Session 3B
Using the Gen-Osc Layer to Fit Data
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Using Gen-Osc to Fit Data

- Pre-built Existing Genosc Layer
- Library optical constants $\rightarrow$ GENOSC
- Cauchy $\rightarrow$ Point-by-Point $\rightarrow$ GENOSC
- Choosing the correct oscillators
  - Fitting out-of-range oscillators
  - Parameter correlation
GENOSC Process Overview

1. Use Oscillator To Fit DATA
2. Create Oscillator Model
3. Reference optical constants
4. Tabulated Optical Constants
5. Pt-by-Pt Fit
6. Existing Oscillator Model

iterate
- Use 7059_u.mat for substrate
- Use a-si_asp.mat as Reference
- Remember to add surface oxide
  - Very important for semiconductors
- Compare Tauc-Lorentz to Cody-Lorentz.
- Use pre-existing Genosc layer for a-Si available in the library and repeat the example.
Procedure for UV Absorbing Films

1. **Cauchy Fit**
   - transparent region only

2. **Pt-by-Pt Fit – all wavelengths**
   - fix thickness, then perform pt-by-pt fit
   - Build Genosc from tabulated ‘cauchy’

3. **Match n,k using Genosc**
   - fit reference – first e2, then e1

4. **Fit ψ & Δ data using new Genosc model**
- Use Si_vuv.mat for substrate
- Cauchy \(\rightarrow\) PBP \(\rightarrow\) Gen-Osc
Example 2: Thin Dielectric on Silicon

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

| 1 cauchy | 22.541 nm |
| 0 si_vuv | 1 mm |

Generated and Experimental

![Graph showing generated and experimental data with labeled parameters and wavelengths.](image-url)
Example 2: Thin Dielectric on Silicon

- Fix Thickness and Cauchy parameters
- Select data at ALL wavelengths
- Fit n & k using Pt-by-Pt fit
Example 2: Thin Dielectric on Silicon

- PBP fit result n, k
Example 2: Thin Dielectric on Silicon

Shortcut: Build GenOsc from **tabulated** ‘cauchy’

<table>
<thead>
<tr>
<th></th>
<th></th>
<th>22.522 nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>genosc</td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>si_v uv</td>
<td>1 mm</td>
</tr>
</tbody>
</table>

If you have tabulated optical constants from any layer you would like to use as reference in Genosc, use right-click menu.
Example 2: Thin Dielectric on Silicon

- Tabulated $n$ & $k$ is loaded as Reference Material
- Note this particular dielectric has Tauc-Lorentz absorption shape in UV
- Select Fit e2 only
Example 2: Thin Dielectric on Silicon

- Add Oscillators to match $\varepsilon_2$ shape of Reference material.
Example 2: Thin Dielectric on Silicon

- Fit Oscillator Parameters to match Reference $\varepsilon_2$. 
Example 2: Thin Dielectric on Silicon

- Select “Fit $e_1$ Only”
- Fit $e_1$ with poles & offset
Example 2: Thin Dielectric on Silicon

Generate data before fitting to insure that the new layer agrees with point-by-point result.

Generated curves should be close to Experimental data.
Example 2: Thin Dielectric on Silicon

- Allow oscillator parameters and thickness to fit.

Generated and Experimental

\[ \text{MSE}=1.36 \]

Watch for correlation between parameters.

SAVE Model File for FUTURE!
Example_3_SiNx_on_Si.dat

- Start from Cauchy to get a Gen-Osc for SiNx layer.

- Minimize number of Genosc parameters.
Out-of-range oscillators, Correlation & sensitivity

- **Fit with 2 Gaussian Oscillators**

![Graph showing Imag(Dielectric Constant) vs. Photon Energy (eV)]
Out-of-range oscillators, correlation & sensitivity

- Note that 3 different oscillators, all fit the measured spectral range equally well!!
- The Gen-Osc function insensitive to the out-of-range Gaussian parameters
- The amplitude, center energy & broadening are correlated!!
Example_4_Resist_on_Si.dat

- Use si_vuv.mat for substrate
- Cauchy → PBP → Gen-Osc
- Gaussians work well to match absorptions from organic film, such as this photoresist.
GENOSC Process Overview

1. Use Oscillator To Fit DATA
2. Pt-by-Pt Fit
3. Existing Oscillator Model
4. Reference optical constants
5. Create Oscillator Model
6. Tabulated Optical Constants

iterate
Using Genosc to Fit Data

✔ Starting with Existing Genosc Layer
✔ Cauchy ➔ Point-by-Point ➔ GENOSC
✔ Choosing the correct oscillators
  ✔ Fitting out-of-range oscillators
  ✔ Parameter correlation
Advanced Genosc

When the pt-by-pt fit fails?
Example_5_Organic_on_Si.dat

- Use si_vuv.mat for substrate

- Is the PBP result KK consistent?
  - Use Gen-Osc to check
What to do when Pt-by-Pt Fails?

1. Ask why did it fail?
   - Abrupt n,k changes (try # Pts. To Avg. = 2)
   - Starting model inaccurate (Roughness, Grading, Depolarization?)

2. Match e2 with oscillators (Gaussians) and match e1 at long-λ. Fit. Go to #4 if needed.

3. Slowly move into absorbing region with Genosc, adding oscillators as needed. Go to #4 if needed.

4. After oscillators come close to solution, do Normal Fit for n,k to develop a “reference” material file.

5. E-mail to us! (measurements@jawoollam.com)
Example 5

- Previous point-by-point fit is not KK consistent. However, we can match $e_2$ at all wavelengths, and $e_1$ at longer wavelengths to get “starting point”.

![General Oscillator Layer interface](image)
Example 5, continued

- Allowing all fit parameters to vary, we get:

Watch for oscillators that get lost.
Is the Point-by-Point Fit KK consistent?

Try # Pts. To Avg. for next guess = 2

Extra Credit, Alternatively Try:
- Match e2 with oscillators (Gaussians) and match e1 at long-l. Fit.
- After oscillators come close to solution, do Normal Fit for n,k to develop a “reference” material file.
Example 6 Results

<table>
<thead>
<tr>
<th></th>
<th>GenOsc</th>
<th>89.853 nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>si_jaw</td>
<td>1 mm</td>
</tr>
</tbody>
</table>

MSE = 2.5
How do we get the answer without reference material file?

Try:
- Slowly move into absorbing region with Genosc, adding oscillators as needed.
- After oscillators come close to solution, do Normal Fit for n,k to develop a “reference” material file.
Example 7

- **Point-by-Point Fit FAILS**

![](Generated and Experimental)

- **Generated and Experimental**
  - **Wavelength (nm)**: 200, 400, 600, 800, 1000, 1200
  - **\( \Psi \) in degrees**: 10, 20, 30, 40, 50, 60, 70, 80
  - **Model Fit**
  - **Exp E 65°**
  - **Exp E 70°**
  - **Exp E 75°**
Cauchy to Sellmeier

- Cauchy Fit up to 1.75eV
  Then, convert to Genosc (Sellmeier)
Extend Data to 2eV

- Range-select to 2eV (Generate), don’t fit yet.

Must need absorption at 1.8eV and above
Add Gaussian, Fit and Repeat

- Difficult, take small steps (.2eV)
- After oscillators come close to solution, do Normal Fit for n,k to develop a “reference” material file.
- Build another Genosc with new “Ref.Mat” file.

MSE = 12
EXTRA CREDIT - Depolarization

- Film was non-uniform and this is required to fit data better.

MSE = 3.9
The following slides provide an additional Example.
The Genosc \textit{psemi} has 9 main variable parameters (11 total*):

1. \(E\) Center energy
2. \(A\) Amplitude
3. \(B\) Broadening
4. \(WL\) Left end point
5. \(WR\) Right end point
6. \(PL\) position left control point
7. \(AL\) amplitude left control point
8. \(PR\) position right control point
9. \(AR\) amplitude right control point.

\[ p_{semi} \]
Psemi-Triangle oscillator

Psemi-TRI

AL = 0.3, AR = 0.5

WL (variable)

WR (variable)

A, Ec (variable)

B (variable)

AL: (variable)

eV

PL = 0.5 (fixed)

PR = 0.5 (fixed)

AR: (variable)
**Psemi-M0 oscillator**

- **A**
  - $B = 0.05\text{eV}$
  - $O2R = 0$
  - (all variable)

- $\varepsilon_2$
  - **Eo** (variable)

- **eV**
  - **WR** (variable)
  - **AR** (variable) = 0.8
  - **AR** = 0.5
  - **AR** = 0.3

- PR = 0.5
  - **PR** (variable)
  - **PR** = 0.6

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- Use SiC_4H_o_g.mat for substrate

- Try to match with Gaussians. How many does it require?

- How many PSEMI oscillators are required?

- Count up the total number of “free” parameters.
Poly-Silicon

- The dielectric function of silicon varies with crystallinity.
- Amorphous films have broad UV absorption: no distinct electronic transitions ($E_1, E_2, \ldots$)
- As crystallinity increases, individual peaks separate & become narrower.
- To quantify crystallinity, optical constants are compared to "reference" measurements where a film with known crystallinity was measured.

\[ \varepsilon_2 \text{ for different silicon films from one "reference" file.} \]
Estimating Crystallinity

- Ellipsometry can be used to estimate the amount of crystallinity by comparing the measured optical constants to the “reference” files. To improve accuracy, a new “reference” file can be created for the particular deposition process.

For high crystalline %, the peak is narrower and eventually separates into two distinct regions.
Estimating Crystallinity - 2

- For amorphous films and small-grain poly-Si, the absorption peak is broad – but there is still a shift of the optical constants as shown below.

![Graph showing Imaginary part of Dielectric Constant (ε₂) vs Photon Energy (eV) for a-Si, 10%, 20%, and 30% poly-Si]
Estimating Bandgap

- The ellipsometer is sensitive to optical constants of film. It will be most sensitive to the shape of absorbing region where $\varepsilon_2$ is larger. Although many models such as Tauc-Lorentz and Cody-Lorentz contain a bandgap term, the indirect gap of silicon films is not directly measurable. The bandgap can be estimated by plotting the decrease in $\alpha$ toward zero (log-scale).

- Discussed in Woollam Newsletter article from year 2012

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**Tauc-Lorentz** model matches different a-Si and poly-Si films. Blue area shows the level of absorption that the SE can detect. Values below are extrapolated from T-L shape.
Estimating Bandgap - 2

- Cody-Lorentz provides more flexibility for amorphous semiconductors. Similar to the Tauc-Lorentz, SE is sensitive to shape primarily from the more absorbing UV region and the bandgap region just shifts as the overall shape changes.

- Lesson: T-L and C-L can provide a qualitative ‘bandgap’ value for comparison, but may not match actual physical property of film.