Session 6 – Absorbing films II: GenOsc Parameterization

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Methods on Absorbing Films

- **Reducing unknowns**
  - Opaque Layer
  - Extrapolation from Transparent Region
  - Optical Constant Parameterization

- **Adding information**
  - SE + Transmission
  - Interference Enhancement
  - Multi-Sample Analysis
  - In-Situ

Above methods are often combined!

Parameterization

-GenOsc -

\[ \varepsilon_2(\lambda) = F(p_1, p_2, \ldots, p_m) \]

\[ \varepsilon_1(\lambda) = F(\varepsilon_2(\lambda)) \] - KK relation

Uniqueness fit

- Use dispersion equations to describe sample optical properties.

- Often combined with other techniques
Optical Absorption

Absorption: Light loses energy to material
Root causes vary with material and spectral regions
- Electronic Transitions
- Molecular Vibrations
- Lattice Vibrations
- Free-carriers

![Diagram showing optical absorption spectrum for Rutile TiO2 from UV to IR with photon energy in eV]
Oscillators

Mass on Spring...

- Have Natural frequency of vibration ($\omega_o$)
- Resonant frequency
  - oscillates at same frequency as the driving force ($F$)

$$\omega_o = \sqrt{\frac{k}{m}}$$

$k$ = Spring force constant
$m$ = mass of object.
$\omega_o$ = resonant Frequency
Dielectric response & Absorption

$\varepsilon_2$ is directly related to the energy absorption (damping) processes.

- $\varepsilon_2$ shape varies due to different quantum mechanical origins of photon absorption
- $\varepsilon_1$ is related to $\varepsilon_2$ through KK-consistency

$n$ and $k$ ($\varepsilon_1$ and $\varepsilon_2$) are not independent!
Kramers-Kronig Consistency

- Kramers-Kronig relation:

\[ n(E) - 1 = \frac{2}{\pi} P \int_{0}^{\infty} \frac{E' k(E')}{E'^2 - E^2} \, dE', \]

\[ \varepsilon_1(E) - 1 = \frac{2}{\pi} P \int_{0}^{\infty} \frac{E' \varepsilon_2(E')}{E'^2 - E^2} \, dE', \]

- K-K consistency is a “necessary but not sufficient” criteria for determining whether a set of optical constants are correct.
Absorption is the “cause”. Through K-K consistency, it describes index (or $\varepsilon_1$)

“bumps” make “wiggles”
Introduction to “Genosc.mat”

ε₁ section

Reference/graph section

ε₂ section & oscillator list
\( \varepsilon_2 \) section: Oscillators

- Mathematical functions that describe \( n \) & \( k \) (\( \varepsilon_1 \) & \( \varepsilon_2 \)).
  - Associated with an absorption resonance
  - Different oscillator types and style
  - Freedom to adjust each parameter.
Typical Oscillators

- **Organics and Dielectrics:** UV Resonant Absorptions
  - Gaussian, Tauc-Lorentz.

- **Semiconductors:**
  - Direct Bandgap: \( \text{Psemi-E0} \)
  - Indirect Gap / Amorphous: Tauc-Lorentz or Cody-Lorentz.
  - Higher Energy Transitions: Gaussian or PSEMI.

- **Metals:** Free Carrier absorption
  - Drude, Lorentz, Harmonic.
Absorption in one spectral region affects all spectral regions...

- Higher energy (shorter wavelength) absorption peaks increase $\varepsilon_1$ (and $n$) at lower energies even in transparent spectral regions.

- Lower energy (longer wavelength) absorption peaks decrease $\varepsilon_1$ (and $n$) at lower energies even in transparent spectral regions.

- These index effects are called “residues.”
Poles: (Sellmeier model)

Poles describe dispersion (curvature) effects from absorptions outside of the spectral range.

Center energies must be **outside** of spectral range.

Valid spectral range

(transparent region)

- \( \varepsilon_1 \) reference
- \( \varepsilon_1 \) Sellmeier

Pole #1 dispersion

Pole #2 dispersion

Photon Energy (eV)
## Why use Oscillators?

<table>
<thead>
<tr>
<th>Method</th>
<th>Advantages</th>
<th>Disadvantages</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oscillators</td>
<td>- Reduces number of fit parameters.</td>
<td>- Can be difficult to set up</td>
</tr>
<tr>
<td>(GENOSC)</td>
<td>- Maintains K-K consistency.</td>
<td>- Need to understand complex dielectric function</td>
</tr>
<tr>
<td></td>
<td>- Flexible for similar samples.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>- Does not require transparent region.</td>
<td></td>
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</tbody>
</table>
OSCILLATOR PROCESS OVERVIEW

I: Existing Oscillator Mat file

II: Tabulated Optical Constants

III: Cauchy fit Transparent region

Pt-by-Pt fit all wavelengths and Save Optical Constants

Create Oscillator Mat file (GenOsc.mat)

Use GENOSC model to fit DATA
Oscillator Approach

- Method I: Use Existing oscillator material file
- Method II: Match tabulated Optical constants
  - Parameterize GENOSC
- Method III: Create GENOSC from Point-by-point results
  - Parameterize from Point-by-point results
    - One oscillator, Multi-oscillators and outrange oscillators
Method I: Use Existing Oscillator Mat File

- Existing oscillator files are available for many materials
- New oscillator files can be saved for future use

Use GENOSC model to fit DATA
Fitting Procedure I

1. Open existing model or add existing Genosc materials layer
2. Adjust Thickness only to match data
   - This prevents oscillator models from getting lost
3. Turn on fit parameters, including oscillator parameters and thickness
   - slowly increase # of fit parameters until no further improvement in fit.
Example: Use Existing Oscillator Mat files

“Example_1_SiN\text{x} on Si.dat”

- Use SiN\text{x}_cl1.mat for SiN\text{x} layer.
- How to further improve fit? (Hint: surface layer?)
Method II: Match Tabulated Optical Constants

- Tabulated optical constants available in publications, WVASE mat library or other sources
- Use tabulated optical constants as reference materials for GENOSC.mat
- May need to iterate before best answer can be found
- Try to use minimum fit parameters
Fitting Procedure II

1. Build model with GenOsc layer
2. Load tabulated optical constants as reference in Genosc
3. Select e2 only: Add and adjust Oscillators to best match e2 shape of Reference material.
4. Select e1 only: fit pole parms and e1 offset to reference
5. Generate data and adjust thickness to match data
6. Normal Fit data
7. May iterate step 3 to 6 until no further improvement.
Demostration: Genosc Fit to Reference

- “Demo_1_a-Si on Glass.dat”
  - use 7059.mat for substrate
  - use a-si_aspnes.mat as reference.

Remember to add surface oxide
- very important for semiconductors.
DEMO_1: a-Si layer on glass

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>genosc</td>
<td>46.743</td>
</tr>
<tr>
<td>sio2</td>
<td>2.576</td>
</tr>
<tr>
<td>7059_u</td>
<td>1</td>
</tr>
</tbody>
</table>

MSE=2.305 (Use Tauc-Lorentz Osc)

- Amp1.1: 188.09±0.418
- En1.1: 3.5554±0.00142
- C1.1: 2.3212±0.00436
- Eg1.1: 1.4487±0.0011
- Thick.1: 46.743±0.00844
- E1Offset.1: 0.61176±0.0185
- Thick.2: 2.576±0.00744
Example: Use Published values as Reference

“Example_2_a-Si on Ge.dat”
- Start with one or two angles
- Use a-Si.mat as reference
- Compare Tauc-Lorentz to Cody-Lorentz.

Remember to add surface oxide
- very important for semiconductors.
Example_2: aSi on Ge

**Step 1: Start with One angle**
Generated and Experimental

**Step 2: Add all angles**
Generated and Experimental
Example_2: aSi on Ge

**Tauc-Lorentz: MSE ~14**

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness</th>
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<tbody>
<tr>
<td>2</td>
<td>sio2_jaw</td>
</tr>
<tr>
<td>1</td>
<td>genosc</td>
</tr>
<tr>
<td>0</td>
<td>ge</td>
</tr>
</tbody>
</table>

**Cody-Lorentz: MSE ~7**

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>sio2</td>
</tr>
<tr>
<td>1</td>
<td>genosc</td>
</tr>
<tr>
<td>0</td>
<td>ge</td>
</tr>
</tbody>
</table>

**Optical Constants**

- **Index of Refraction (n)**
- **Extinction Coefficient (k)**

![Optical Constants Graph](image-url)
Method III: Create oscillator model
From Pt-by-Pt

III: Cauchy fit
Transparent region

Pt-by-Pt fit all wavelengths
and Save Optical Constants

Create Oscillator Mat file
(GenOsc.mat)

iterate

Use GENOSC model
to fit DATA
Fitting Procedure III

1. **Cauchy Fit transparent region only**
   - Add surface layer as needed

2. **Pt-by-Pt Fit all wavelengths**
   - Turn off all other fit parameters EXCEPT n and k
   - Point-by-point fit
   - Save tabulated optical constants or save environment file

3. **Build Genosc**
   - Replace Cauchy layer with Genosc
   - Use tabulated pt-by-pt fit results as reference
   - Fit reference – e2 first, then e1

4. **Generate data before fitting data**

5. **Fit \( \Psi \) & \( \Delta \) data using new Genosc layer model**

6. **Adjust oscillators to get best fit**
Demo_2: Genosc procedure

- “Demo_2_thin dielectric on Si.dat”
  (Use si_vuv.mat for substrate)
Demo_2: Thin Dielectric on Silicon- Step 1

- Range select Transparent Region
- Build Model with Single-layer Cauchy
- Fit thickness and Cauchy parameters
- Extend range further toward absorbing region until MSE climbs

<p>| | | |</p>
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<tr>
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<tbody>
<tr>
<td>1</td>
<td>cauchy</td>
<td>22.439 nm</td>
</tr>
<tr>
<td>0</td>
<td>si_vuv</td>
<td>1 mm</td>
</tr>
</tbody>
</table>

Generated and Experimental

- Model Fit
- Exp E 60°
- Exp E 75°
Demo_2: Thin Dielectric on Silicon - Step 2

- Turn off thickness and Cauchy parameters
- Range select data at ALL wavelengths
- Fit n & k using Pt-by-Pt Fit
- Save tabulated n and k or environment file
Demo 2: Thin Dielectric on Silicon - Step 3

- **Build Genosc**
  - Method 1:
    - right-click on Cauchy layer
    - Genosc will have pt-by-pt results loaded in reference
  - Method 2:
    - Replace Cauchy with Genosc
    - Manually load tabulated pt-by-pt results into reference
- Generate data before fitting to insure that the new layer agrees with point-by-point result.
  - Generated curves should be close to Experimental data.
Demo_2: Thin Dielectric on Silicon - Step 5

- Genosc to fit experimental data
  - Fit thickness and oscillator params
- May need to adjust fitting parameters in Genosc
- Become sensitive to surface conditions toward UV

<table>
<thead>
<tr>
<th></th>
<th>GenOsc</th>
<th>22.418 nm</th>
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<tr>
<td>1</td>
<td>si_vuv</td>
<td>1 mm</td>
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</table>

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Amp1.1</td>
<td>74.529±1.87</td>
</tr>
<tr>
<td>En1.1</td>
<td>8.2541±0.0392</td>
</tr>
<tr>
<td>C1.1</td>
<td>6.4983±0.11</td>
</tr>
<tr>
<td>Eg1.1</td>
<td>2.6189±0.0219</td>
</tr>
<tr>
<td>PoleMag.1</td>
<td>14.971±6.08</td>
</tr>
<tr>
<td>E1Offset.1</td>
<td>1.1795±0.0352</td>
</tr>
<tr>
<td>Thick.1</td>
<td>22.418±0.0273</td>
</tr>
</tbody>
</table>

MSE=1.391
Examples: Genosc Procedure

“Example_3_dielectric on Si.dat”
- Follow procedure in Demo_2
- Model the data using Demo_2 genosc material file

“Example_4_resist on Si.dat”
- Gaussian oscillators work well to match absorptions in organic films

Is the Point-by-Point Fit KK consistent?
Example_3: dielectric on Si

<p>| | | |</p>
<table>
<thead>
<tr>
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<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>example_4_dielectric on si_g</td>
<td>151.956 nm</td>
</tr>
<tr>
<td>2</td>
<td>srough</td>
<td>1.879 nm</td>
</tr>
<tr>
<td>0</td>
<td>si_vuv</td>
<td>1 mm</td>
</tr>
</tbody>
</table>

MSE ~2.6
One Tauc-Lorentz
Example 4: resist on Si

<table>
<thead>
<tr>
<th></th>
<th>GenOsc</th>
<th>161.051 nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>si_vuv</td>
<td>1 mm</td>
</tr>
</tbody>
</table>

MSE ~3.3
Six Gaussians

Generated and Experimental

\[
\begin{align*}
\Psi \text{ in degrees} & \\
\Delta \text{ in degrees} &
\end{align*}
\]

Photon Energy (eV)

\[
\begin{align*}
\text{Model Fit} & \\
\text{Exp E 55°} & \\
\text{Exp E 65°} & \\
\text{Exp E 75°} &
\end{align*}
\]
Example 4: resist on Si

Point-by-point fit results are mainly K-K consistent.
What to watch for...

**Goal:** Find minimum number of model parameters to fit the experimental data.

1. **Watch for parameters which reach limits or not physical**
   - e.g. Oscillator amplitude goes to zero or negative

2. **Check correlation and sensitivity**
   - Check for large error bars. Is each parameter sensitive?
   - Check correlation matrix.
   - Can out-of-range oscillators be replace by pole?

**Use RESET often!!**
Out-of-range Oscillators

The genosc function can be **less sensitive** to the out-of-range oscillators

- Parameters, such as amplitude, center energy & broadening will be **correlated** !!
- Out-of-range oscillators can sometimes be replaced with poles

Note that **3 different oscillators all fit** the measured spectral range equally well !!
OSCILLATOR PROCESS OVERVIEW

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III: Cauchy fit Transparent region

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Create Oscillator Mat file (GenOsc.mat)

Use GENOSC model to fit DATA

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