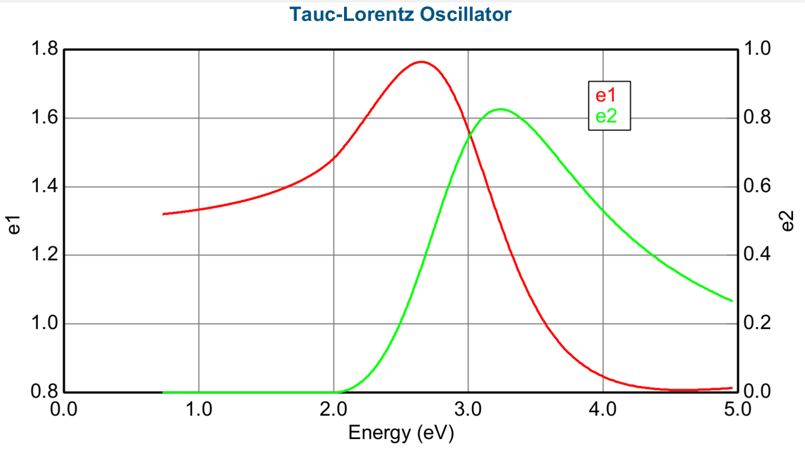
Describes the effect on ε1 from out-of-range absorptions

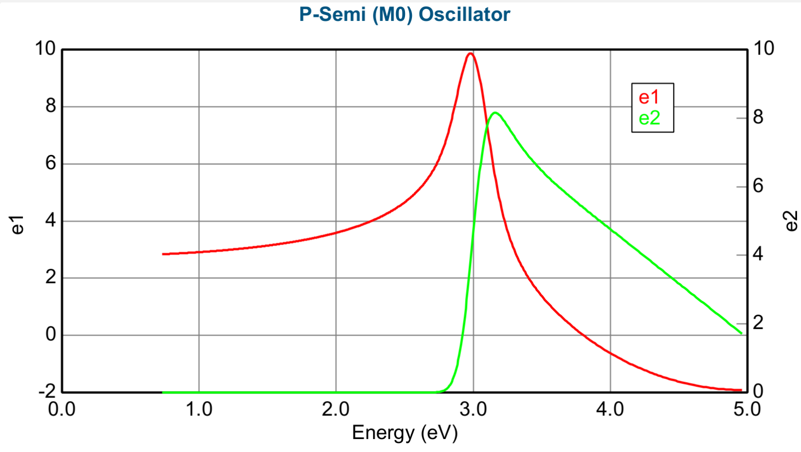
e2 - Oscillator List:

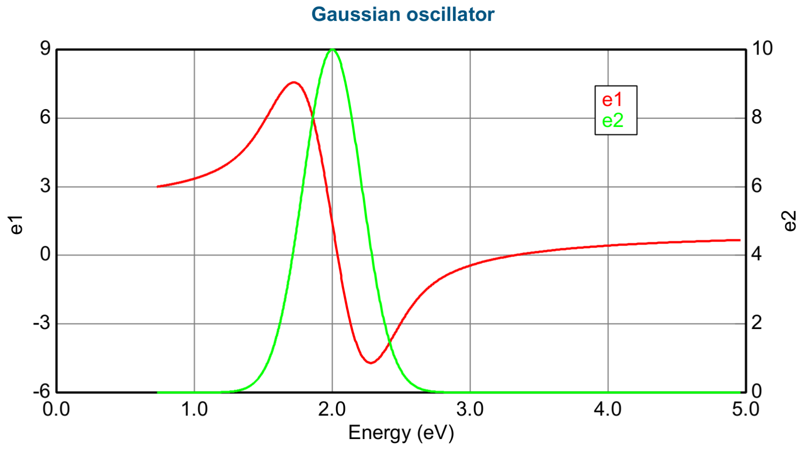
Describe absorptions within the analysis range, affecting ε_2 and KK transformed ε_1 shape

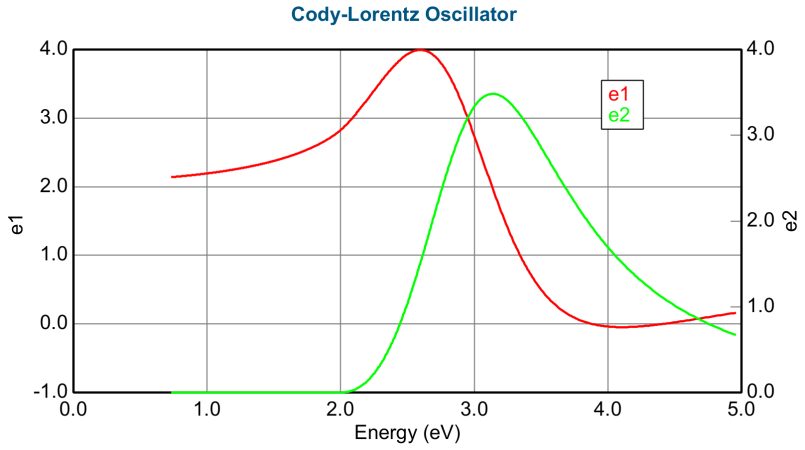
Common Oscillator Types

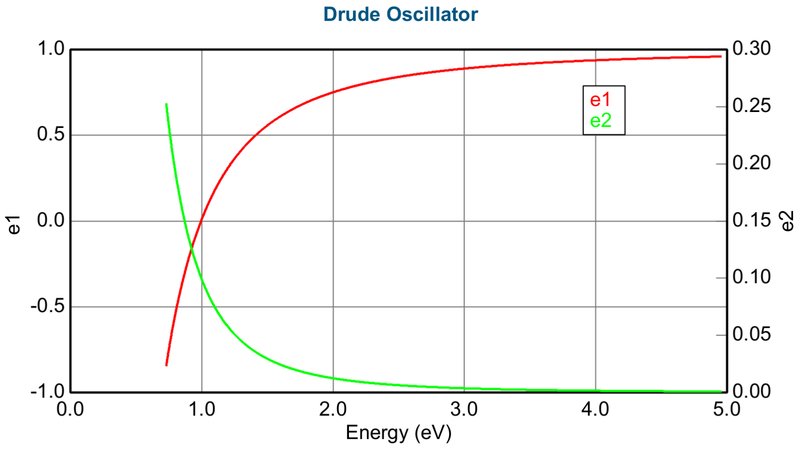






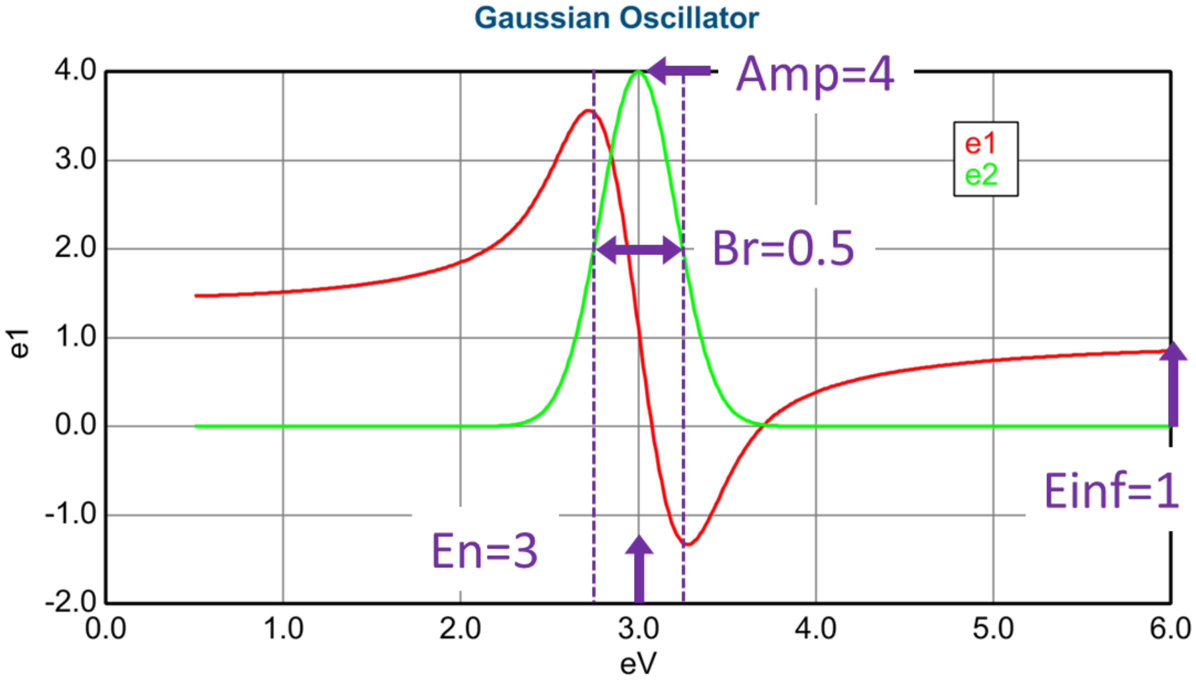


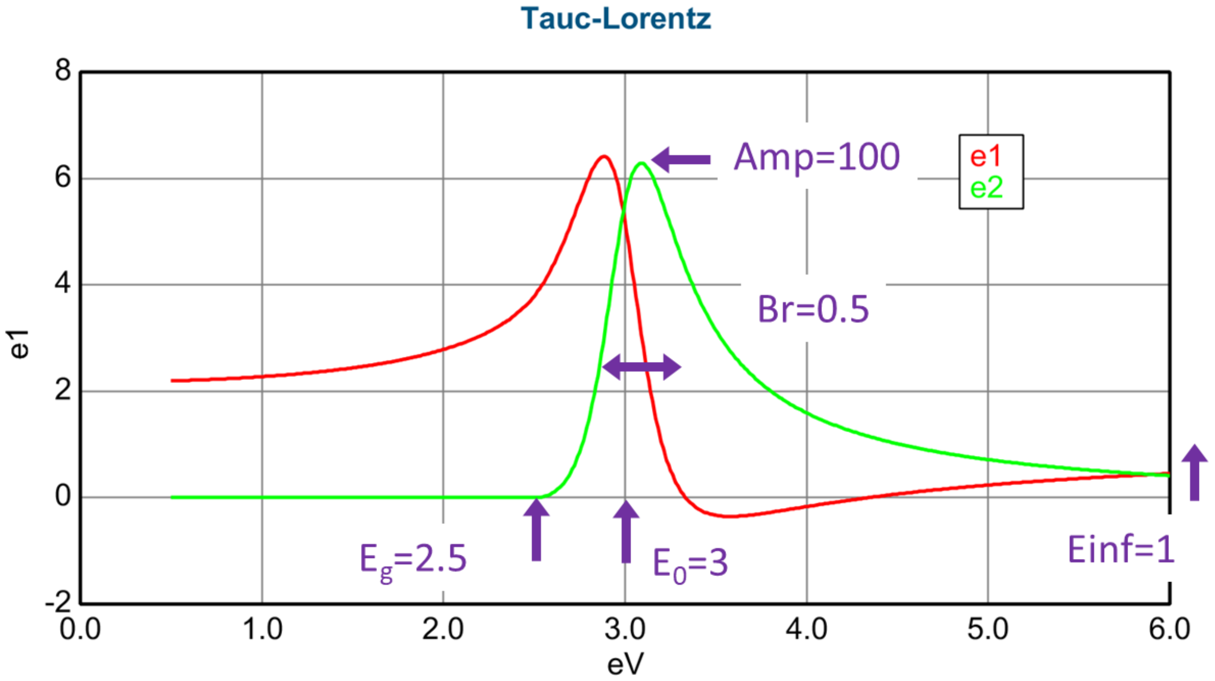




Describing Absorption Shapes

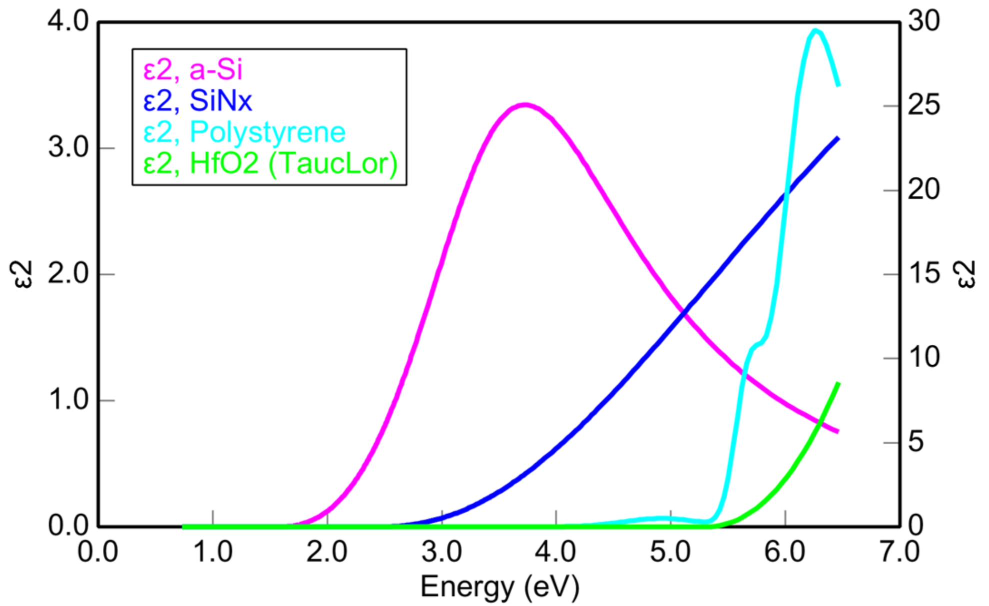
- Most oscillators have Amplitude, Broadening, and Center Energy to describe the shape of ε_2.
- Some also include Bandgap Energy –separates absorbing and transparent regions.

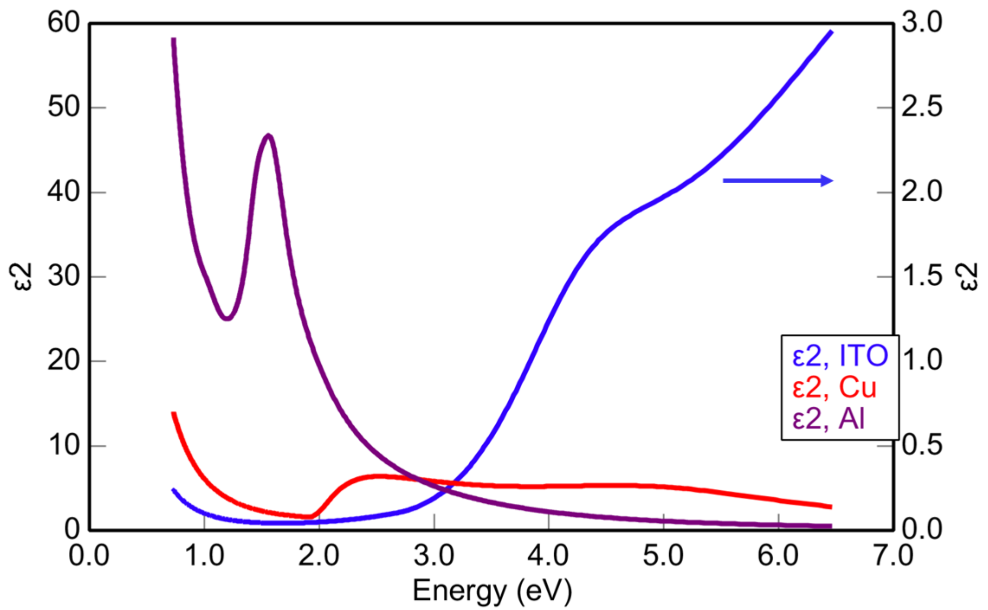




Which oscillators should I choose?

- **Gaussian**: organics, dielectric, semiconductors
- **Tauc-** and **Cody-Lorentz**: amorphous dielectrics and semiconductors
- **PSEMI**: crystalline materials, especially direct bandgap
- **Lorentz**: Metals and mid-IR phonons
- **Drude**: Conductive materials (metals, TCOs, heavily doped semis)

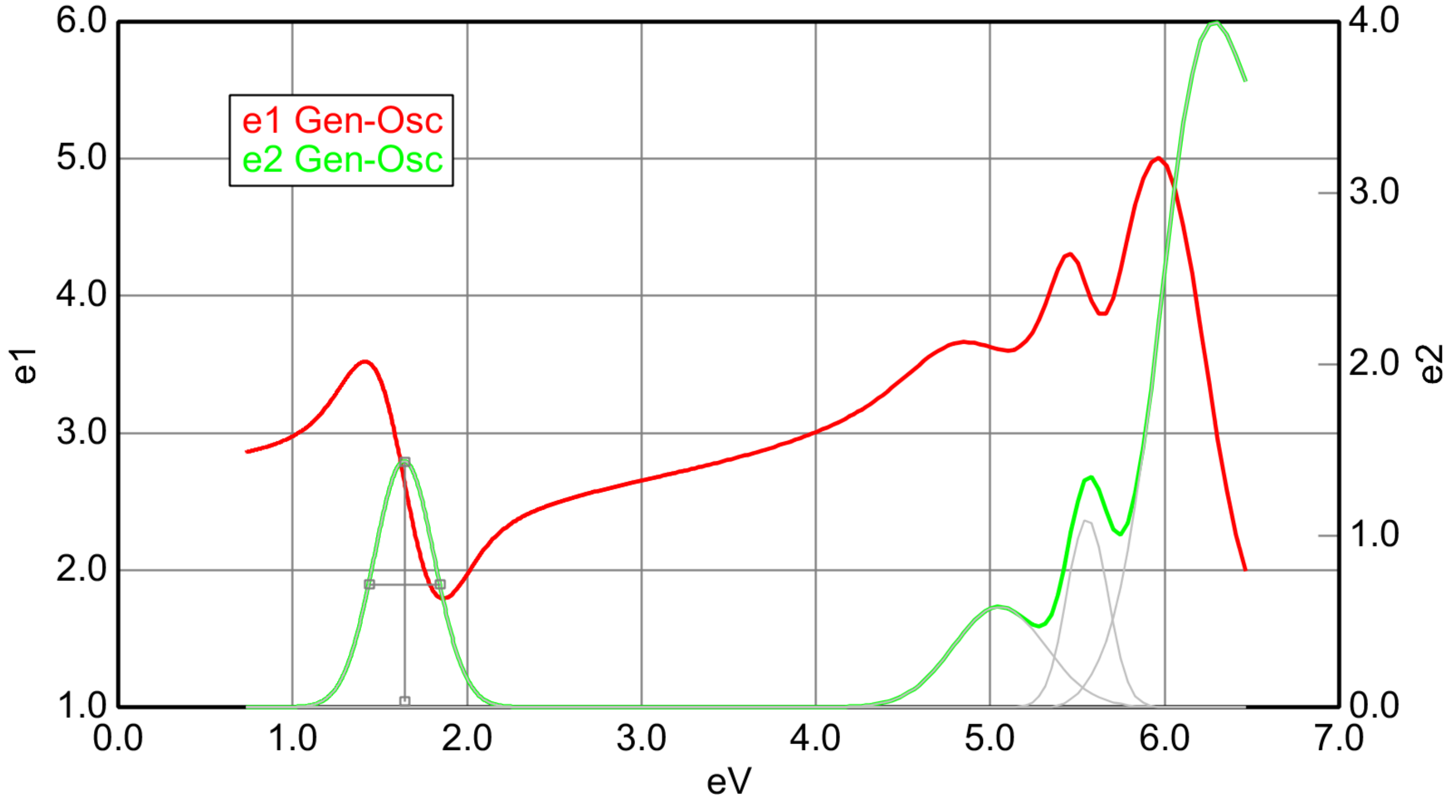




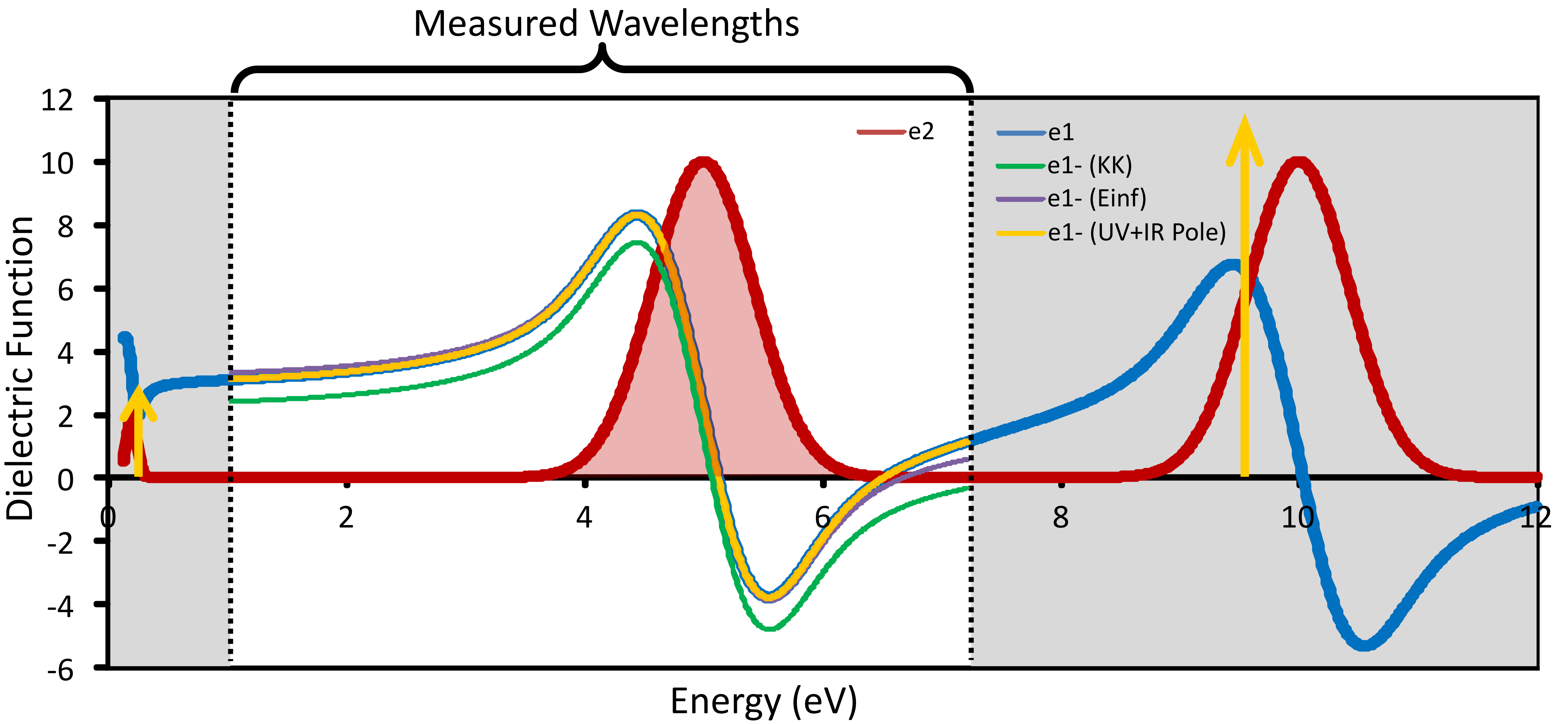
Optical Properties of Real Materials

- Absorption from different sources occurs at different wavelengths
- Integration <u>under all absorptions</u> is required to get the correct real part from KK transformation

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



Using Einf and Poles



Gen-Osc Methods

METHOD 1:

Fit Data with Pre-built Gen-Osc

METHOD 2:

Constructing your Own Gen-Osc

METHOD 3:

Cauchy ▶ B-Spline

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Build Gen-Osc from B-spline n,k

Demonstration 1: Using existing Gen-Osc

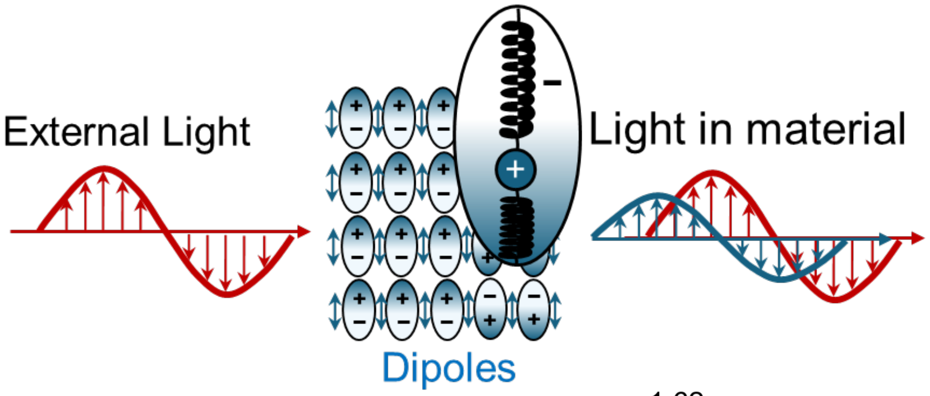
- Amorphous silicon thin film on 1737 Glass

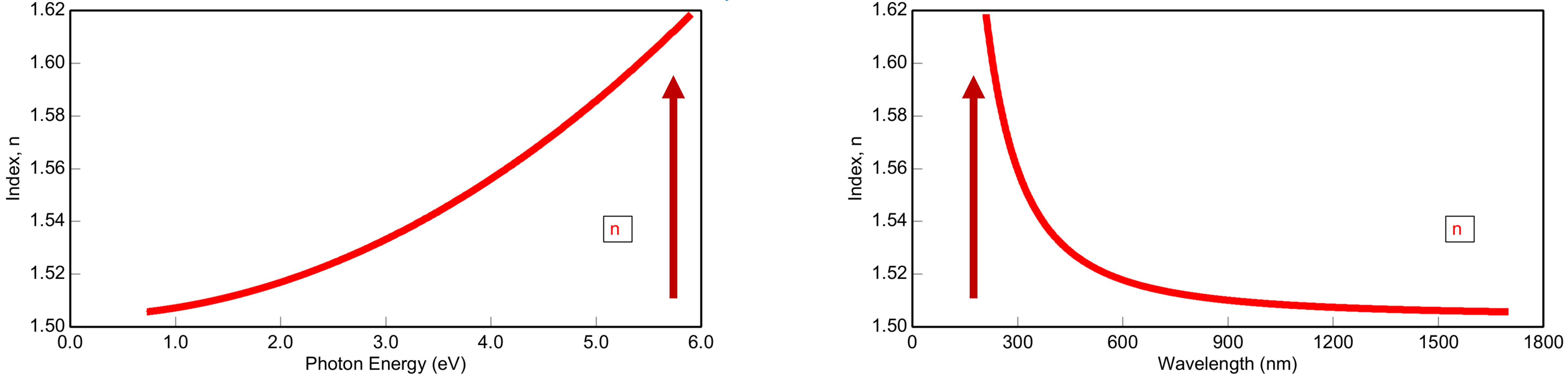
Roughness = **5.33 nm** (fit)
- Layer # 1 = a-Si_Aspnes_cl Thickness # 1 = **335.66 nm** (fit)
  Show Dialog
  - **e1 Components**
    Einf = **1.133** (fit)
    UV Pole Amp. = 0.000 UV Pole En. = 11.000
    IR Pole Amp. = 0.000
  - **e2 Components**
    Oscillator Menu: **Add** **Delete** **Delete All** **Sort**
    Fit Menu: All None **Amp.** **Br.** **En.** Display Units = OFF
    1: Type = Cody-Lorentz Amp1 = **83.943** (fit) Br1 = **2.681** (fit)
    Eo1 = **3.871** (fit) Eg1 = **1.791** (fit) Ep1 = **1.545** (fit)
    + Urbach Absorption Parameters
+ Substrate = 1737 Glass_Genosc

MSE = 3.456
Roughness = 5.33 ± 0.015 nm
Thickness # 1 = 335.66 ± 0.085 nm
Einf = 1.133 ± 0.0116
Amp1 = 83.943 ± 0.7446
Br1 = 2.681 ± 0.006380
Eo1 = 3.871 ± 0.006881
Eg1 = 1.791 ± 0.001238
Ep1 = 1.545 ± 0.0164

Normal Dispersion

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

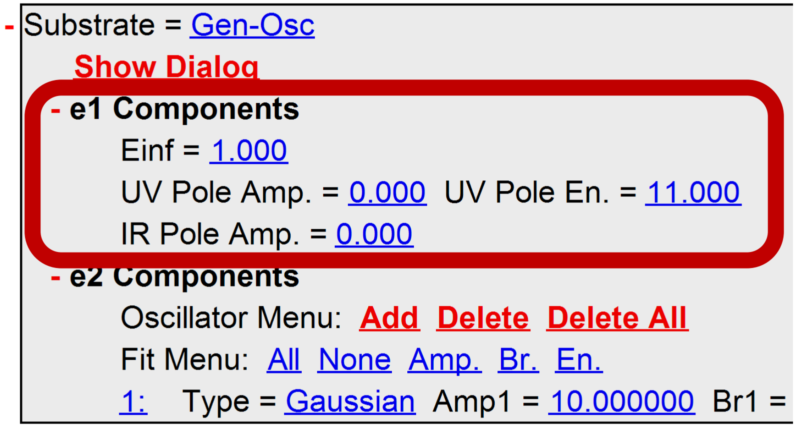


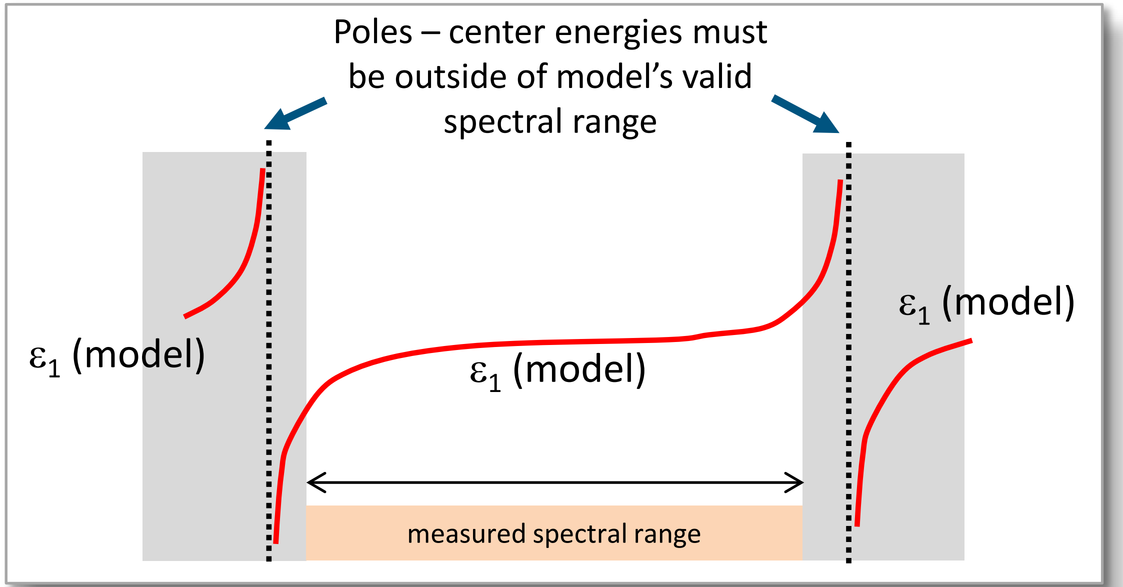


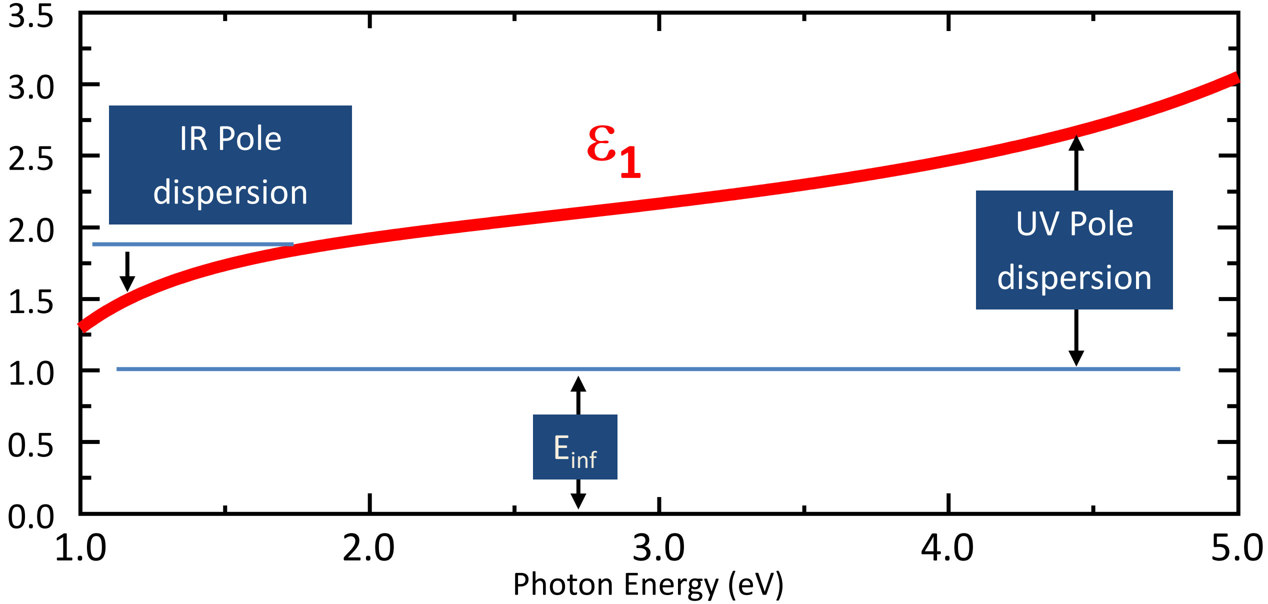
Poles and Einf

Poles add dispersion (curvature) to the ends of the transparent spectral range

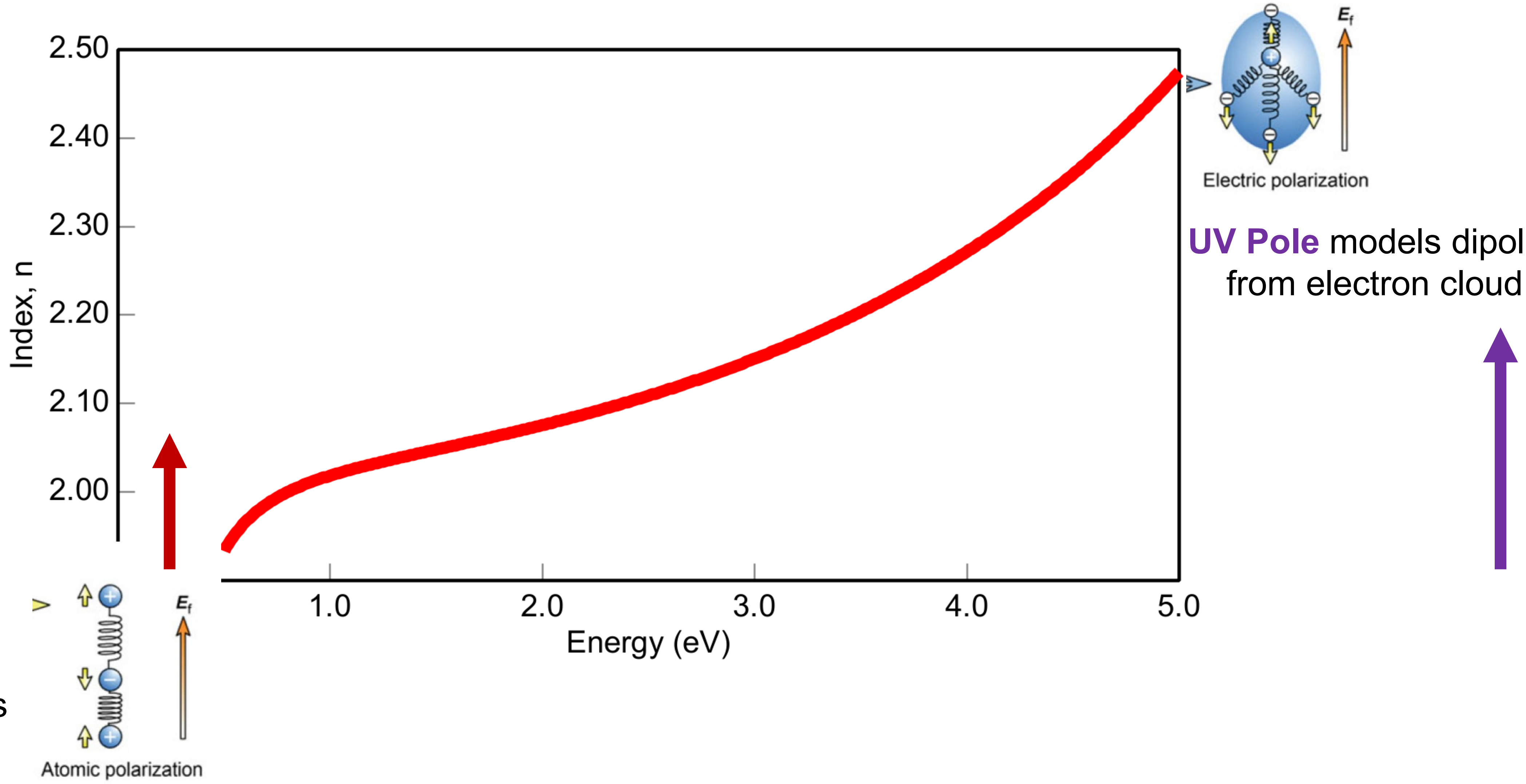
$$\varepsilon(E)=\sum_{n}\frac{A_n}{E_n^2-E^2}$$







Physics behind "2 Poles"



IR Pole models dipoles from atoms/molecules

UV Pole models dipoles from electron cloud

Demonstration 2: BK7 Substrate

- Fit data with both Sellmeier and Cauchy – compare results

Include Surface Roughness = ON Roughness = **13.44 Å** (fit)

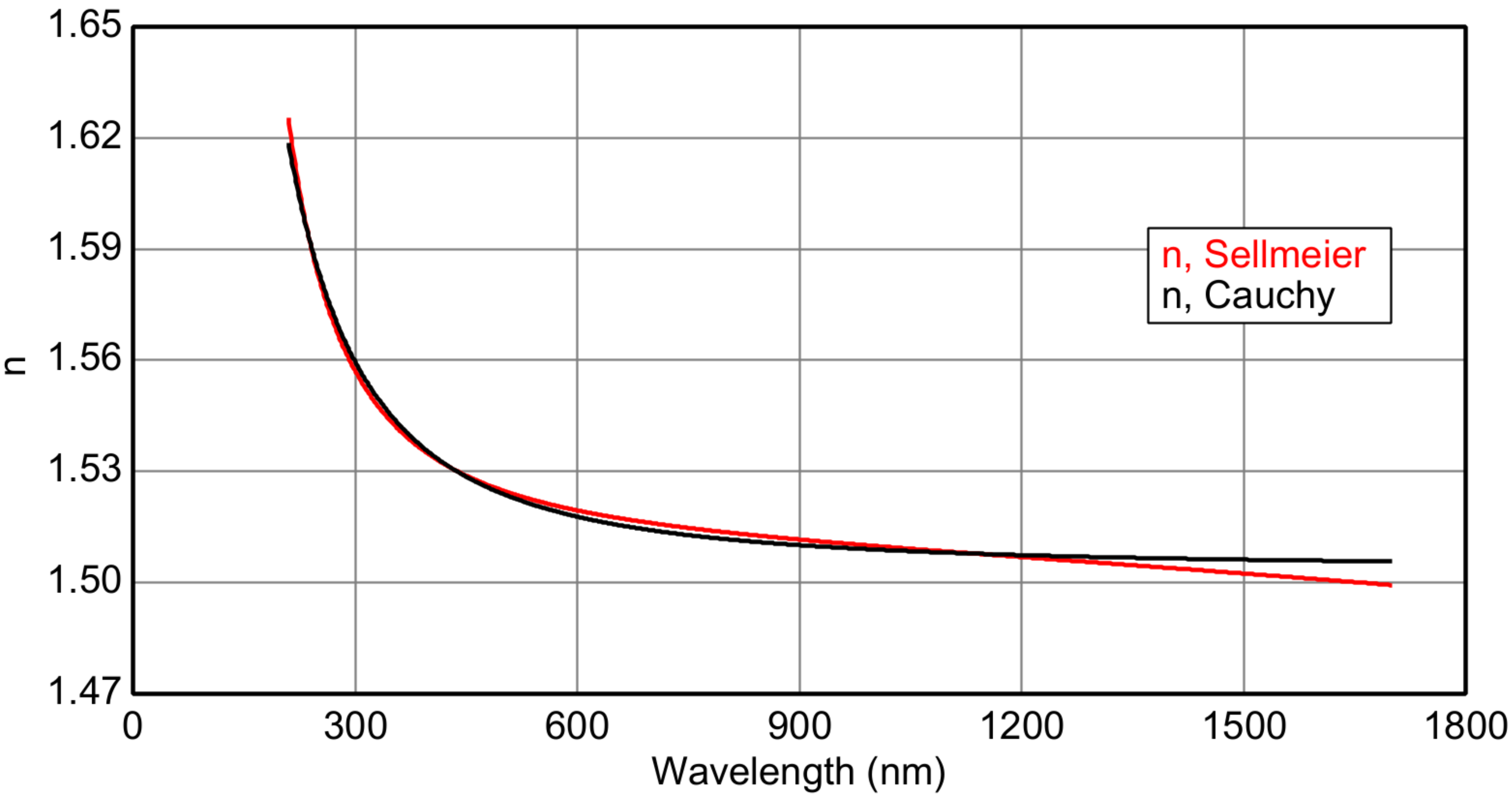
- Substrate = Gen-Osc
  - **Show Dialog**
  - **e1 Components**
    - Einf = **1.466** (fit)
    - UV Pole Amp. = **92.7823** (fit) UV Pole En. = **10.665** (fit)
    - IR Pole Amp. = **0.0200** (fit)
  - **e2 Components**
    - Oscillator Menu: **Add** **Delete** **Delete All** **Sort**
    - Fit Menu: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

MSE = 1.054
Roughness = 13.44 ± 0.039 Å
Einf = 1.466 ± 0.0117
UV Pole Amp. = 92.7823 ± 2.28468
UV Pole En. = 10.665 ± 0.0560
IR Pole Amp. = 0.0200 ± 0.00017652

BK7 Substrate: Sellmeier or Cauchy?

Full Wavelength Range:
MSE (Sellmeier) = 1.054
MSE (Cauchy) = 1.536

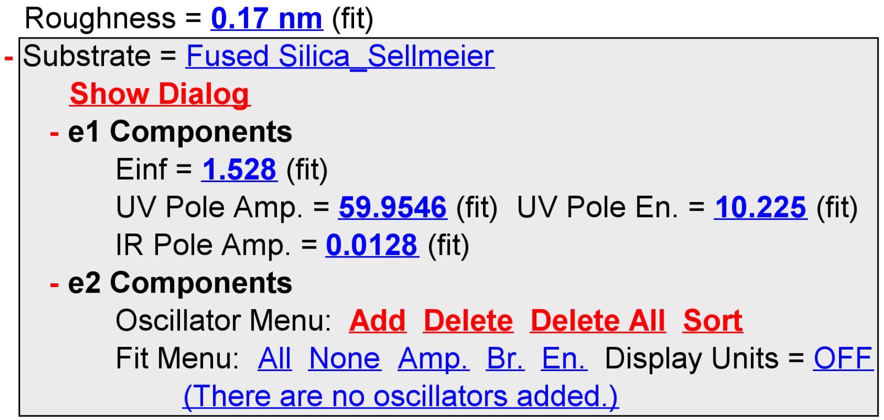
Limited 250-1000 nm:
MSE (Sellmeier) = 0.723
MSE (Cauchy) = 0.734

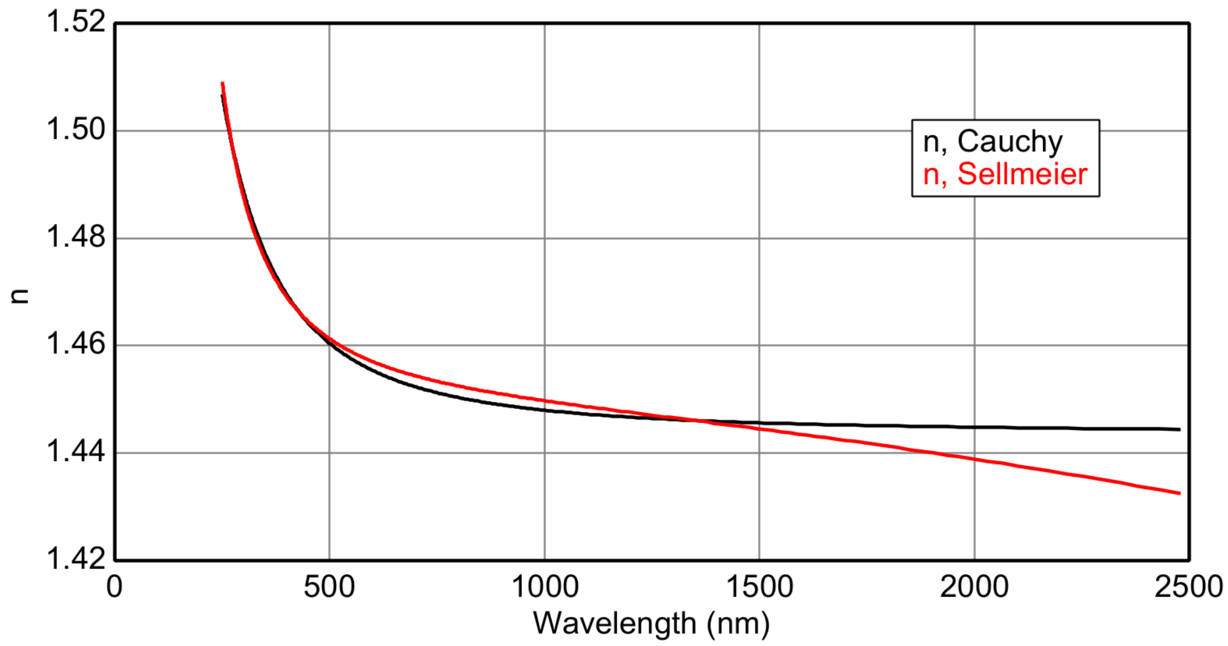


4-01: Fused Silica Substrate

- Fit data with both Sellmeier and Cauchy – compare results

MSE (Sellmeier) = 0.626
MSE (Cauchy) = 1.188





Gen-Osc Methods

METHOD 1:

Fit Data with Pre-built Gen-Osc

METHOD 2:

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⇩

Build Gen-Osc from B-spline n,k

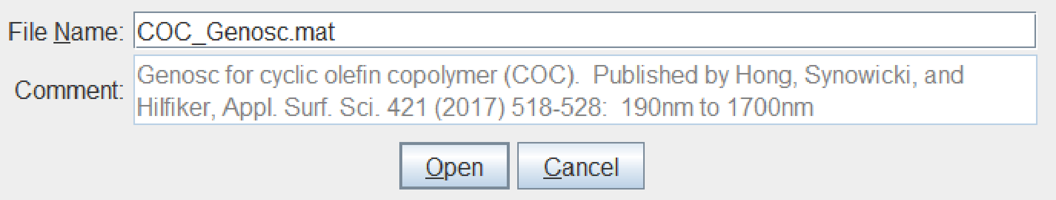
Pre-Built Gen-Osc

Fit Data with
Pre-Built Gen-Osc

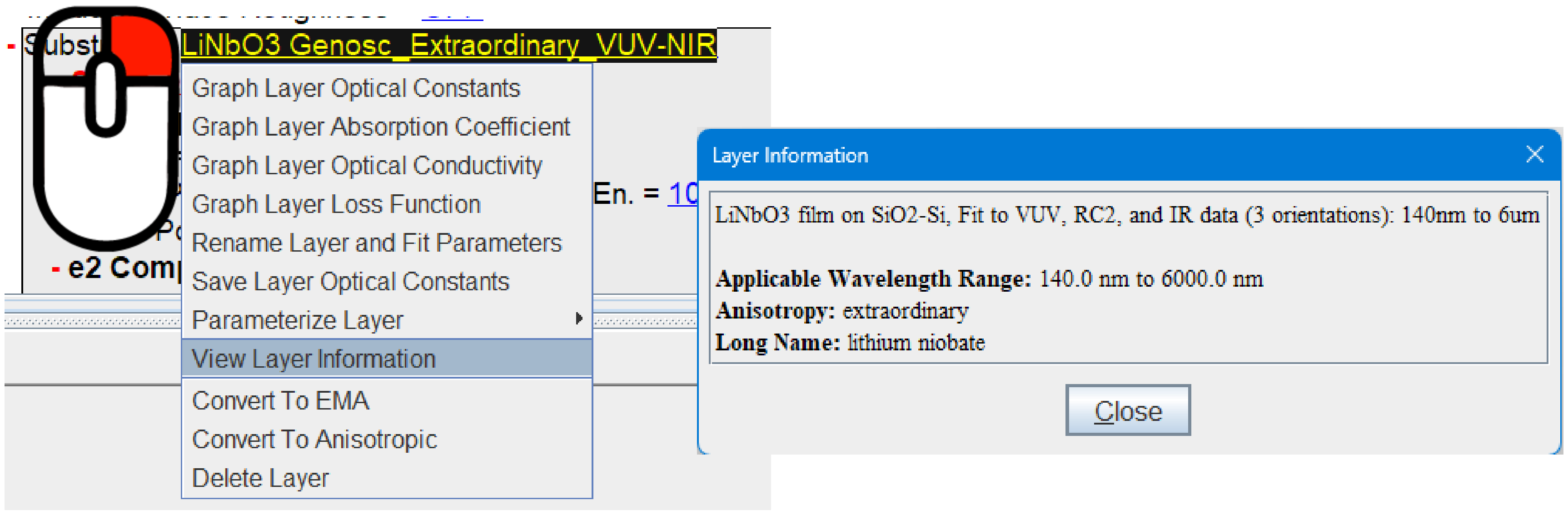
1. Add pre-built Gen-Osc layer in your model.
2. Adjust and fit Thickness-only to match data.
    - prevents oscillator parameters from getting lost.
3. Turn on Oscillator Fit parameters.
4. Watch for “lost” parameters – simplify your model.

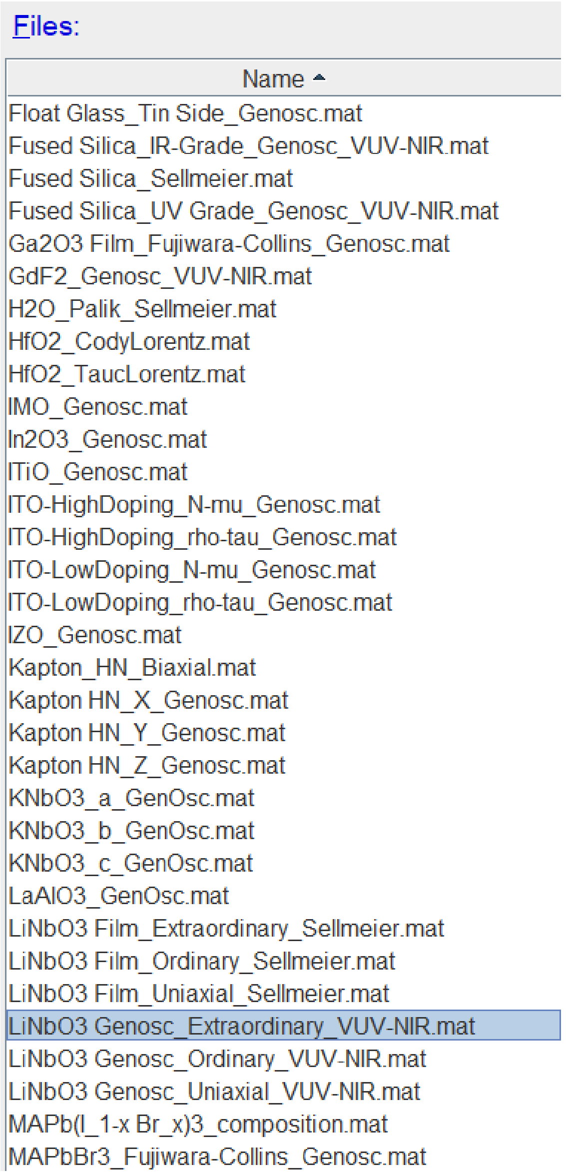
Material File Names and Comments

- The new material files tell you they are a “Genosc”.
- Click on a file to see **Comment**



- Right-click layer name to **View Layer Info**.





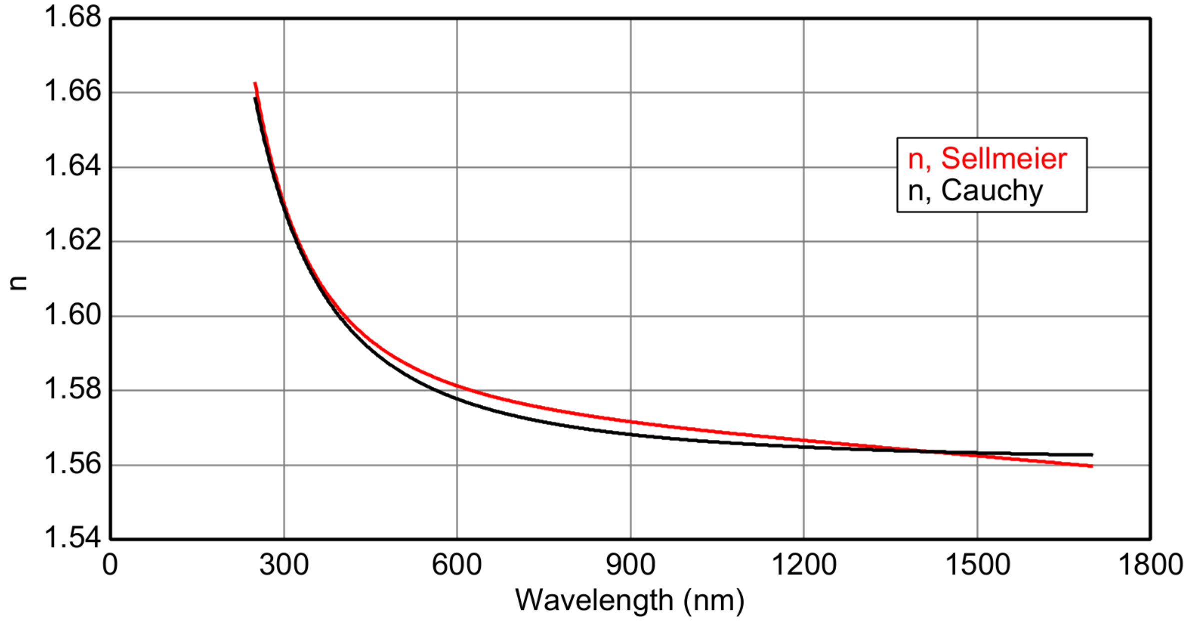
4-02: Using Existing Genosc: Al_2O_3 thin film on Si

- Fit data with both Sellmeier and Cauchy – compare results
  - *Hint: Delete the oscillator (we are fitting the transparent region)*

MSE (Sellmeier) = 3.552
MSE (Cauchy) = 8.941

- Layer # 1 = Gen-Osc Thickness # 1 = **2971.24 Å** (fit)
  Show Dialog
  - **e1 Components**
    Einf = **1.485** (fit)
    UV Pole Amp. = **100.6613** (fit) UV Pole En. = **10.142** (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.)

Substrate = SI_JAW



Which Gen-Osc Parameters to Use?

- Are oscillators in the same energy range as your data?
- What parameters have been used?
- Which parameters have a big effect?
- Test parameters – do they improve fit quality (lower MSE)?
  - If no, press **RESET** and turn them off.

Lost Parameters may include:
i) negative amplitudes, ii) very small broadenings, and iii) out-of-range energies

4-03: Use Prebuilt Gen-Osc: SiNx on Si

- Use Prebuilt SiNx GenOsc mat file
- Match thickness
- Fit parameters and check for correlation

HINTS:

- Did you try surface roughness?

Fit Data with
Pre-Built Gen-Osc

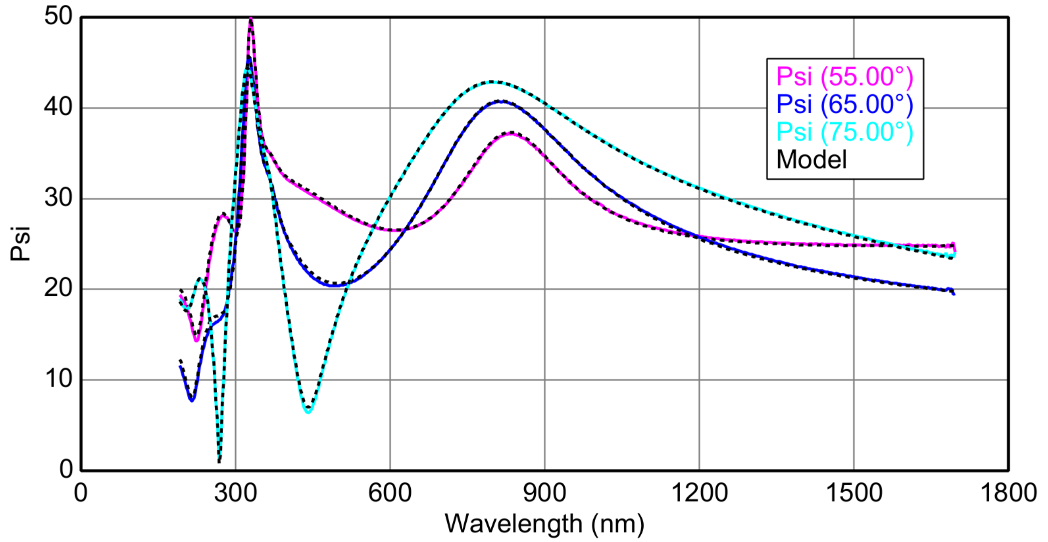
SiNx on Si: Results

Roughness = 51.07 Å (fit)
- Layer # 1 = SiNx (CodyLor) Thickness # 1 = 1180.04 Å (fit)
  - Show Dialog
  - e1 Components
    - Einf = 1.025
    - UV Pole Amp. = 97.2437 (fit) UV Pole En. = 9.460 (fit)
    - IR Pole Amp. = 0.000
  - e2 Components
    - Oscillator Menu: Add Delete Delete All Sort
    - Fit Menu: All None Amp. Br. En. Display Units = OFF
    - 1: Type = Cody-Lorentz Amp1 = 29.204 (fit) Br1 = 6.587 (fit)
      Eo1 = 7.851 (fit) Eg1 = 2.226 (fit) Ep1 = 3.671 (fit)
      + Urbach Absorption Parameters

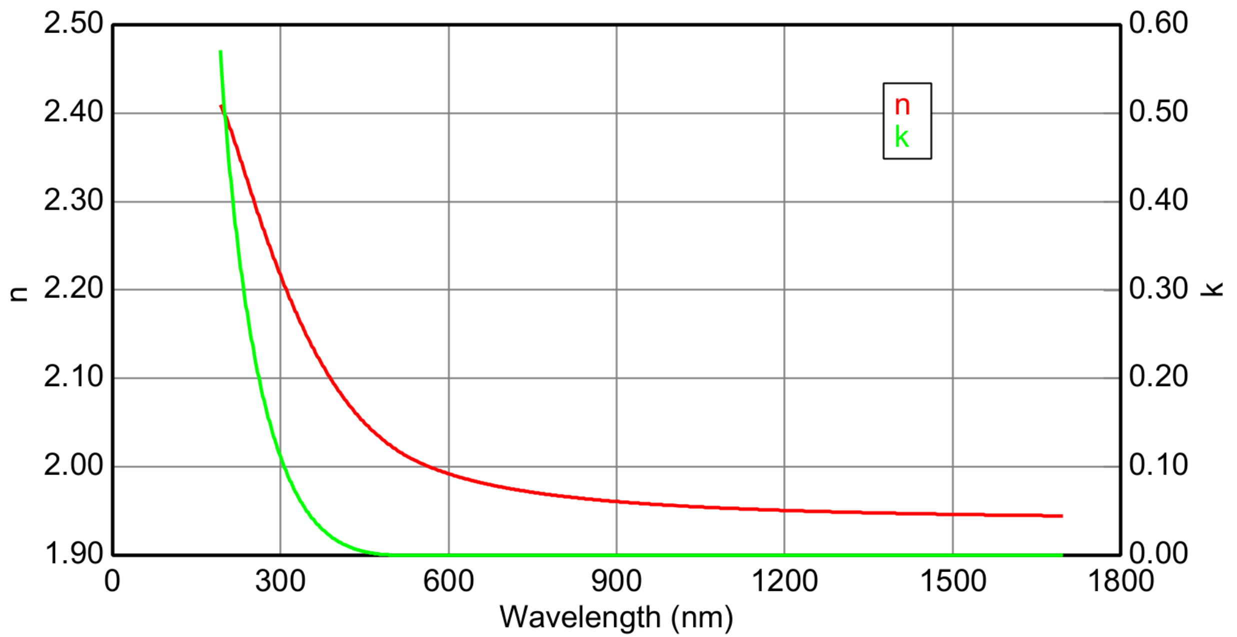
Substrate = Si_JAW

MSE = 5.342
Roughness = 51.07 ± 0.238 Å
Thickness # 1 = 1180.04 ± 0.116 Å
UV Pole Amp. = 97.2437 ± 8.91036
UV Pole En. = 9.460 ± 0.0826
Amp1 = 29.204 ± 3.1452
Br1 = 6.587 ± 0.4039
Eo1 = 7.851 ± 0.1154
Eg1 = 2.226 ± 0.0111
Ep1 = 3.671 ± 0.2445

Variable Angle Spectroscopic Ellipsometric (VASE) Data



Optical Constants of SiNx (CodyLor) vs. nm



4-04: Use Prebuilt Gen-Osc: Nb_2O_5 on Si

- Use Prebuilt Nb2O5_GenOsc.mat file
- Match thickness
- Fit parameters and check for correlation

Hints:

- Any non-idealities?

Fit Data with
Pre-Built Gen-Osc

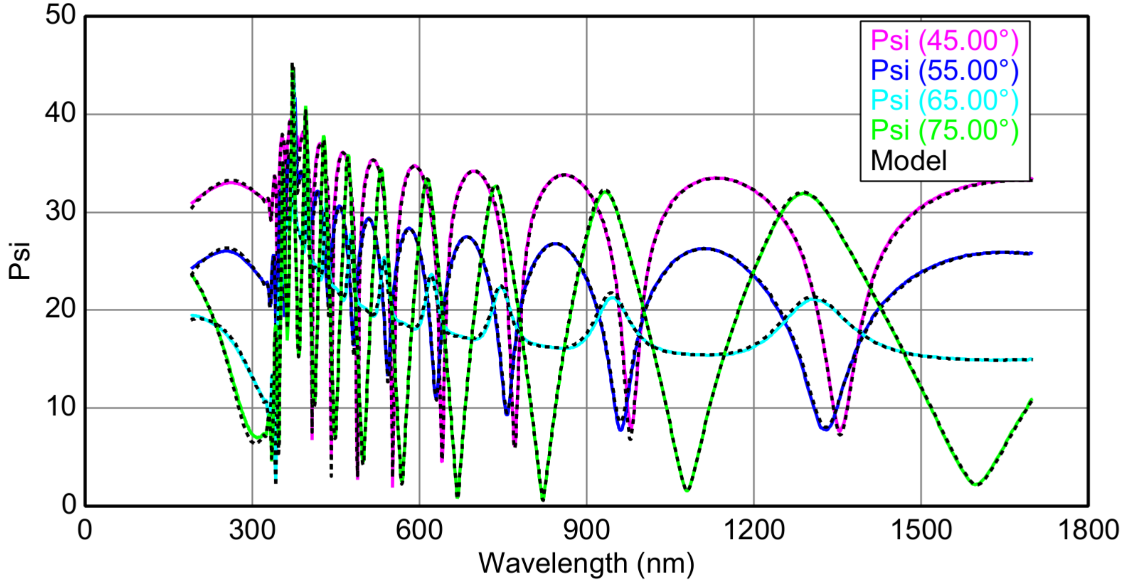
Nb_2O_5 on Si: Results

- Layer # 1 = Nb2O5_Genosc Thickness # 1 = **8091.86 Å** (fit)
  Show Dialog
  - **e1 Components**
    Einf = 1.000
    UV Pole Amp. = 107.0559 UV Pole En. = 10.443
    IR Pole Amp. = 0.0374
  - **e2 Components**
    Oscillator Menu: **Add** **Delete** **Delete All** **Sort**
    Fit Menu: All None **Amp.** **Br.** **En.** Display Units = OFF
    1: Type = Cody-Lorentz Amp1 = **313.841** (fit) Br1 = **1.521** (fit)
    Eo1 = **4.397** (fit) Eg1 = **3.364** (fit) Ep1 = **6.444** (fit)
    + Urbach Absorption Parameters

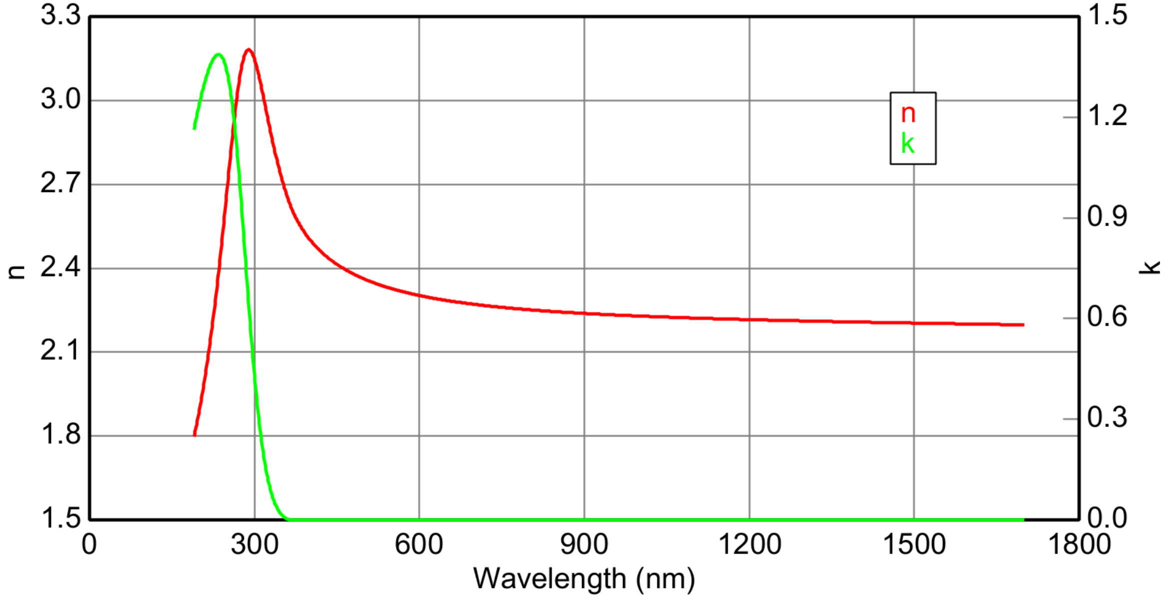
Substrate = Si_JAW

MSE = 10.798
Thickness # 1 = 8091.86 ± 1.221 Å
Amp1 = 313.841 ± 4.2777
Br1 = 1.521 ± 0.006641
Eo1 = 4.397 ± 0.002294
Eg1 = 3.364 ± 0.001027
Ep1 = 6.444 ± 0.0553
Bandwidth (nm) = 3.024 ± 0.0125

Variable Angle Spectroscopic Ellipsometric (VASE) Data



Optical Constants of Nb2O5_Genosc vs. nm



4-05: Using Existing Gen-Osc: amorphous Silicon on Glass

- Start by fitting the Glass substrate (or use Glass Substrate_4-05.mat)
- Add the a-Si Genosc, roll-in the thickness and oscillator parameters.
- Fit to get thickness and optical constants.

Fit Data with
Pre-Built Gen-Osc

Results: a-Si on Glass

Roughness = **48.62 Å** (fit)

\- Layer # 1 = a-Si_Aspnes_cl Thickness # 1 = **923.60 Å** (fit)

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** **Sort**

Fit Menu: All None Amp. Br. En. Display Units = OFF

1: Type = Cody-Lorentz Amp1 = **611.390** (fit) Br1 = **2.683** (fit)

Eo1 = **3.424** (fit) Eg1 = **1.450** (fit) Ep1 = **11.896** (fit)

\+ Urbach Absorption Parameters

\+ Substrate = Glass Substrate_4-03

MSE = 2.413

Roughness = 48.62 ± 0.098 Å

Thickness # 1 = 923.60 ± 0.105 Å

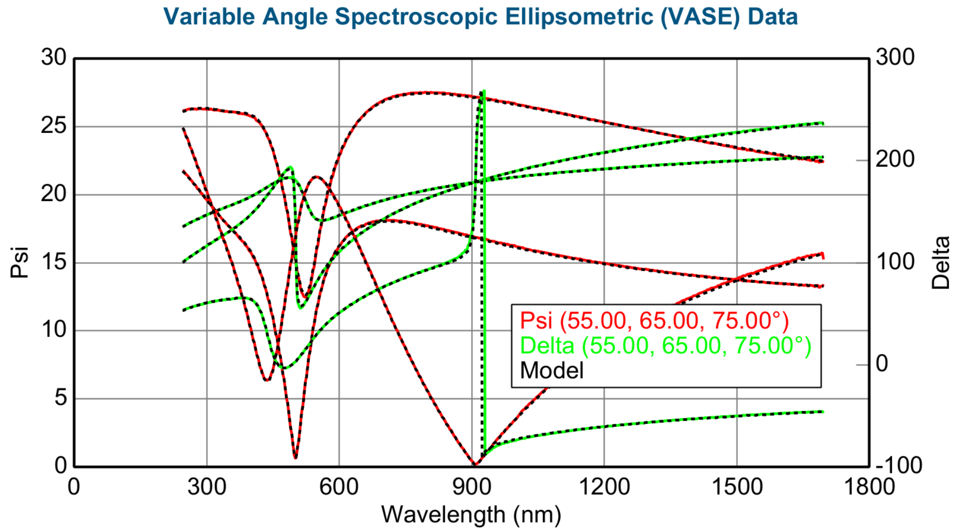
Amp1 = 611.390 ± 8.4071

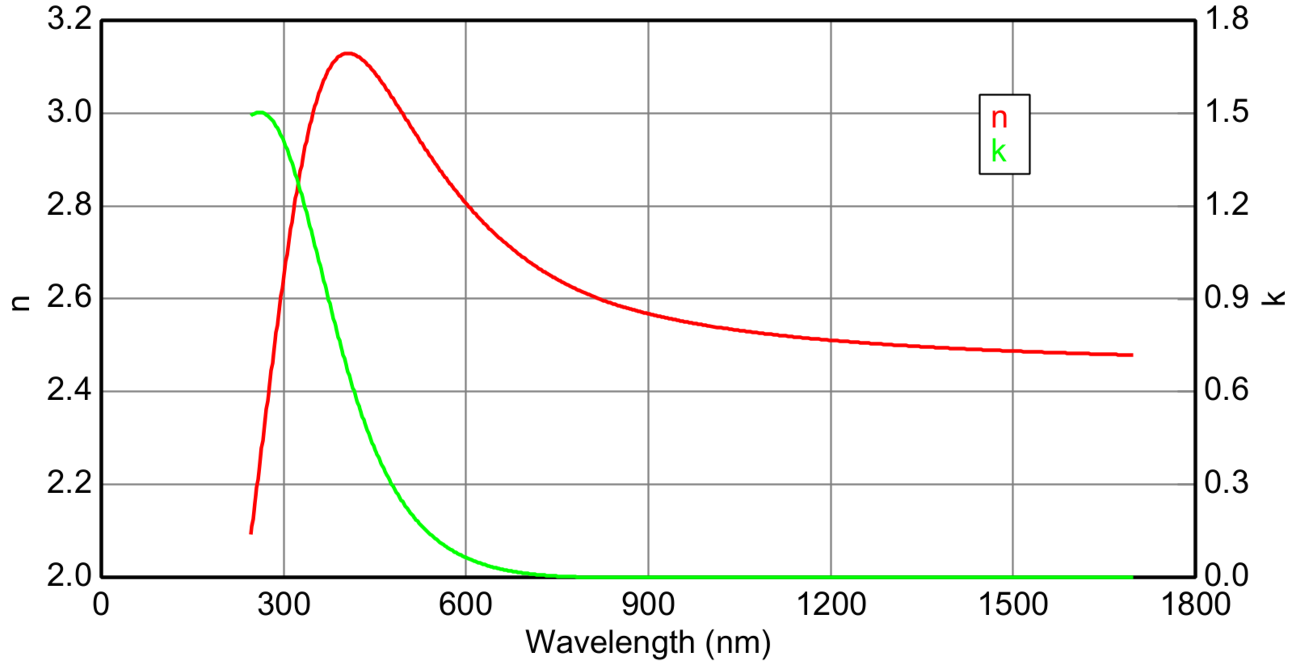
Br1 = 2.683 ± 0.005517

Eo1 = 3.424 ± 0.001935

Eg1 = 1.450 ± 0.002748

Ep1 = 11.896 ± 0.1049





Gen-Osc Methods

METHOD 1:

Fit Data with Pre-built Gen-Osc

METHOD 2:

Constructing your Own Gen-Osc

METHOD 3:

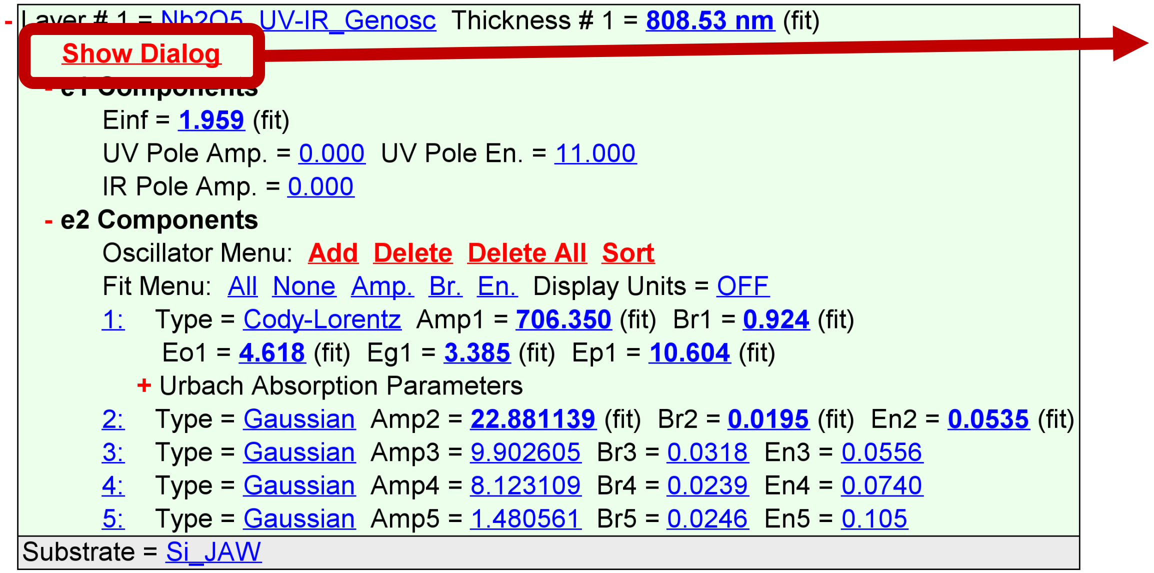
Cauchy ▶ B-Spline

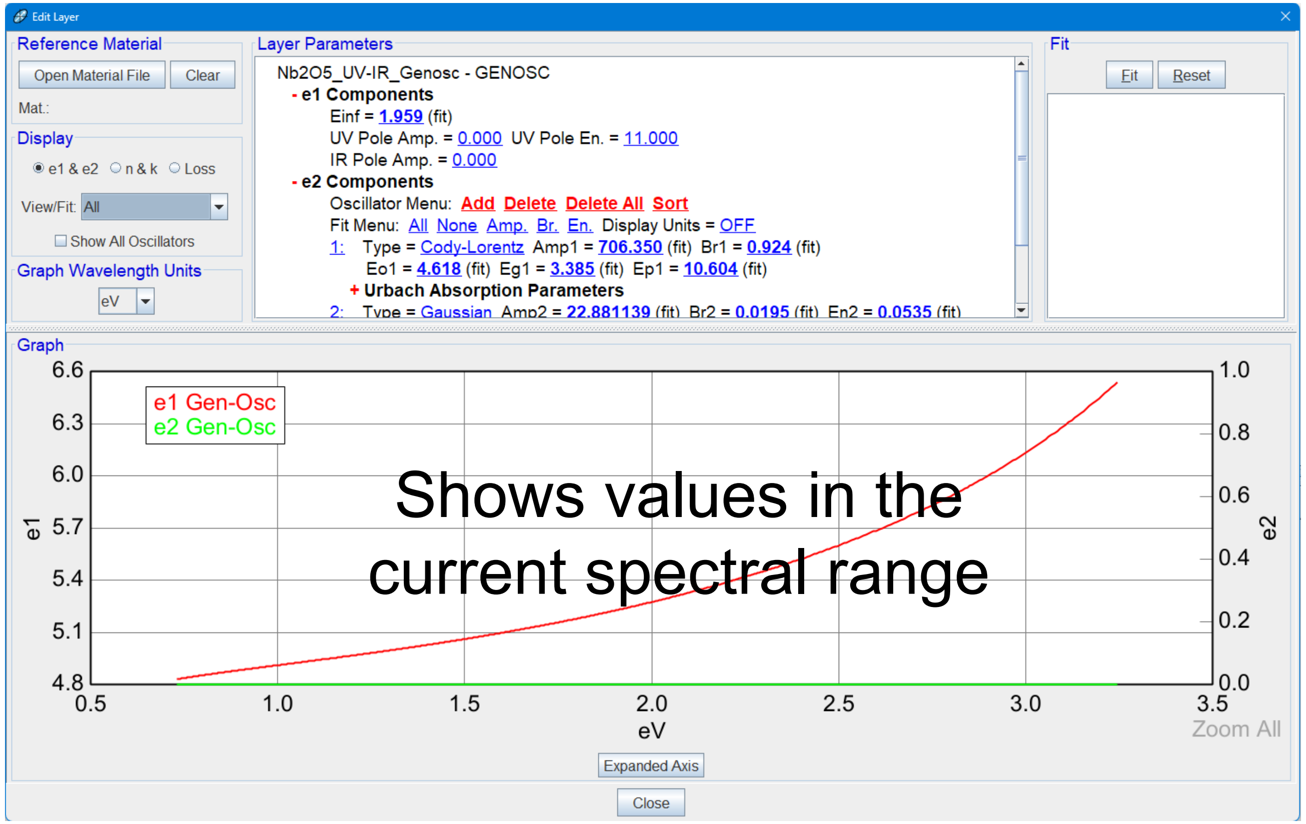
⇩

Build Gen-Osc from B-spline n,k

Simplify my Genosc

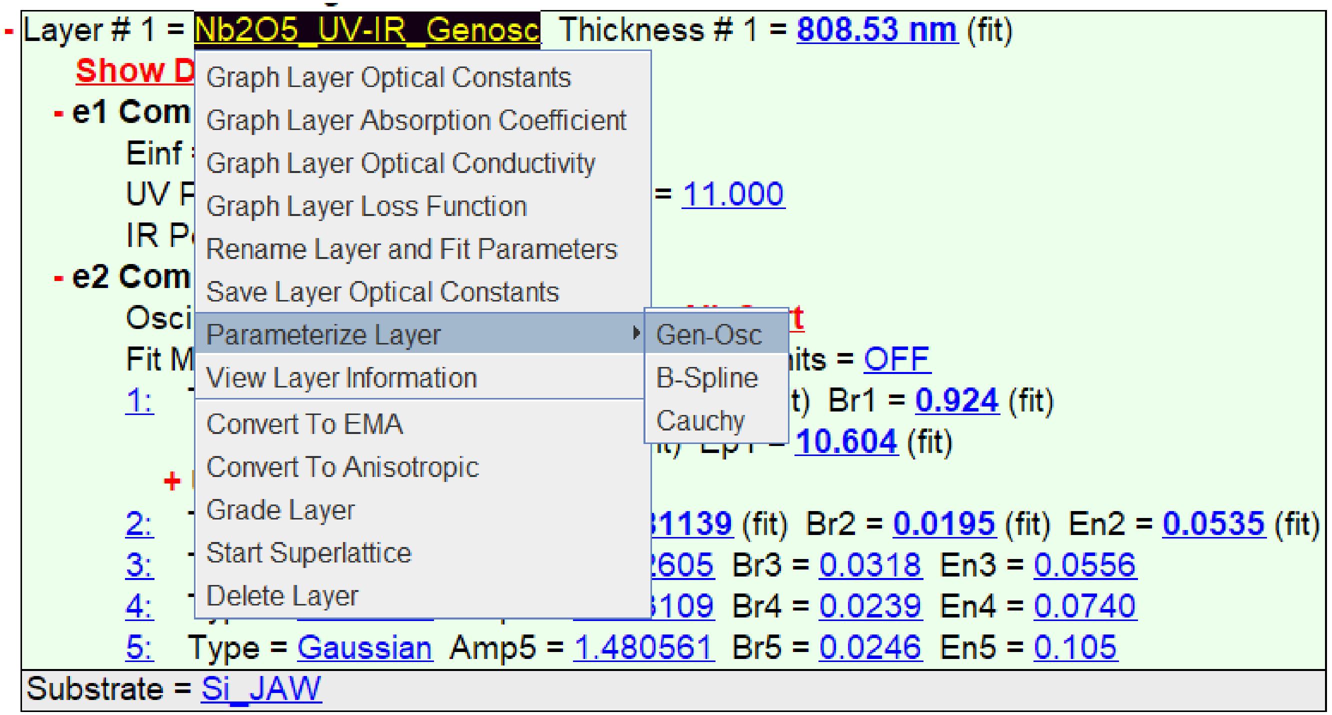
- Check to see if your oscillators are outside the data energy range. If yes, they only contribute to the KK integration (ε_1).





Replacing Oscillators with Poles

- Strategy 1: Delete the unnecessary oscillators – change pole values
- Strategy 2: "Start Over" - use the Parameterize Layer command to use your current values as reference for a new Genosc.



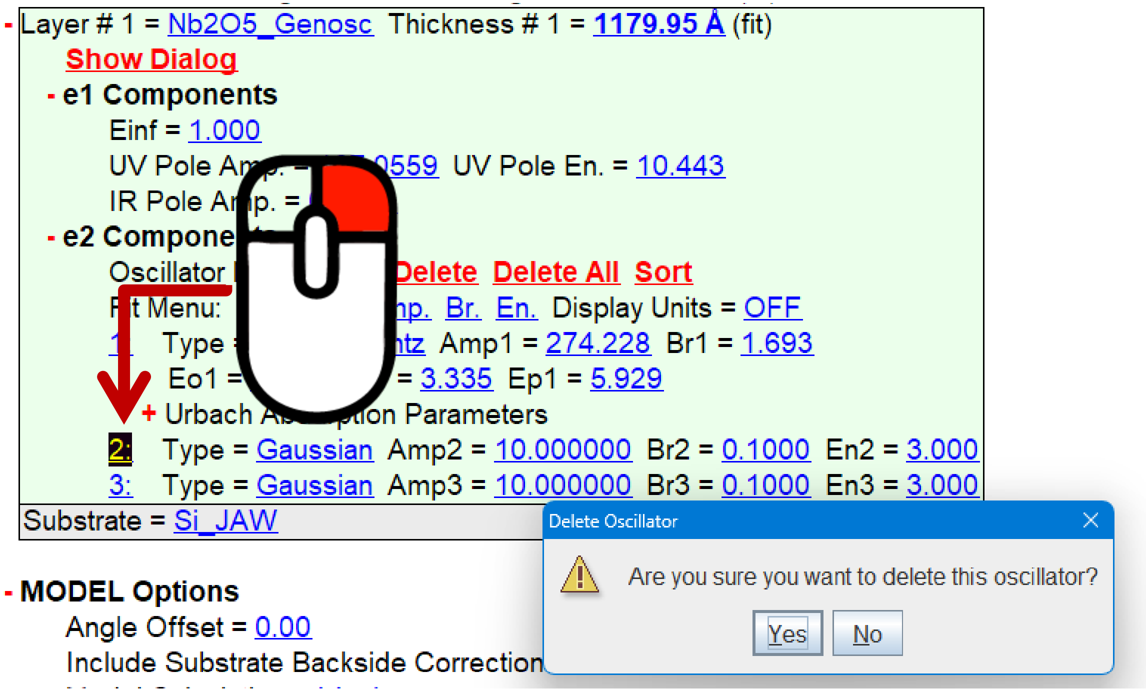
Disabling or Deleting oscillators

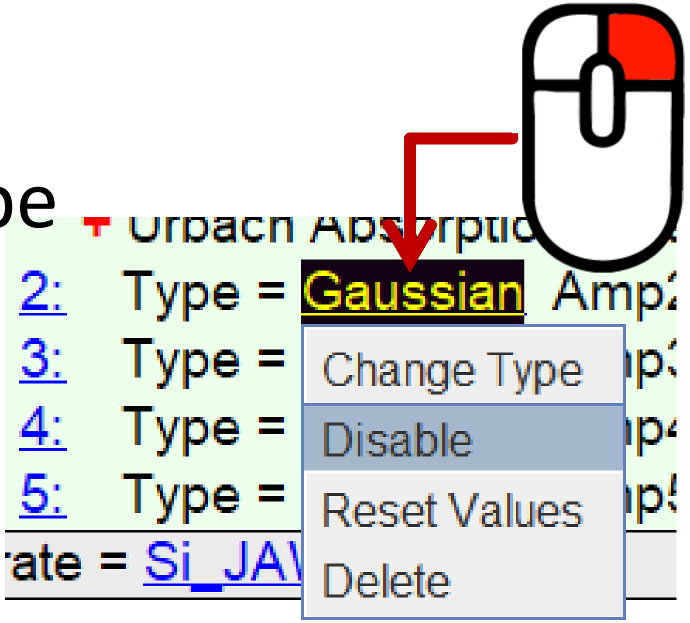
DELETE

- Right-Click “#”
  - Shift-Right-Click “#” deletes without warning

DISABLE

- Right-Click Oscillator Type



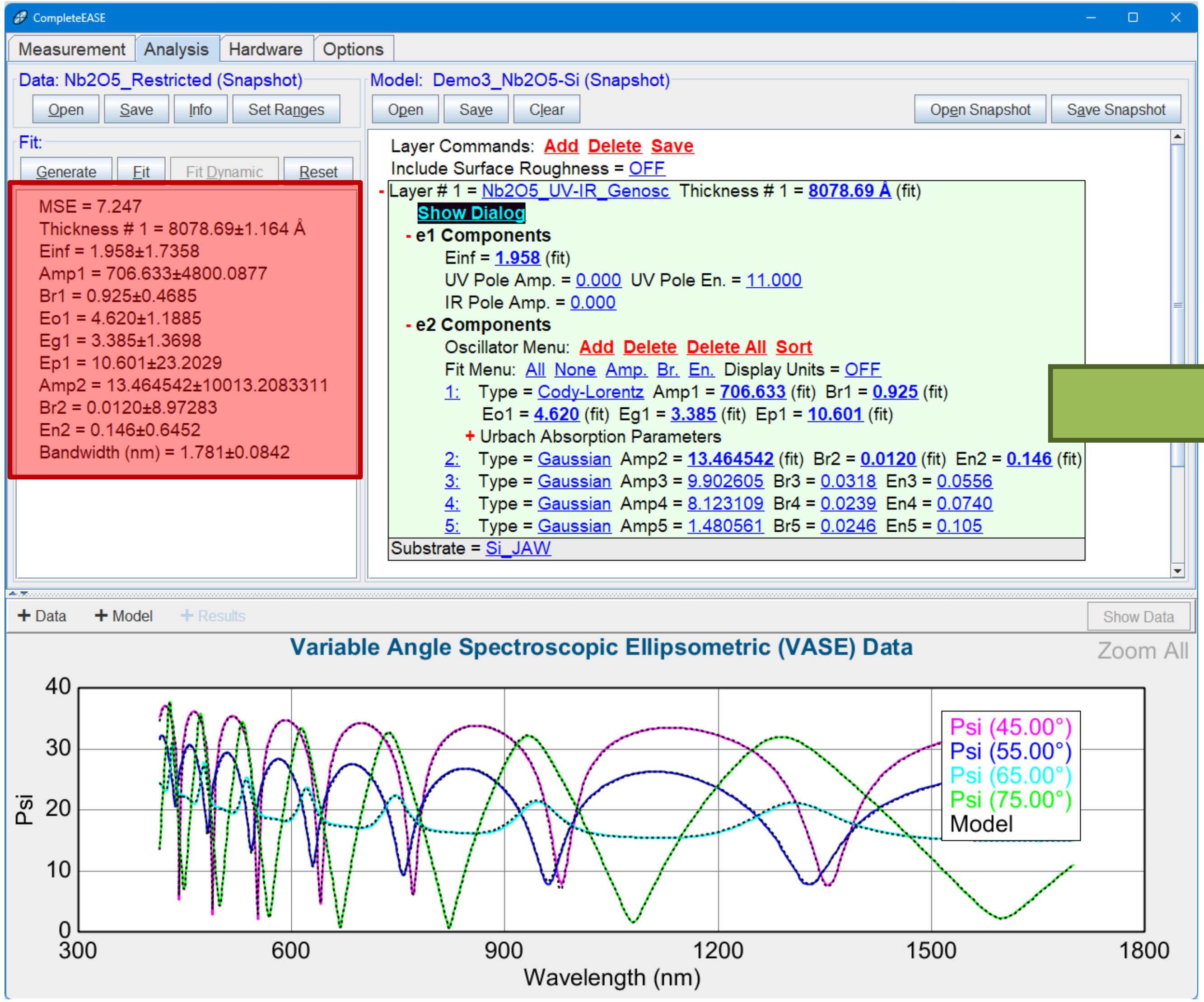


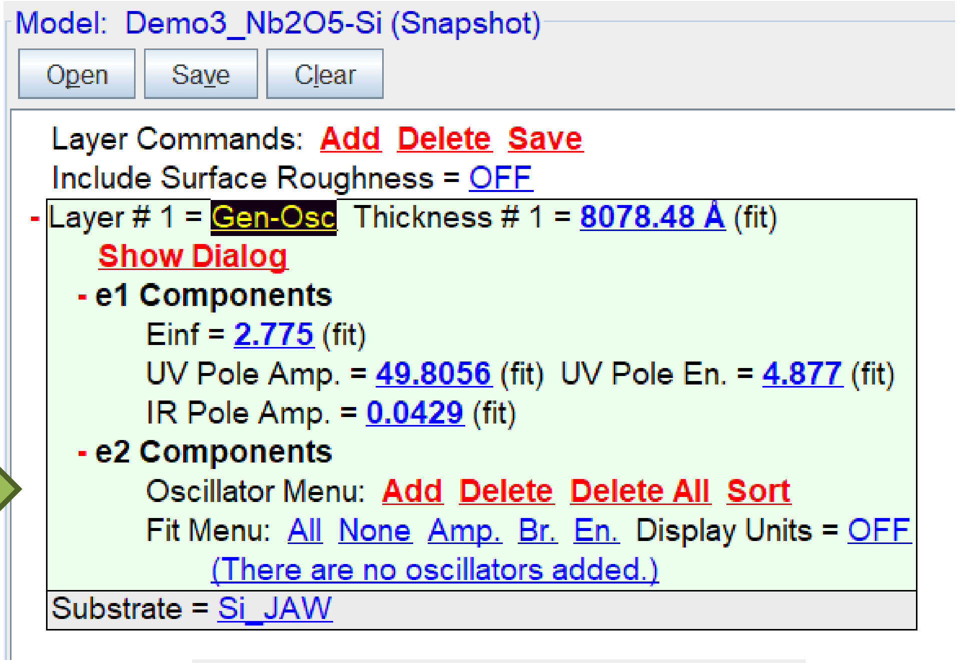
Demonstration 3: Simplify Existing Gen-Osc: Nb_2O_5 on Si

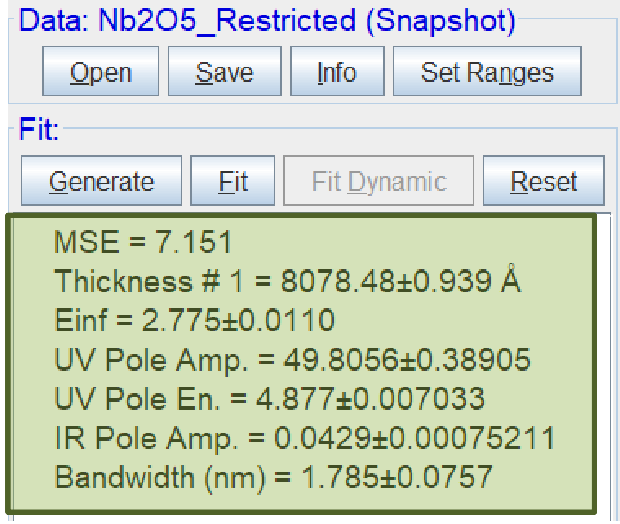
- Open SNAPSHOT: Demo3_Nb2O5-Si
- Simplify the existing model.

Constructing your Own Gen-Osc

Nb_2O_5 Demonstration: Results







4-06: Making a Genosc: Ta_2O_5 on Fused Silica

- **Fit the data with existing Genosc**
- **Simplify the Genosc for the limited wavelength range**

HINTS:

- Is the backside smooth or rough?

Constructing your Own Gen-Osc

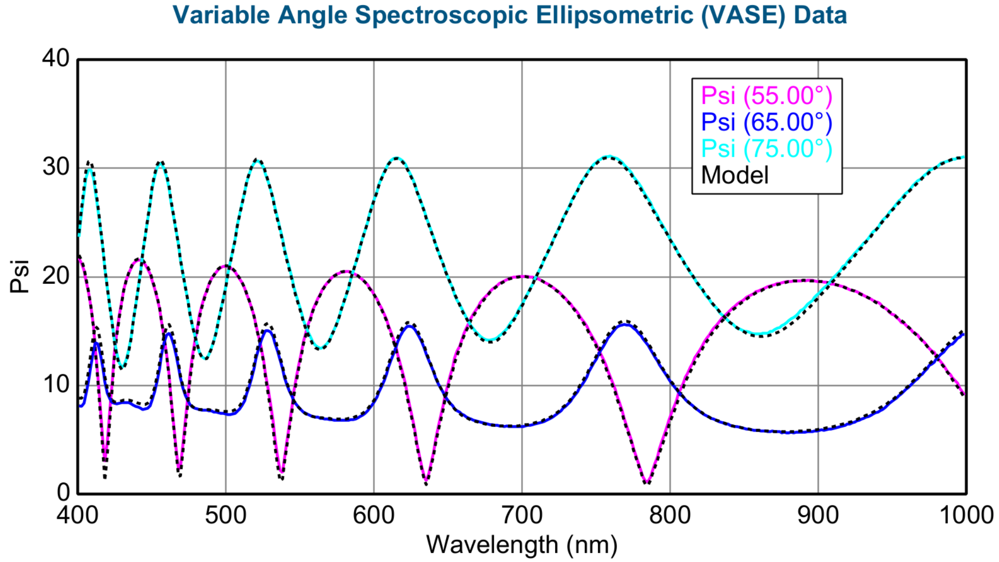
Ta_2O_5 on Fused Silica: Results

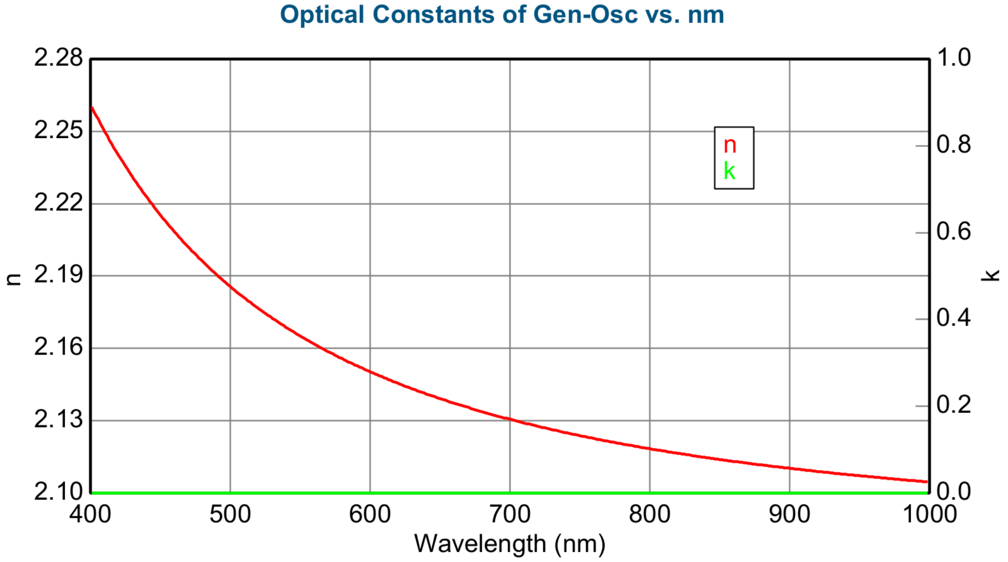
Include Surface Roughness = OFF
- Layer # 1 = Gen-Osc Thickness # 1 = **8021.94 Å** (fit)
  Show Dialog
  - **e1 Components**
    Einf = **2.290** (fit)
    UV Pole Amp. = **72.3690** (fit) UV Pole En. = **5.934** (fit)
    IR Pole Amp. = **0.0175** (fit)
  + **e2 Components**

+ Substrate = Fused Silica_Sellmeier Substrate Thickness = 1.0000 mm

- **MODEL Options**
  Angle Offset = 0.00
  Include Substrate Backside Correction = ON
    Transmission SE Data = OFF Reverse Direction = OFF
    # Back Reflections = **1.543** (fit)
    % 1st Reflection = 100.00

MSE = 6.367
Thickness # 1 = 8021.94 ± 2.181 Å
Einf = 2.290 ± 0.0974
UV Pole Amp. = 72.3690 ± 5.39413
UV Pole En. = 5.934 ± 0.0877
IR Pole Amp. = 0.0175 ± 0.00682
Back Reflections = 1.543 ± 0.0339





Gen-Osc Methods

METHOD 1:

Fit Data with Pre-built Gen-Osc

METHOD 2:

Constructing your Own Gen-Osc

METHOD 3:

Cauchy ▶ B-Spline

⇩

Build Gen-Osc from B-spline n,k

Procedure: Building your own Gen-Osc

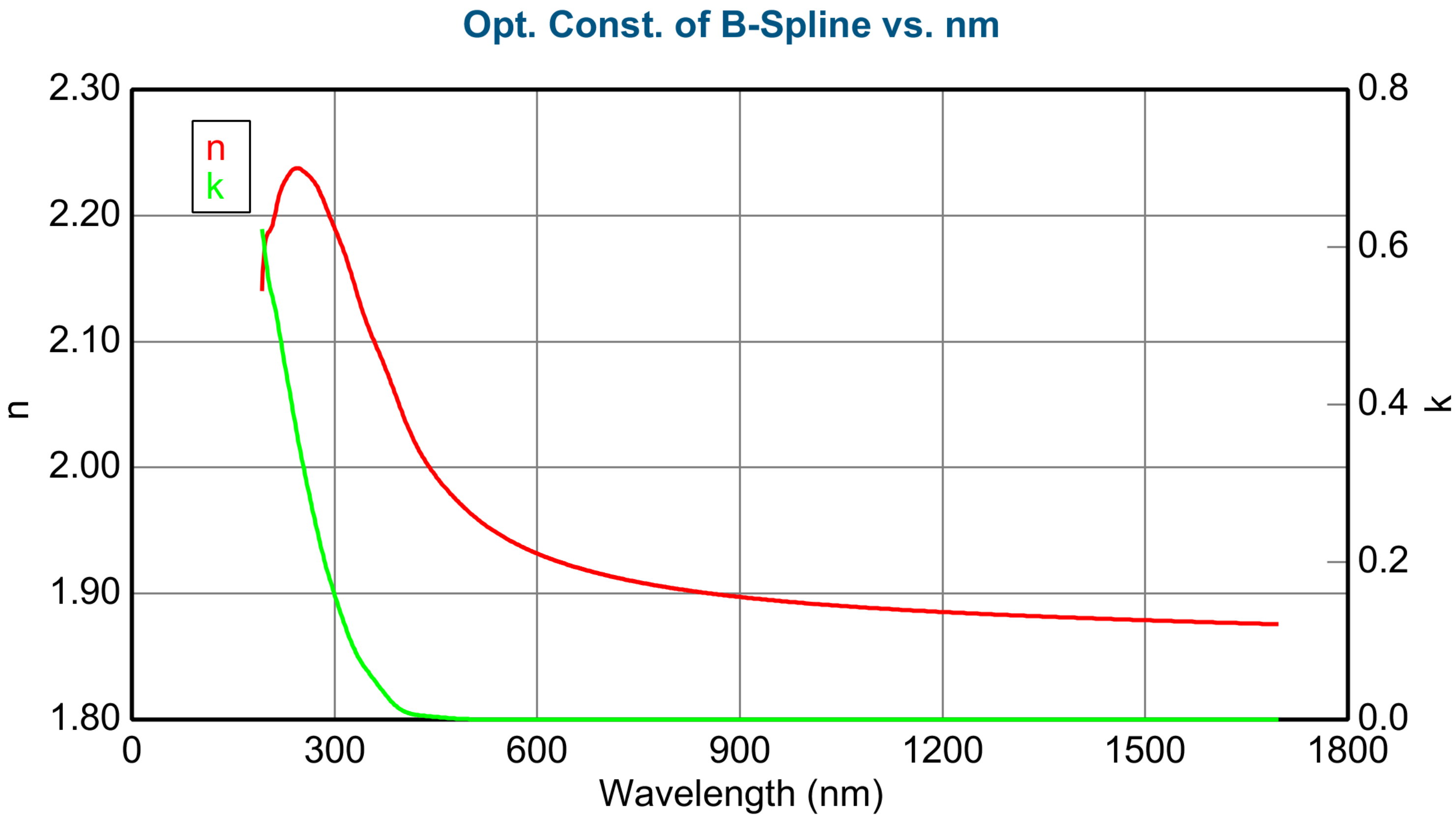
Match ε_2

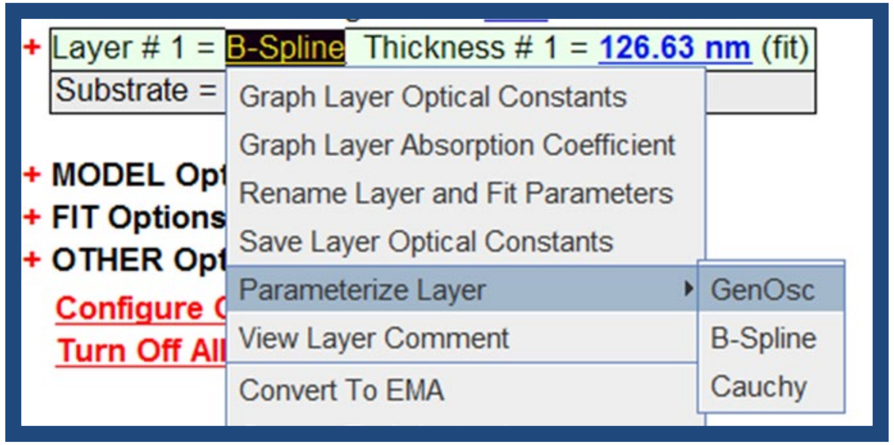
Match ε_1

Building Oscillator Model

Fit Data with Oscillators

Using Current Results as Reference

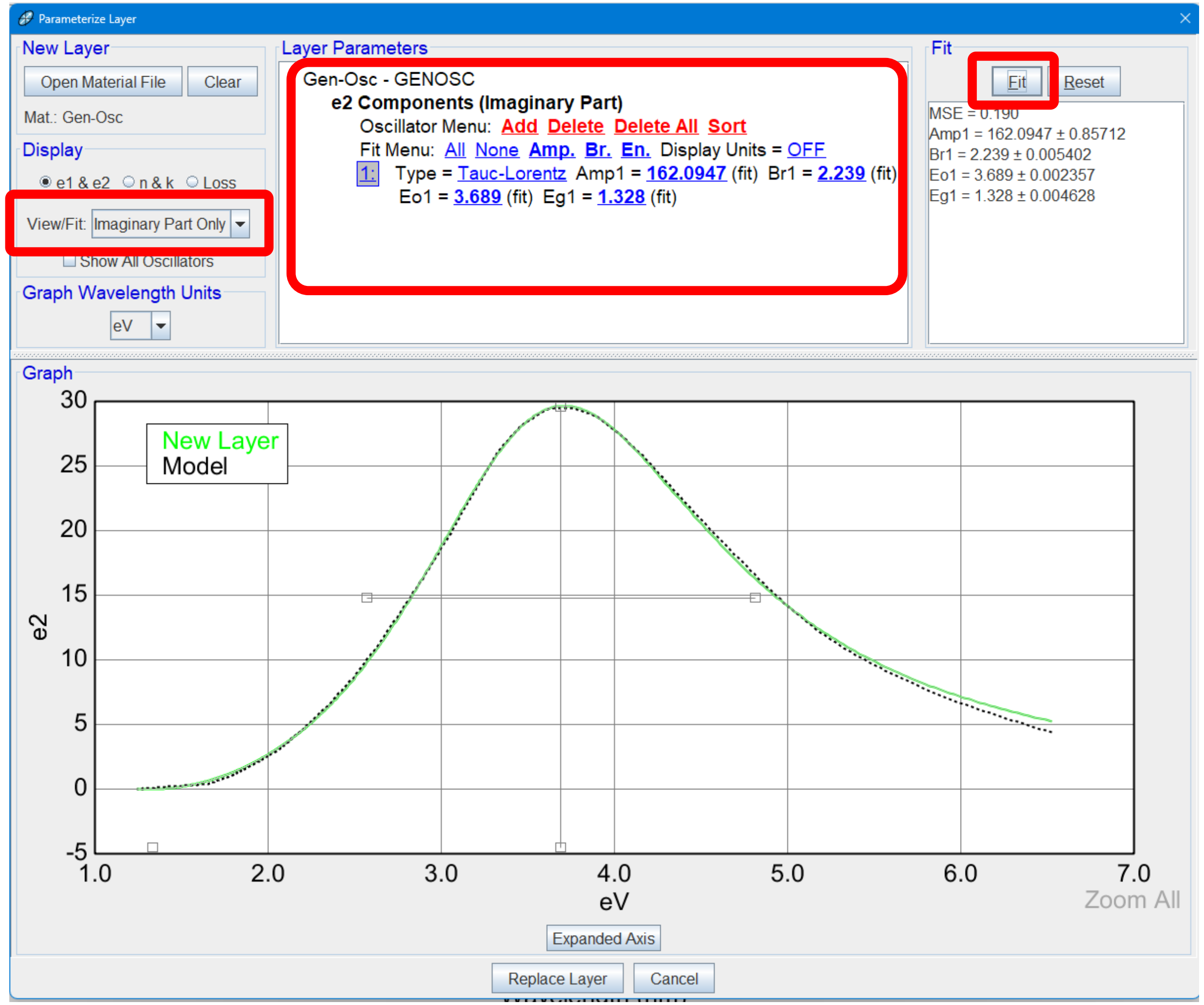


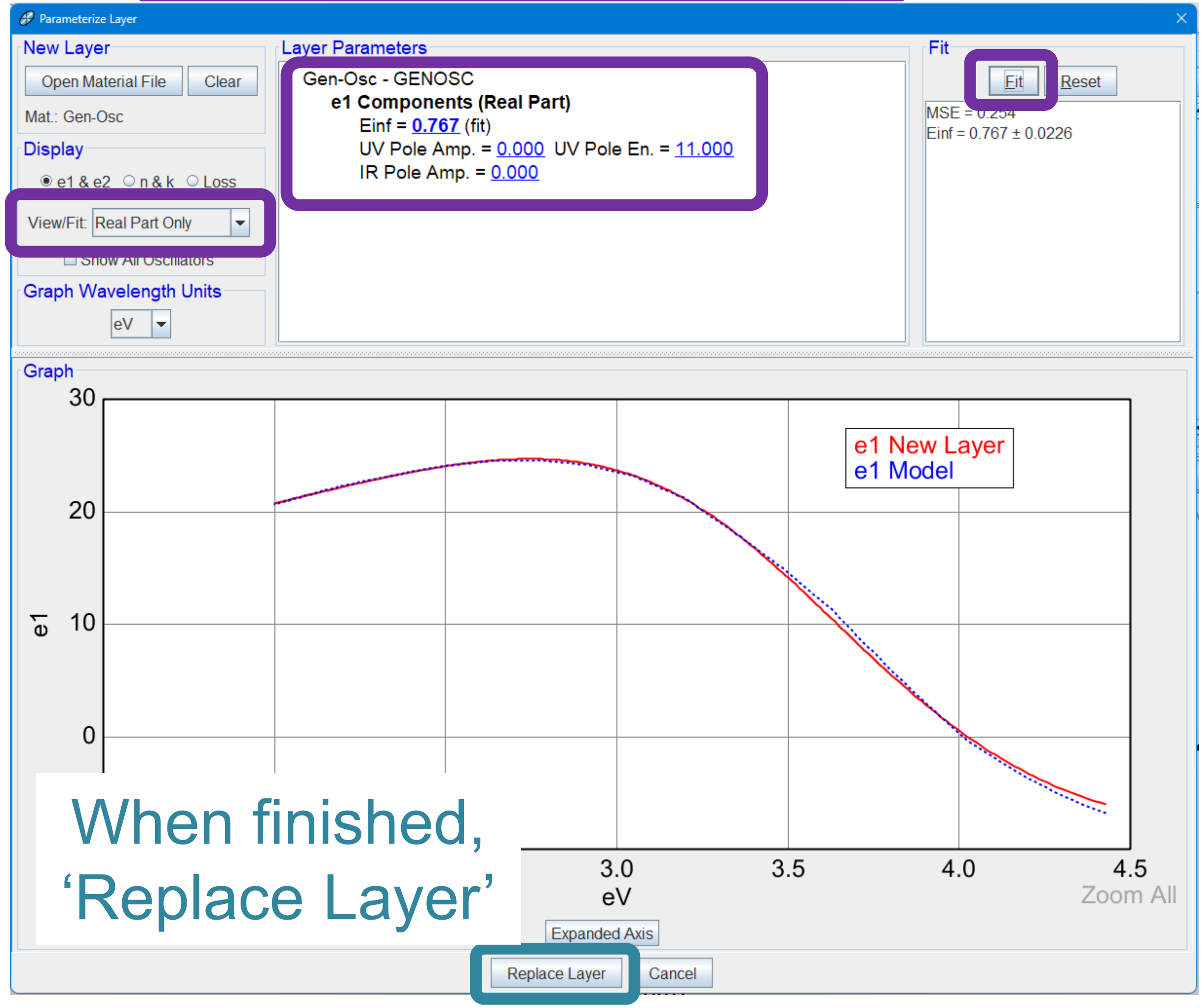


Building a Gen-Osc

Match ε_2 with oscillators

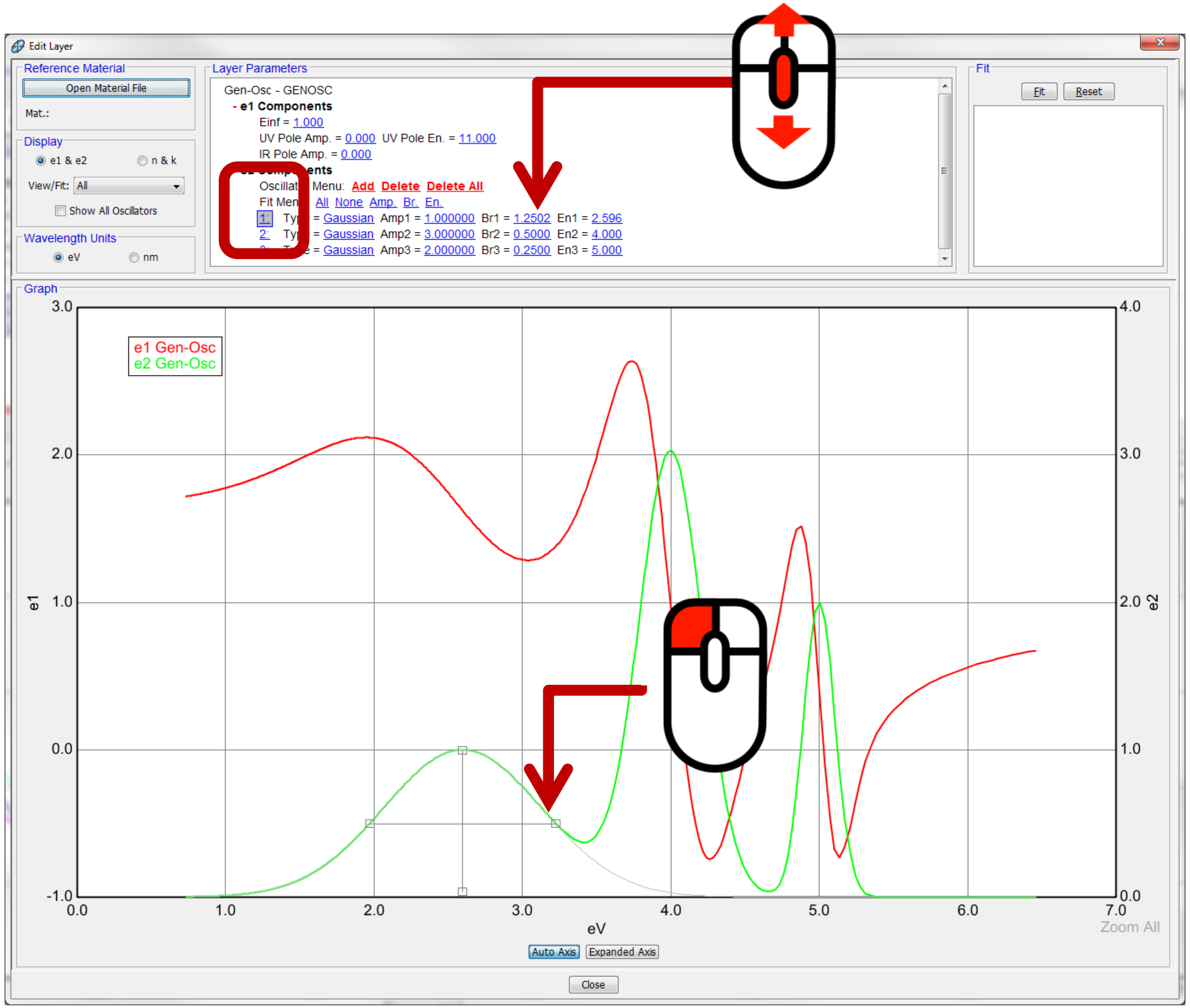
Match ε_1 with Einf, Poles





Manipulating oscillators

- SHIFT- “Mouse-Roll” on Parm.
  - CTRL-SHIFT for smaller step
- Left-Click # to view “handles”
  - Drag grey boxes with mouse



4-07: Making a Genosc: a-Ge Thin Film

- **B-spline fit is already completed > saved as Snapshot**
- **Convert the b-spline to a Genosc**
  - **Can you get similar MSE?**
  - **How do your Genosc optical constants compare to B-spline**

HINTS:

- It will take more than one oscillator to find a great match to the b-spline.

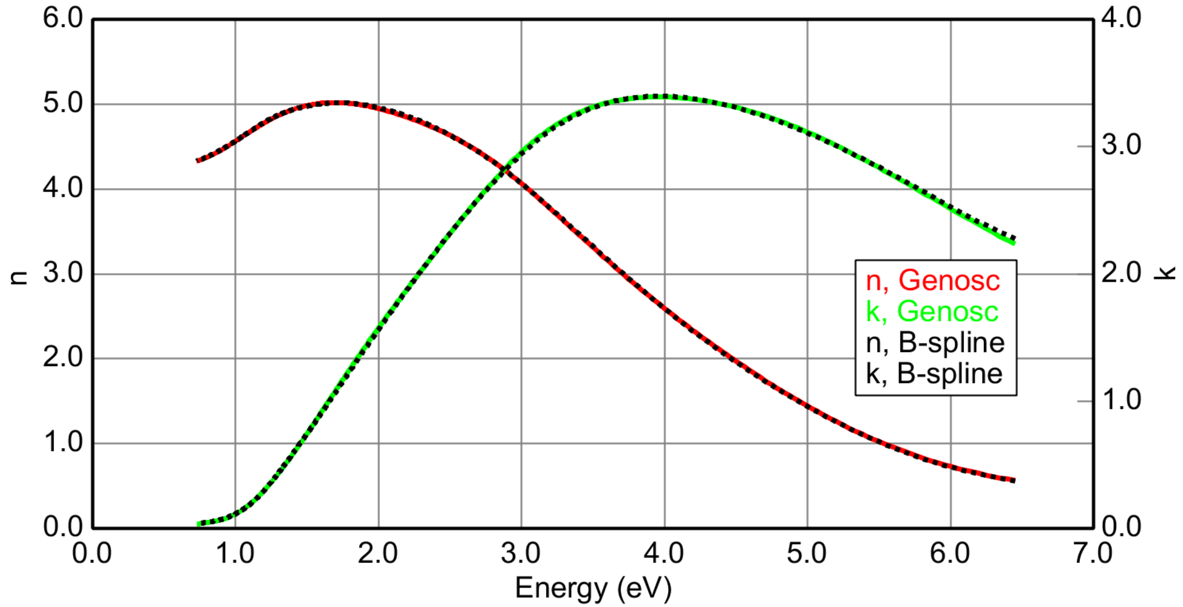
Constructing your Own Gen-Osc

a-Ge Thin Film : Results

Roughness = **46.83 Å** (fit)

- Layer # 2 = a-Ge_Adachi_cl Thickness # 2 = **3179.79 Å** (fit)
  - **Show Dialog**
  - **- e1 Components**
    - Einf = **1.296** (fit)
    - UV Pole Amp. = 0.000 UV Pole En. = 11.000
    - IR Pole Amp. = 0.000
  - **- e2 Components**
    - Oscillator Menu: **Add** **Delete** **Delete All** **Sort**
    - Fit Menu: All None **Amp.** **Br.** **En.** Display Units = OFF
    - 1: Type = Cody-Lorentz Amp1 = **55.015** (fit) Br1 = **2.642** (fit)
      Eo1 = **3.101** (fit) Eg1 = **0.878** (fit) Ep1 = **0.699** (fit)
      + Urbach Absorption Parameters
    - 2: Type = Gaussian Amp2 = **3.483783** (fit) Br2 = **1.1284** (fit) En2 = **1.857** (fit)
    - 3: Type = Gaussian Amp3 = **6.358459** (fit) Br3 = **2.5087** (fit) En3 = **3.876** (fit)
- Layer # 1 = SiNx_Film Thickness # 1 = **955.45 Å** (fit)
- Substrate = Glass Substrate

Genosc MSE = 2.803
B-spline MSE = 2.485



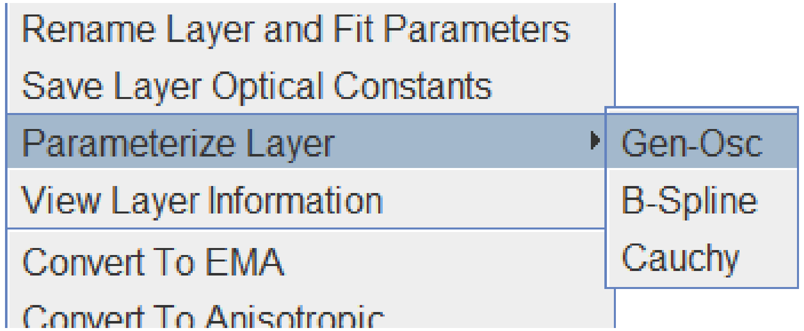
4-08: Making a Genosc: ZnO Thin Film

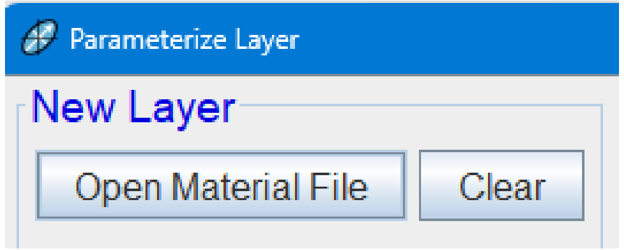
- **B-spline fit is already completed > saved as Snapshot**
- **Convert the b-spline to a Genosc**
  - **Can you get similar MSE?**
  - **How do your Genosc optical constants compare to B-spline**

Constructing your Own Gen-Osc

HINTS:

- Why build your own when there is an existing ZnO gen-osc?
  - Parameterize to Genosc, then “Open Material File” and choose ZnO_Genosc.mat





ZnO Thin Film : Results

Roughness = **126.29 Å** (fit)

\- Layer # 1 = ZnO_Genosc Thickness # 1 = **926.09 Å** (fit)

Show Dialog

\- **e1 Components**

Einf = 1.000

UV Pole Amp. = **219.7595** (fit) UV Pole En. = **11.035** (fit)

IR Pole Amp. = **0.0446** (fit)

\- **e2 Components**

Oscillator Menu: **Add** **Delete** **Delete All** **Sort**

Fit Menu: All None **Amp.** **Br.** **En.** Display Units = OFF

1: Type = PSemi-M0 Amp1 = **1.871** (fit) Br1 = **0.0765** (fit)

Eo1 = **3.301** (fit) WR1 = **5.1752** (fit) PR1 = **0.354** (fit)

AR1 = **0.666** (fit) O2R1 = **-0.394** (fit)

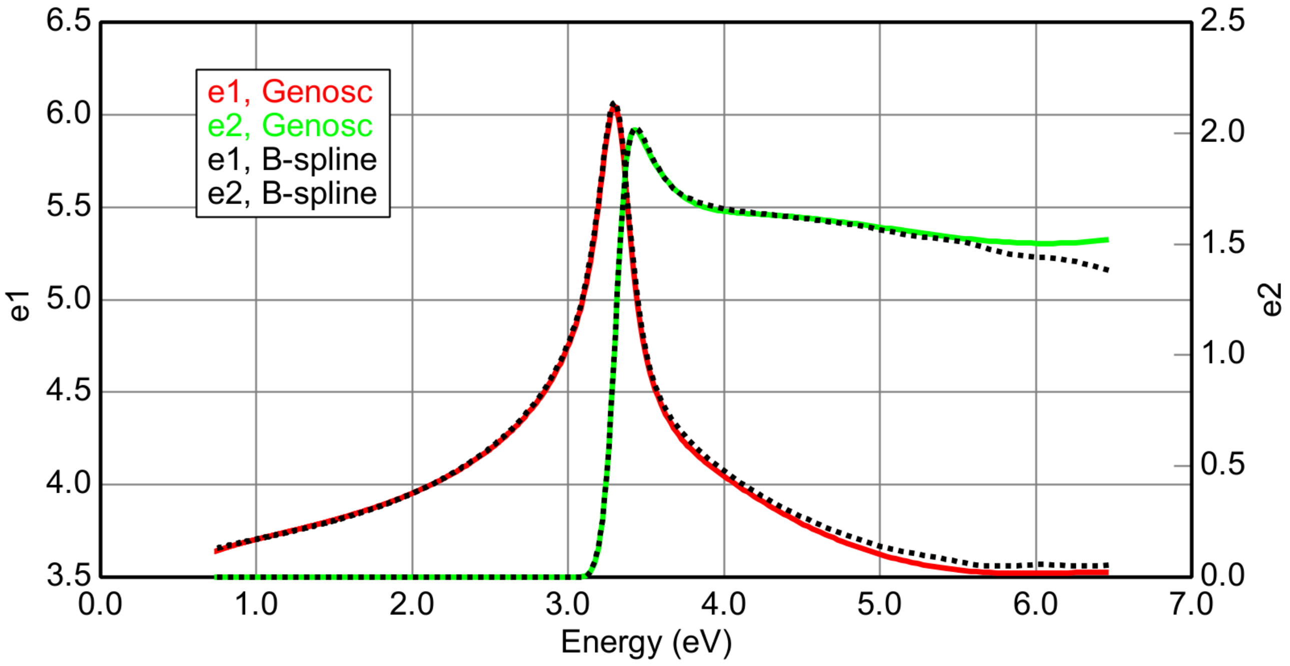
2: Type = Gaussian Amp2 = **0.270272** (fit) Br2 = **0.2460** (fit) En2 = **3.398** (fit)

3: Type = Gaussian Amp3 = **0.551993** (fit) Br3 = **0.9438** (fit) En3 = **6.960** (fit)

\+ Substrate = 7059_Genosc

B-spline MSE = 3.329

Genosc MSE = 3.206



Gen-Osc Methods

METHOD 1:

Fit Data with Pre-built Gen-Osc

METHOD 2:

Constructing your Own Gen-Osc

METHOD 3:

Cauchy ▶ B-Spline

⇩

Build Gen-Osc from B-spline n,k

Procedure: Building your own Gen-Osc

Cauchy ► B-Spline

↓

Match ε_2

↓

Match ε_1

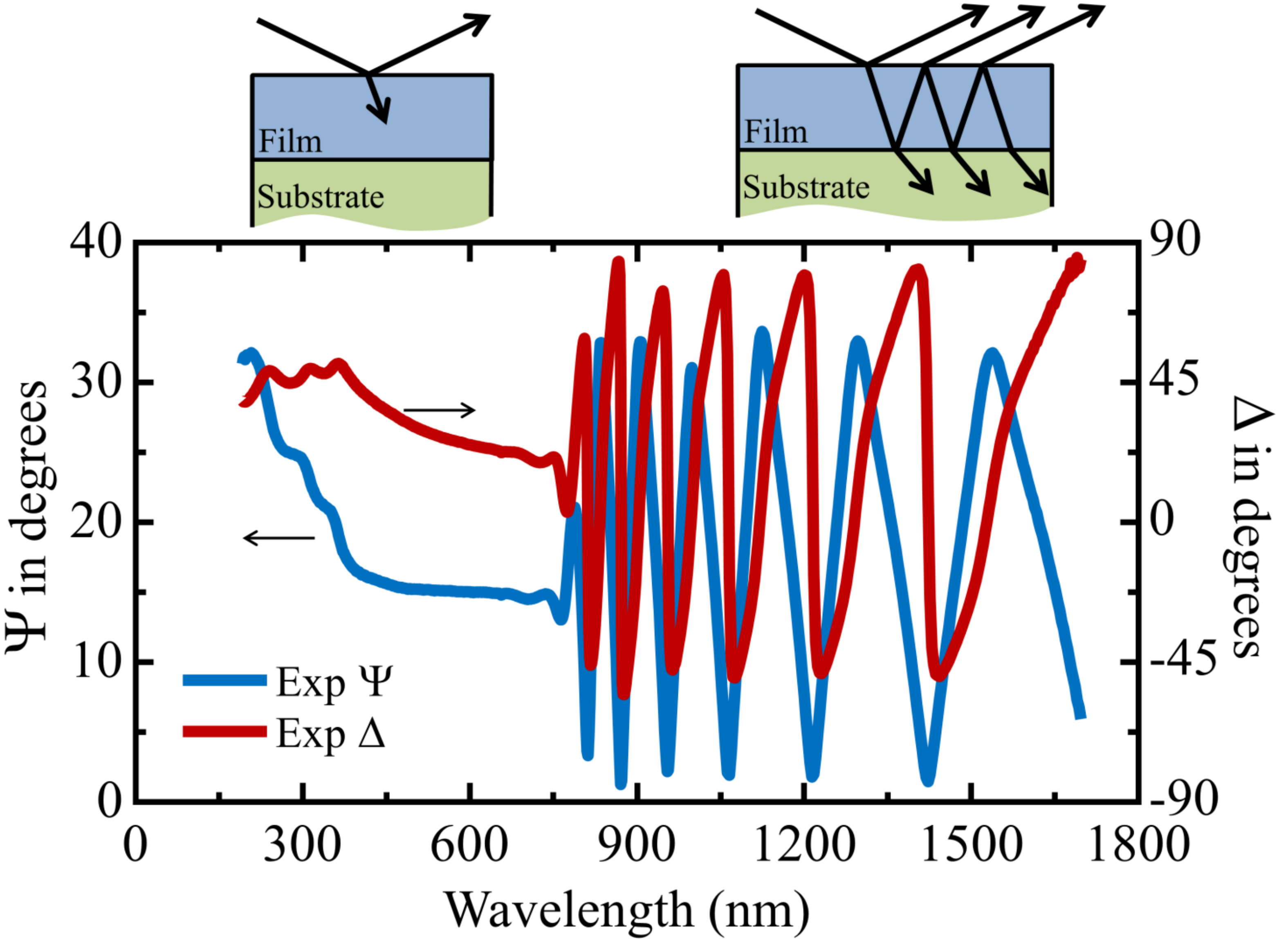
↓

Fit Data with Oscillators

Building Oscillator Model

Cauchy → B-Spline → Gen-Osc

- Putting all the pieces t



Build Gen-Osc from B-spline fit results

Cauchy ▶ B-Spline

⇩

Build Gen-Osc from B-Spline n,k

⇩

Fit Data with Gen-Osc

1. Cauchy Fit transparent region only
2. B-Spline fit to all wavelengths
3. Build Gen-Osc from B-spline *n,k* results
   - Fit reference – ε_2 first, then ε_1
   - Generate data before fitting
4. Fit Data (Ψ & Δ) using Gen-Osc

4-09: Fit Chalcogenide Glass Substrate with Genosc

- Start with Cauchy Fit (> 900 nm)
- Extend to all wavelengths with B-spline
- Convert to Genosc

Cauchy ▶ B-Spline

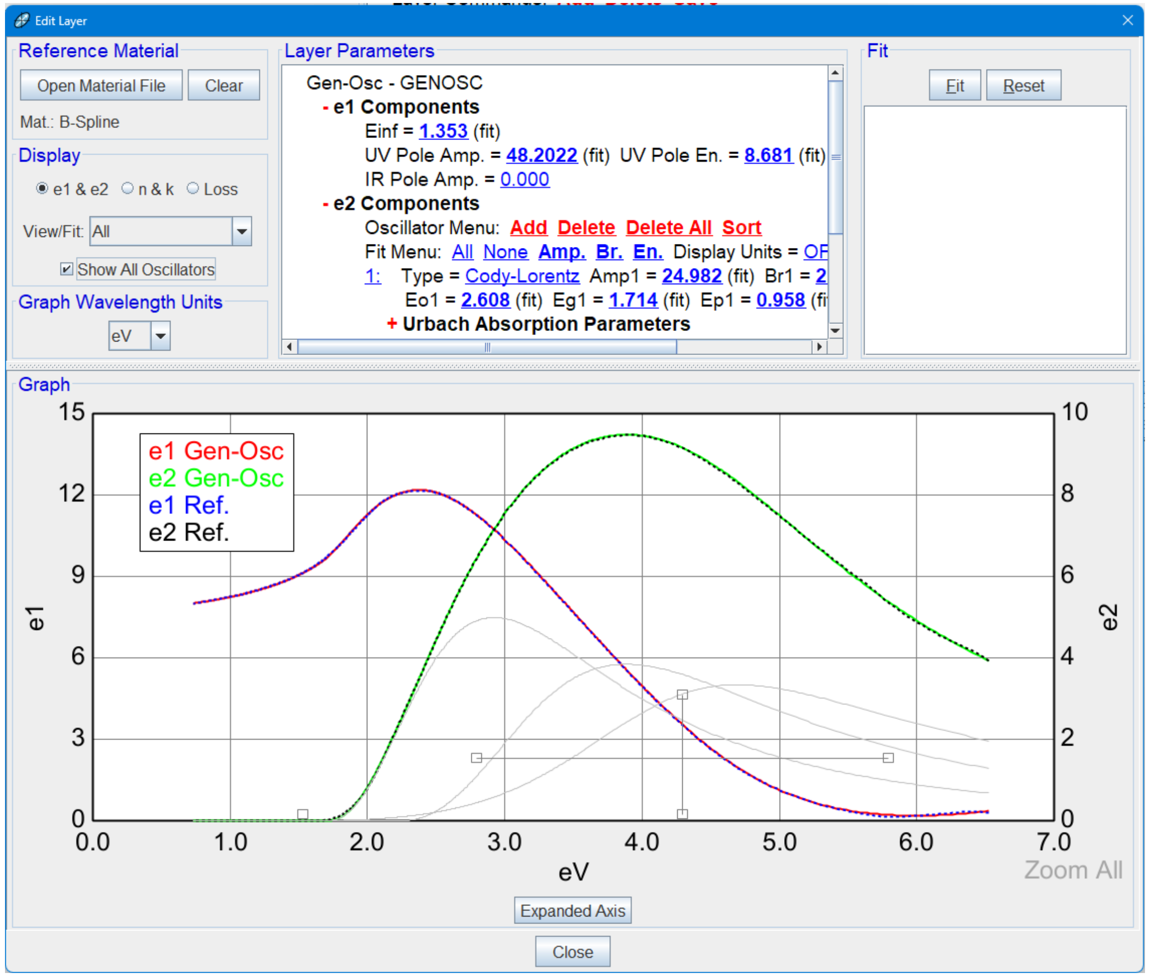
⇩

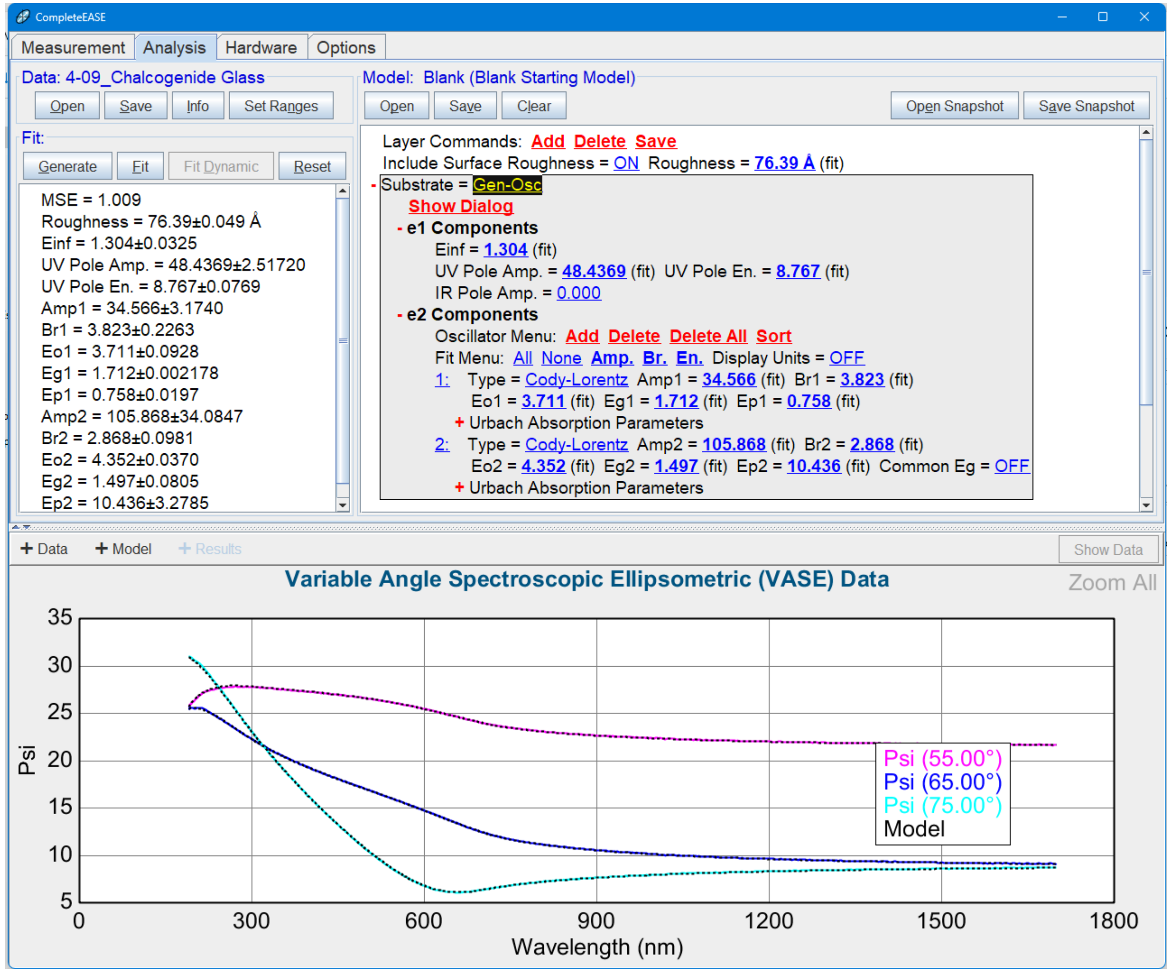
Build Gen-Osc from B-Spline n,k

⇩

Fit Data with Gen-Osc

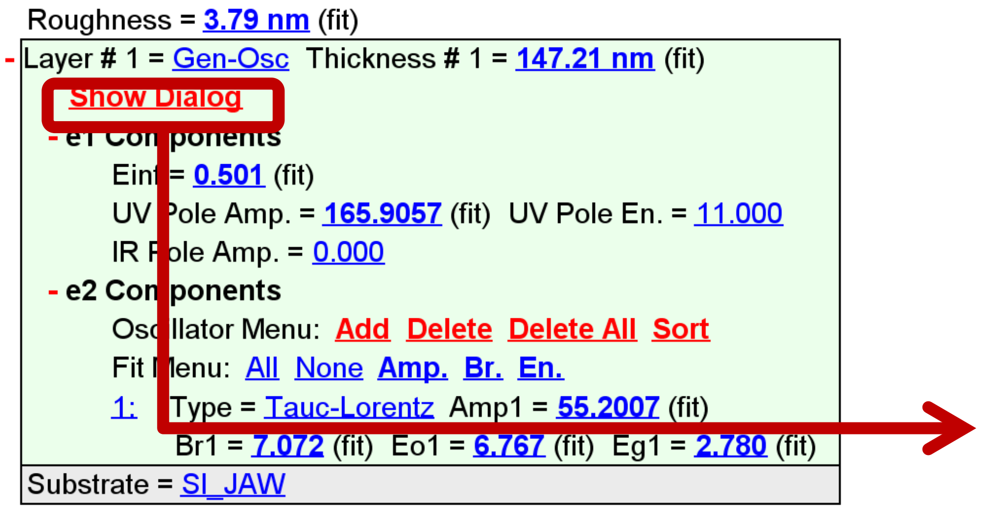
Chalcogenide Substrate: Results





B-spline MSE = 0.947
Genosc MSE = 1.009

Are Additional Oscillators necessary?

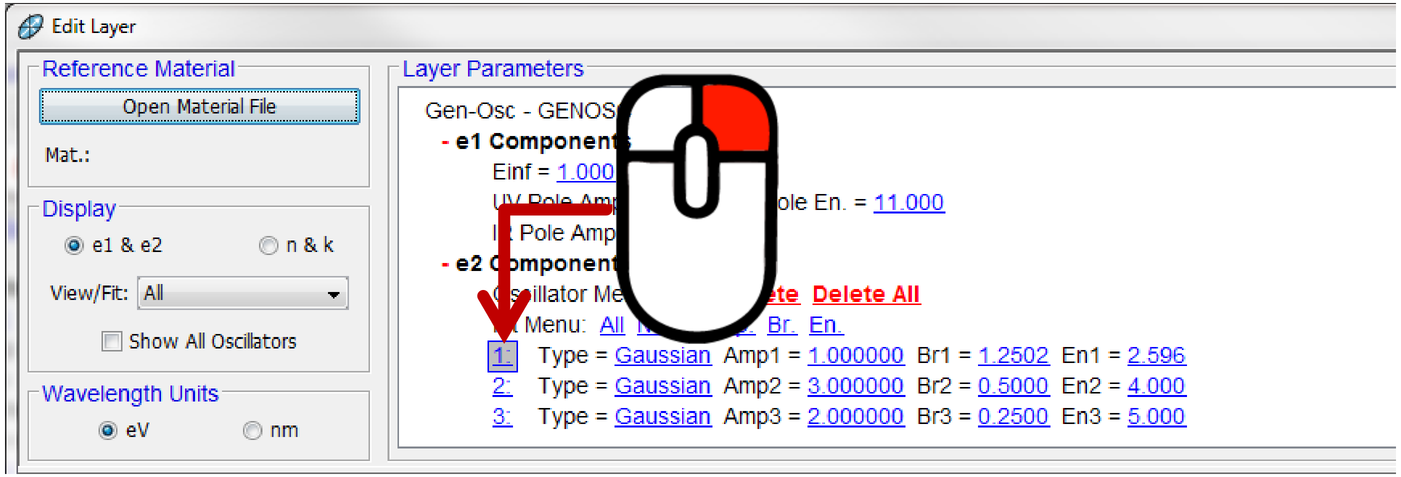


- <u>Add</u> from Oscillator Menu
- SHIFT-“Left-Click” on graph

Disabling or Deleting oscillators

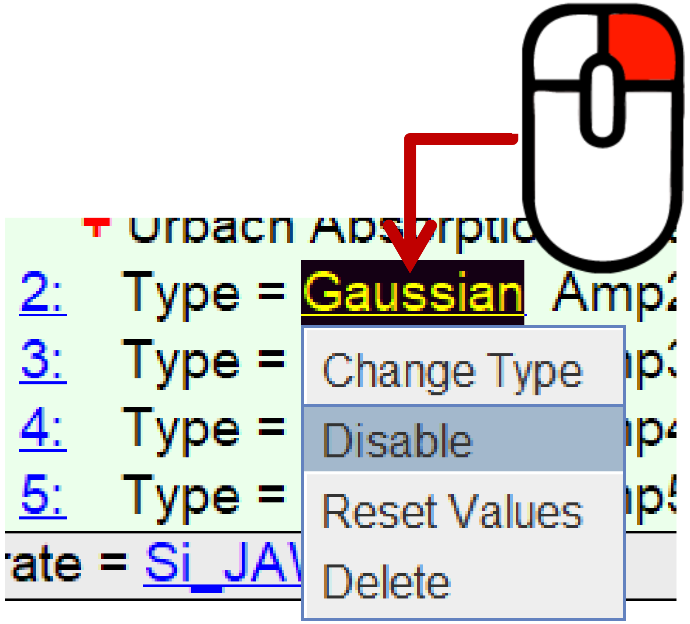
DELETE

- Right-Click "#"
  - Shift-Right-Click "#" deletes without warning



DISABLE

- Right-Click Oscillator Type



4-10: Photoresist on Silicon: Cauchy → B-Spline → Genosc

- Build a Genosc for this Photoresist.
- If you have trouble with the b-spline, I saved my snapshot – start there

Cauchy ▶ B-Spline

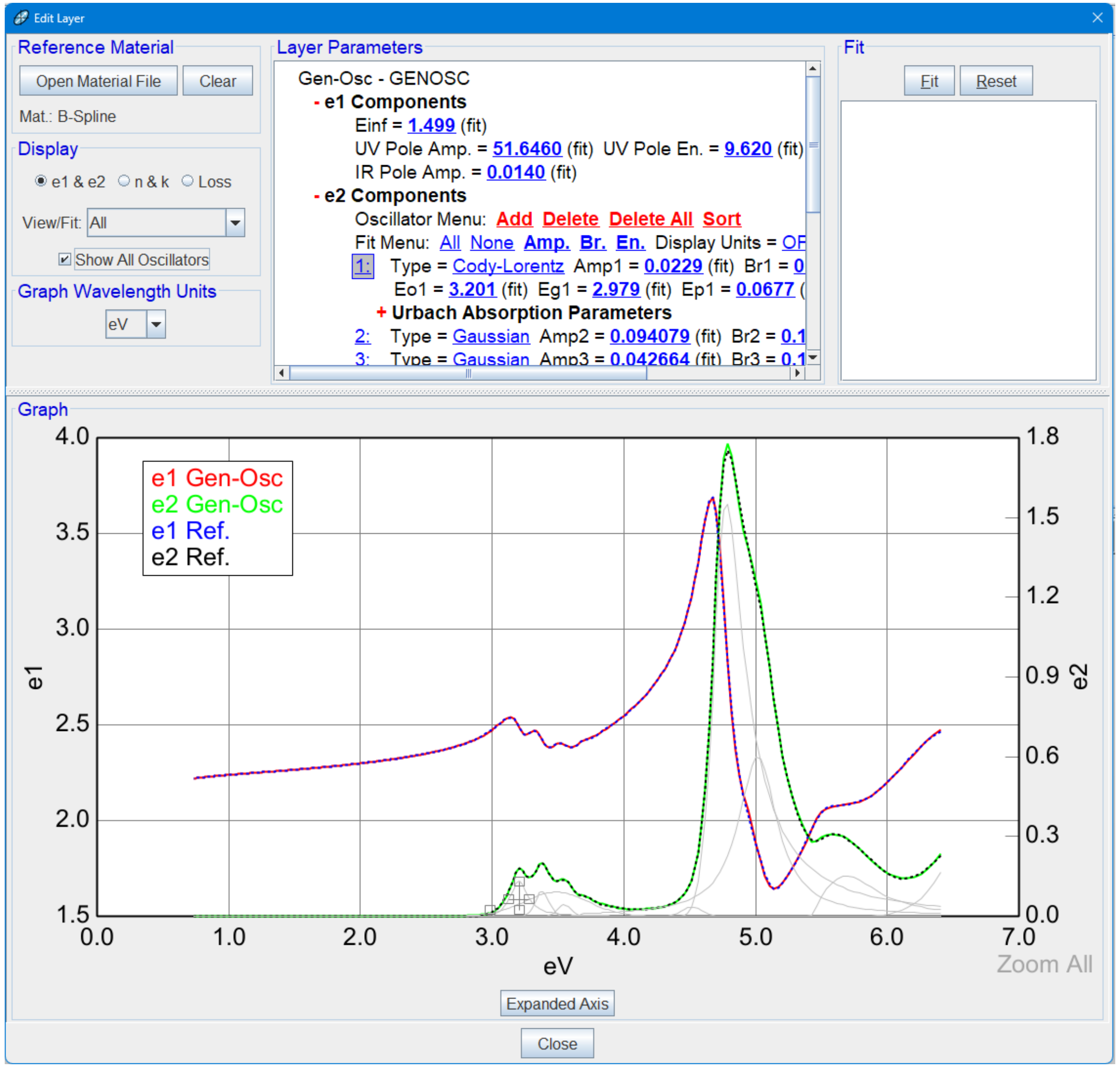
⇩

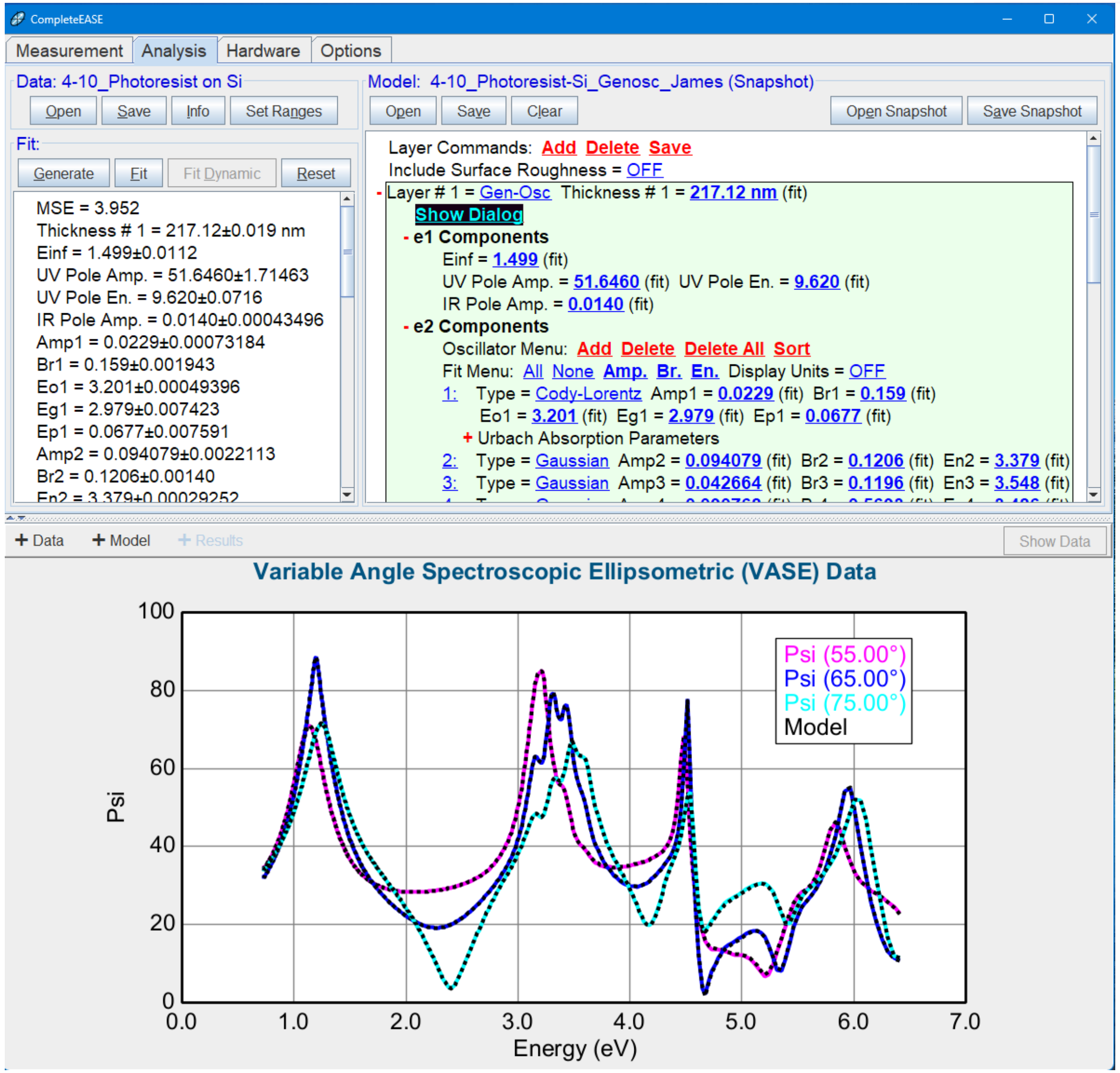
Build Gen-Osc from B-spline n,k

HINTS:

- Can you match MSE of your b-spline fit?
- How many oscillators did it take?

Photoresist on Si: Results

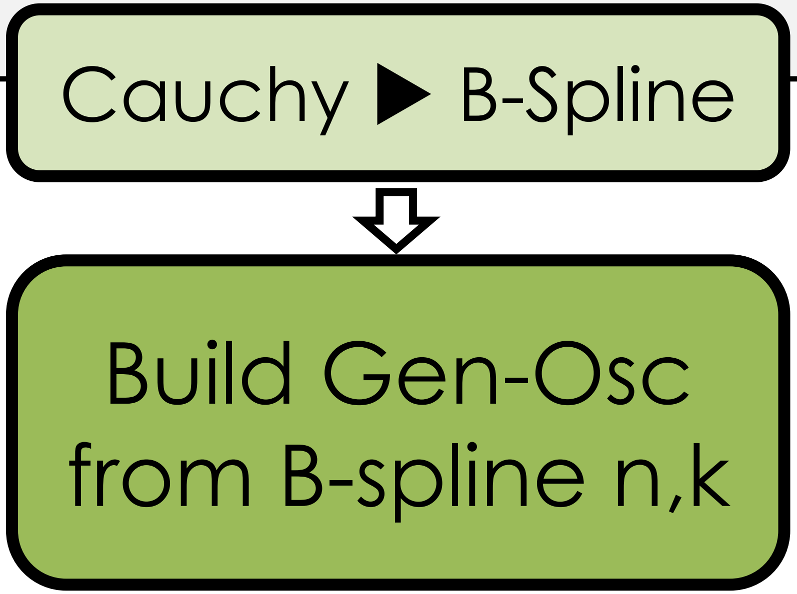




4-10B: Photoresist on Silicon: Diagnosing Genosc Problems

Open Snapshot: 4-10B_Photoresist-Si_Genosc_PROBLEMS

- I quickly made a Gen-osc to match the b-spline for this photoresist.
- Please diagnose (and fix) any problems with my Gen-Osc

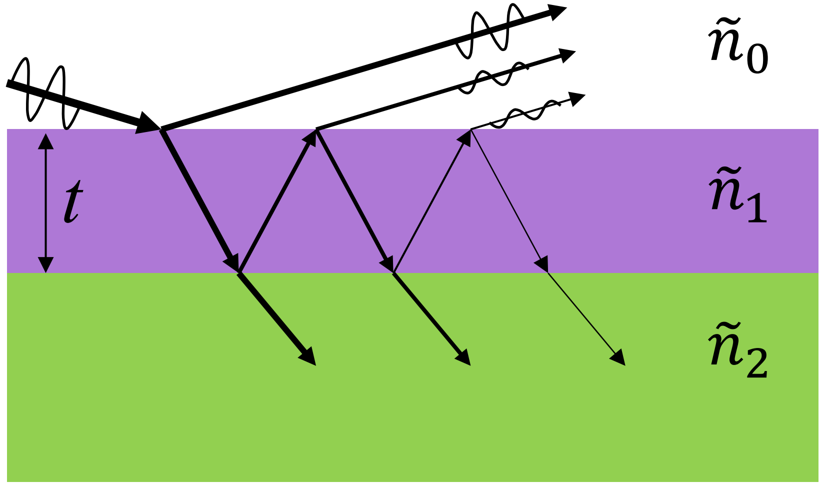


Model Comparison

Model	Advantages	Disadvantages	Recommend
B-spline	▪ Easy to use. ▪ Smooth functions. ▪ Customize node spacing. ▪ Kramers-Kronig consistent.	▪ No physical basis – just "curve fitting". ▪ Large number of fit parameters. ▪ Easy to use incorrectly.	▪ Best for **metals**, **organics**, and **crystalline materials**. *can capture all details in *n,k* *perfect for sharp features when using custom node spacing
Gen-osc	▪ Few Fit parameters. ▪ Kramers-Kronig consistent. ▪ May be physically related to absorption phenomena	▪ Can be tedious. ▪ May not capture all features.	▪ Best for **amorphous dielectrics** and **semiconductors**. *can be described with 1-2 oscillators. ▪ Better for constraining certain parameters for similar materials (or for anisotropic optical constants)

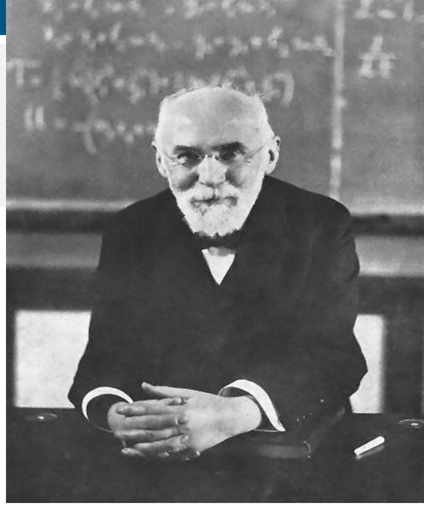
Course Outline

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



EXTRA SLIDES

Lorentz oscillator



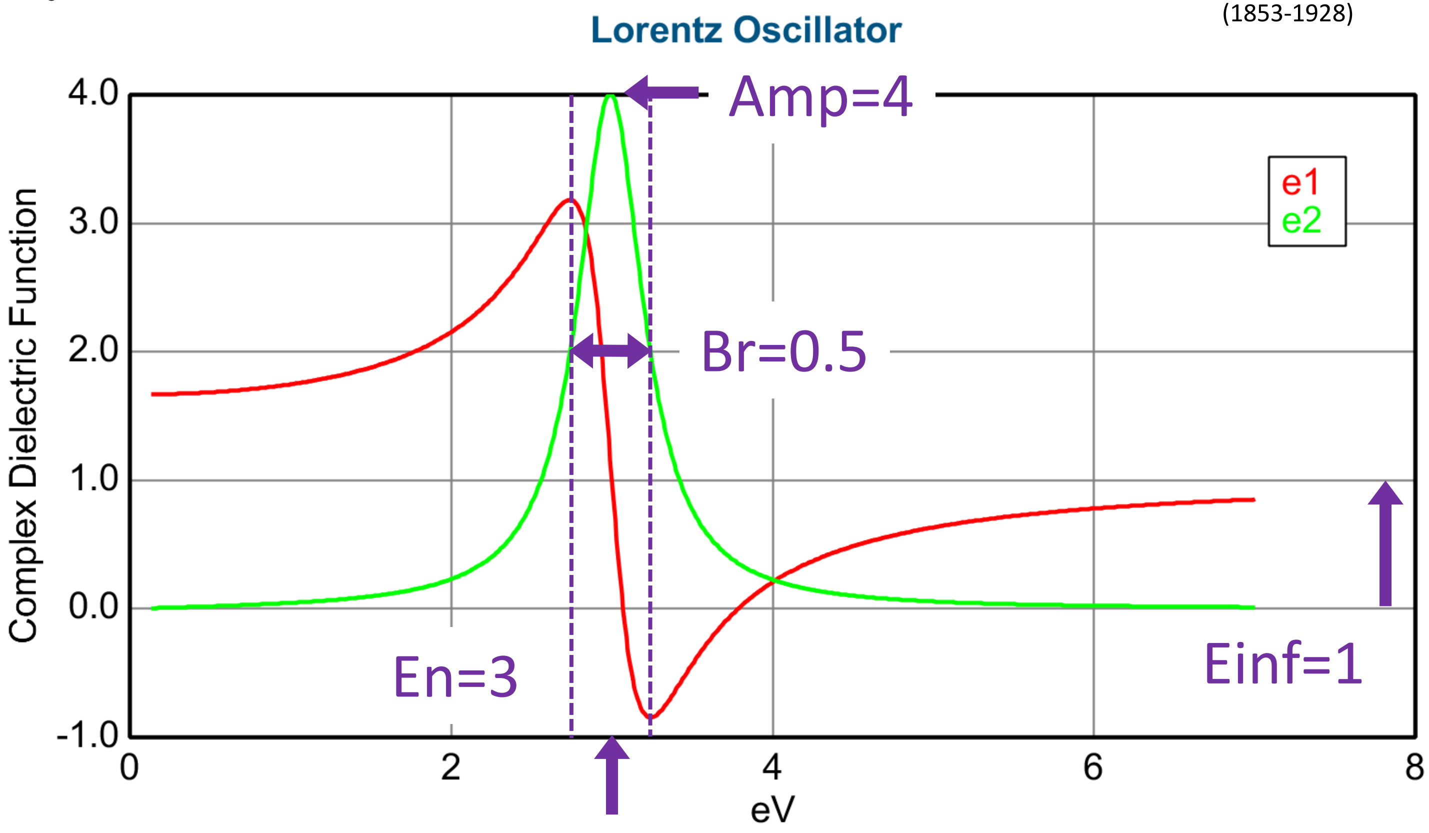
Hendrik Antoon Lorentz
(1853-1928)

- Classic "Harmonic" Oscillator

$$\tilde{\varepsilon}(E) = \varepsilon_1(\infty) + \frac{A\Gamma E_0}{E_0^2 - E^2 + i\Gamma E}$$

- 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 = Lorentz Amp1 = 4.000000 Br1 = 0.5000 En1 = 3.000

- 3 ε_2 Parameters: **Amp, En, Br**
- Broad Absorption
- Useful for metals

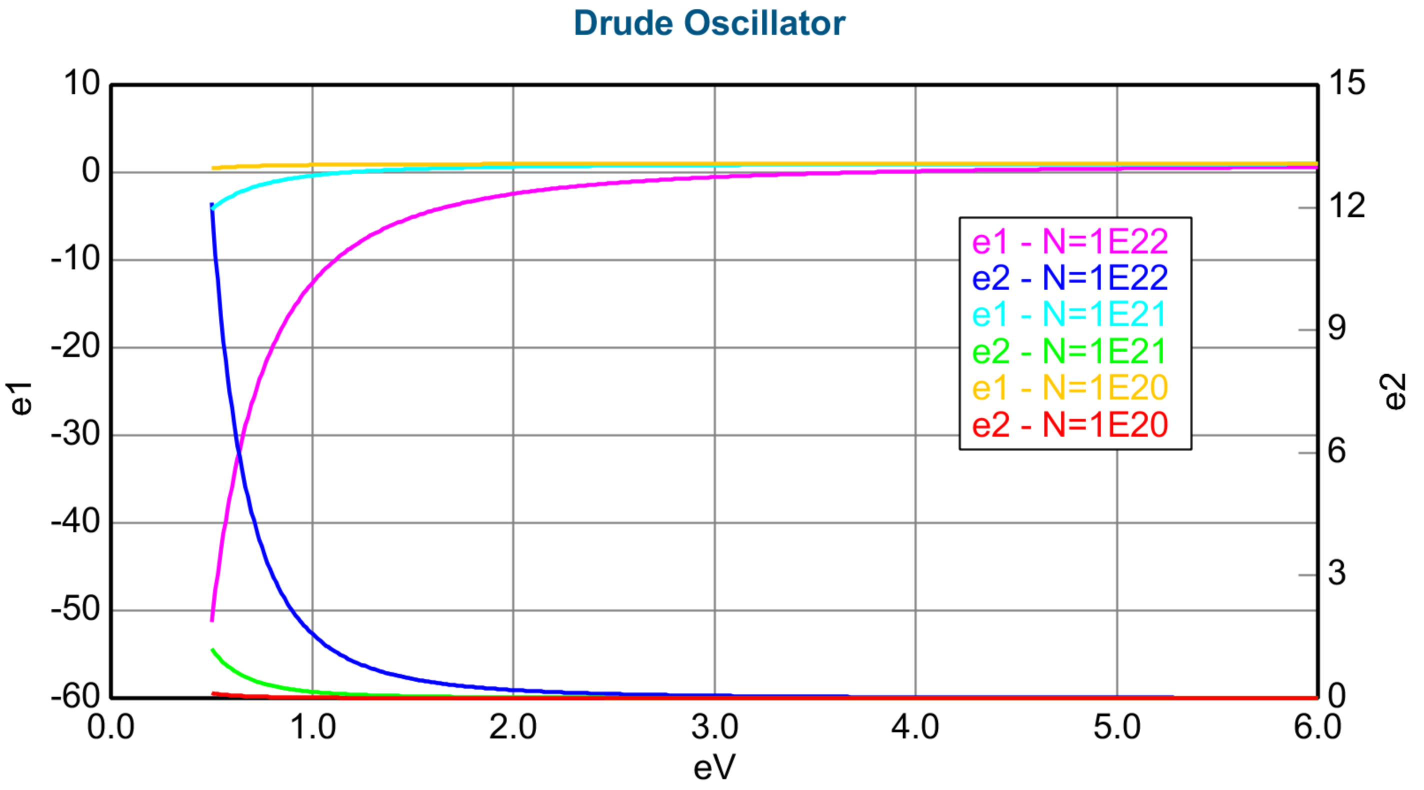


Drude Oscillator

- Lorentz oscillator with $E_0 = 0$
- Describes unbound charge - no restoring force

Paul Drude
(1863-1906)

- 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 = Drude(RT) Resistivity (Ohm·cm)1 = 0.001000 Scat. Time (fs)1 = 5.000
    - 2: Type = Drude(NMu) N2 = 1.0000E+20 mu2 = 10.000
      mstar2 = 1.000



- 2 ε_2 Parameters: **R, T** or **N, Mu**
- Describe long-wavelength absorption from conductivity: metals, doped semiconductors & conductive oxides

Gaussian Oscillator

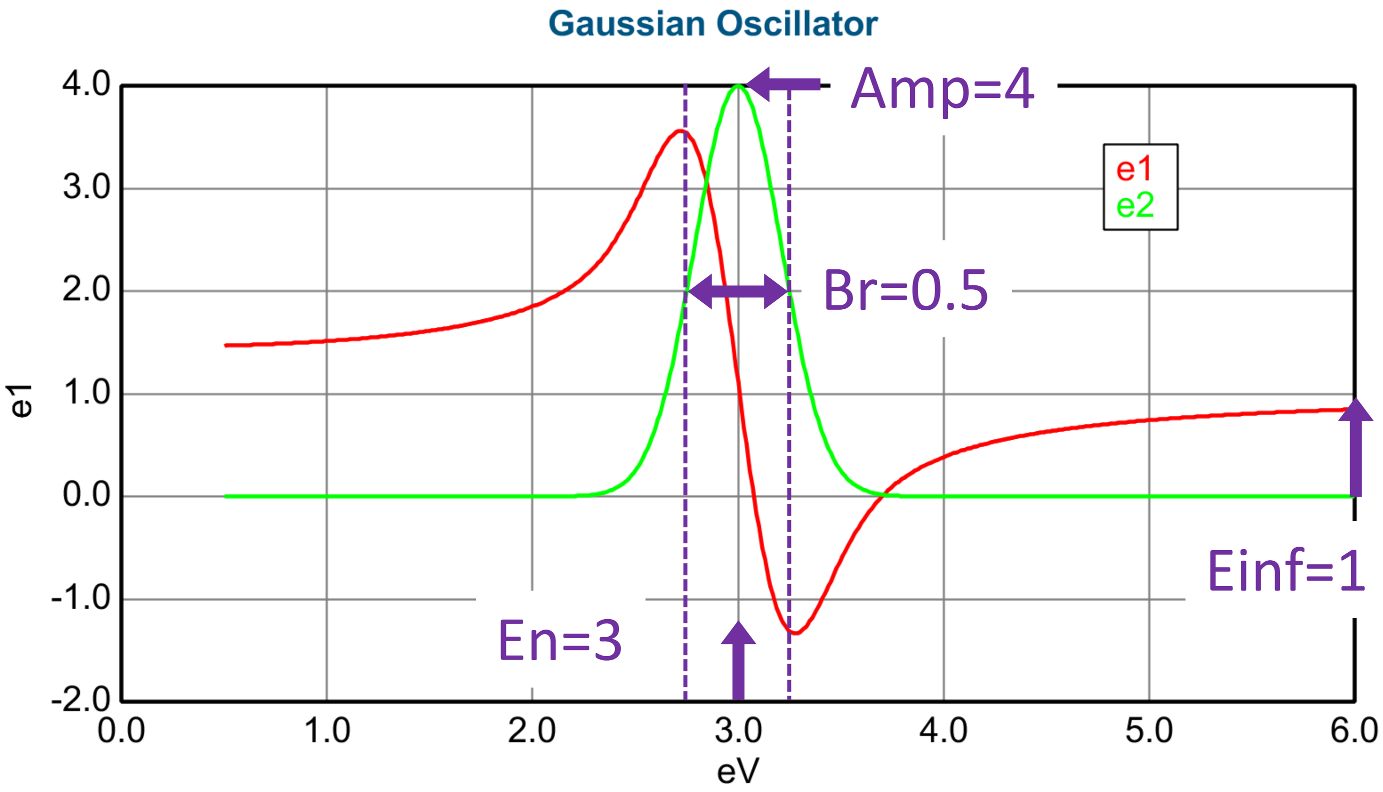
Carl Friedrich Gauss
(1777-1855)

- Gaussian line-shape for ε_2, KK for ε_1

$$\varepsilon_2(E) = Ae^{-\left(\frac{E-E_0}{\sigma}\right)^2} - Ae^{-\left(\frac{E+E_0}{\sigma}\right)^2} \quad \text{with} \quad \sigma = \frac{\Gamma}{2\sqrt{\ln(2)}}$$

- Shorter absorption tails than Lorentz

- 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



- 3 Parameters: **Amp, Br, En**

Very useful for:

- Materials with bandgaps
- Multiple UV absorptions in amorphous materials

Tauc-Lorentz Oscillator

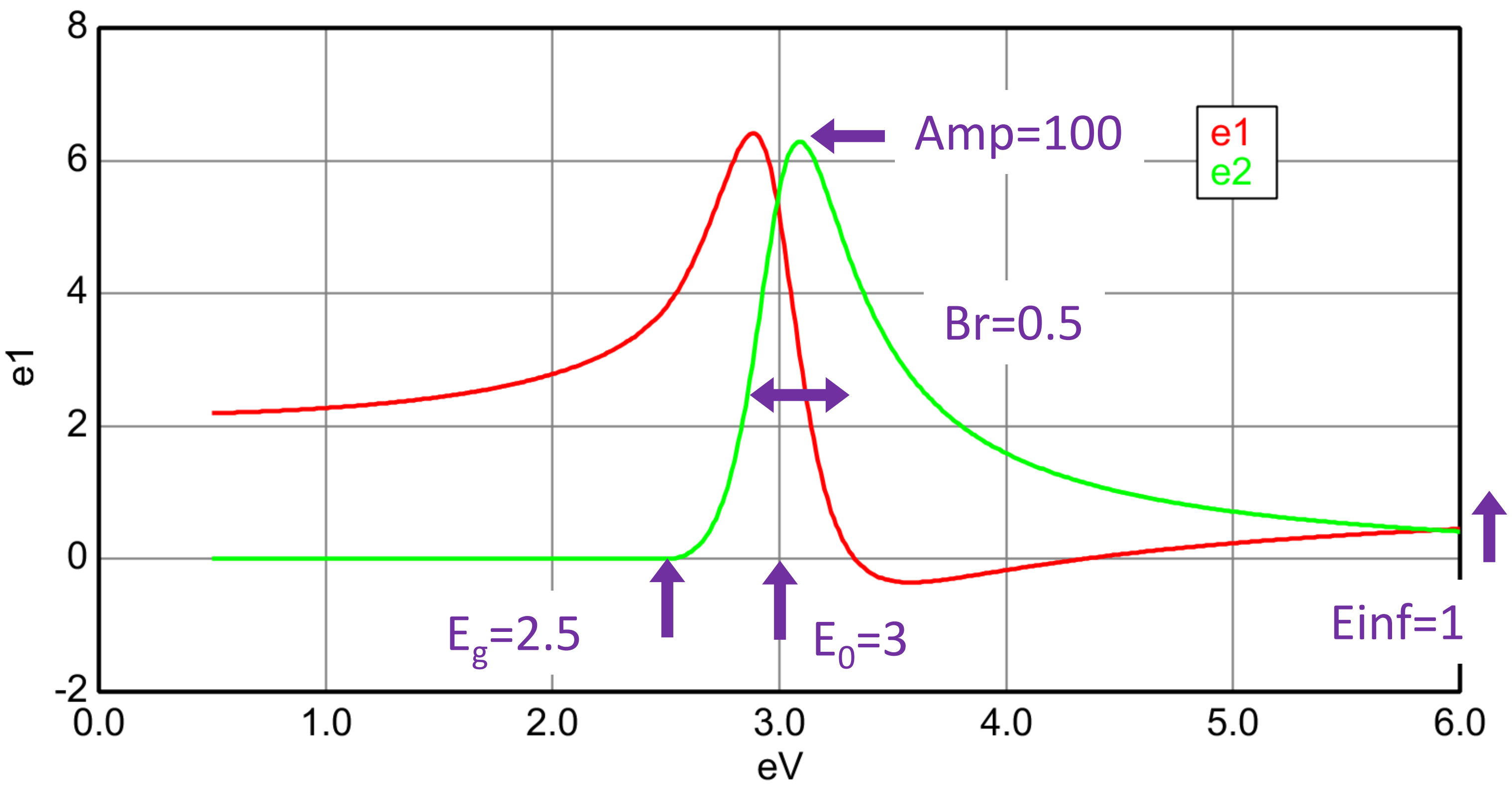
G.E. Jellison Jr.
(Oak Ridge NL)

- Adds Bandgap Energy (E_g)
  - NO absorption at energies below Eg
- Near band edge, ε_2 follows Tauc-law formula:
- Asymmetric shape of ε_2

$$\varepsilon_2(E) \propto \frac{\left(E - E_g\right)^2}{E^2}$$

- 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 = Tauc-Lorentz Amp1 = 100.0000
      Br1 = 0.500 Eo1 = 3.000 Eg1 = 2.500 Common Eg = OFF

Tauc-Lorentz



- 4 ε_2 Parameters: **Amp**, **Br**, **Eo**, **Eg**
- Amorphous semiconductors and dielectrics (UV absorptions)

G.E. Jellison, Jr. and F.A. Modine, *Appl. Phys. Lett.* **69**, 371 (1996), Erratum, *Appl. Phys. Lett.* **69**, 2137 (1996)

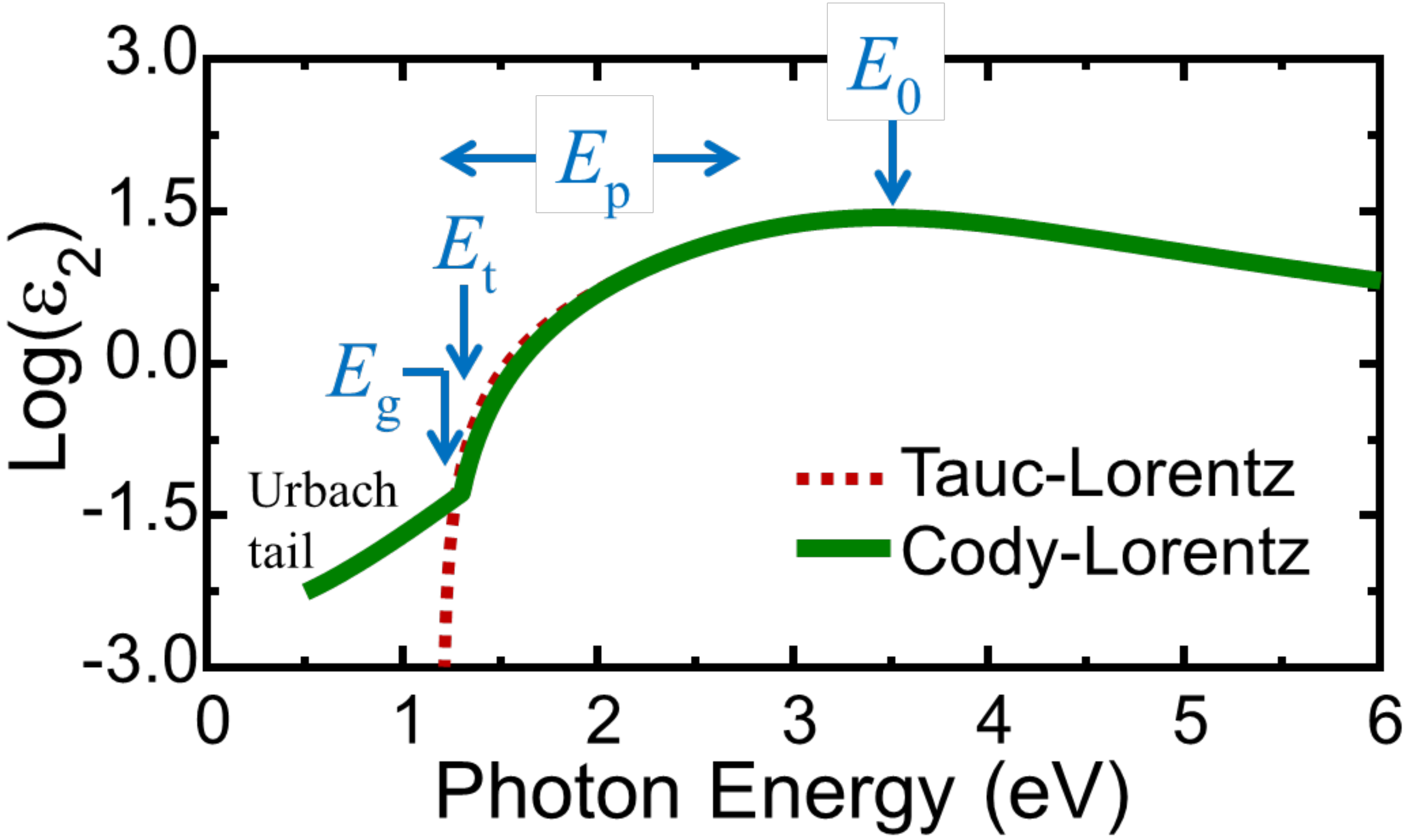
Cody-Lorentz Oscillator

- Defines band-gap and optional Urbach tail below the gap
- Follows Cody absorption:

$$\varepsilon_2(E) \propto \left(E - E_g\right)^2$$

Robert Collins (Univ-Toledo)

- 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** **Sort**
    - Fit Menu: All None Amp. Br. En.
    - 1: Type = Cody-Lorentz Amp1 = 20.000 Br1 = 6.000
      Eo1 = 6.000 Eg1 = 1.000 Ep1 = 1.000
    - + Urbach Absorption Parameters



- 7 (5) Parms: **Amp**, **Br**, **Eo**, **Eg**, **Ep**, **Et**, **Eu**
- Amorphous semiconductors and dielectrics (UV absorptions)

Hint: Leave Et=0, Eu=0.5

A.S. Ferlauto, G.M Ferreira, J.M. Pearce, C.R. Wronski, R.W. Collins, Xunming Deng, and Gautam Ganguly, J. Appl. Phys. **92**, 2424 (2002).

Parametric Grading

- Allow individual parameter to vary with depth through the film
- Select main parameters, such as amplitudes, bandgap energies, resistivities
- Keep balance between # of slice and model complexities

Roughness = 7.04 nm (fit)

\- Graded Layer Thickness # 1 = 199.60 nm (fit)

Grade Type = Parametric # of Slices = 51

Profile = Two Segment Position (%) = 84.04 (fit)

\- Material = ITO (GenOsc)

Show Dialog

\- e1 Components

Name	Value	Grade	Bottom Value	Middle Value	Top Value	Graph
Einf	1.595	OFF				
UV Pole Amp.	0.000	OFF				
UV Pole En.	11.000	OFF				
IR Pole Amp.	0.000	OFF				

\- e2 Components

Oscillator Menu: Add Delete Delete All Sort

Fit Menu: All None Amp. Br. En.

1: Type = Tauc-Lorentz

Name	Value	Grade	Bottom Value	Middle Value	Top Value	Graph
Amp1	(Graded)	ON	40.4117	31.8177	66.5203	Draw
Br1	30.893	OFF				
Eo1	15.000	OFF				
Eg1	2.424	OFF				

2: Type = Gaussian

Name	Value	Grade	Bottom Value	Middle Value	Top Value	Graph
Amp2	6.094700	OFF				
Br2	2.0850	OFF				
En2	6.787	OFF				

3: Type = Drude(RT)

Name	Value	Grade	Bottom Value	Middle Value	Top Value	Graph
Resistivity (Ohm·cm)3	(Graded)	ON	0.00012887	0.00016768	0.00027680	Draw
Scat. Time (fs)3	(Graded)	ON	7.845	6.367	12.741	Draw

\+ Substrate = 7059_Cauchy Substrate Thickness = 1.0000 mm

Demonstration #4: ITO on Silicon

- Fit the data with existing ITO layer.
- Improve fit with “Parametric Gradient”

Fit Data with
Pre-Built Gen-Osc

ITO on Si: Results