Session 1B
Transparent Materials
Andrew Martin
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Overview

- Transparent substrates & films
  - Cauchy equation
  - Common complexities

- Evaluating, comparing, & saving results
  - Normal dispersion
  - Environment Files
What do you mean transparent?

- **No or very little absorption**
  - Extinction coefficient $k=0$ or very small ($k<10^{-3}$)

- **Wavelength dependent!**
  - Typical transparent materials in visible wavelength range: polymers, glasses, oxides, etc...
Dispersion Equations

Definition:
Mathematical description of the optical constants as a function of wavelength \((\text{not a list of } n, k)\)

Advantages:
- Reduces the number of unknowns
- Adjust optical constants with only a few parameters
- Avoid noise in the data
- Better for interpolating and extrapolating
- Some maintain \(K-K\) consistency
Cauchy Dispersion Equation

- Cauchy relationship is empirical description of index \((n)\) of transparent materials.

\[
n(\lambda) = A + \frac{B}{\lambda^2} + \frac{C}{\lambda^4}
\]
Cauchy Dispersion Equation

- Describes index \( n \) as a function of wavelength \( \lambda \)
- For transparent materials only (\( k = 0 \) or very small)

\[
n(\lambda) = A + \frac{B}{\lambda^2} + \frac{C}{\lambda^4}
\]

\[
k(\lambda) = 0
\]
Transparent Substrates

- Typical examples (VIS/NIR) include:
  - Glass
  - Bulk polymers
  - Other examples?
Data Features

- **Psi** = flat and smooth
- **Delta** = 0° or 180°, unless absorbing or surface film is present
Common Complexities

- Backside Reflections
- Surface Roughness
- Index Grading
Avoiding Backside Reflections

1. Roughen backside with grinder, sandpaper, or sandblaster.

2. Spatially Separate Front & Back reflections.
   - Focusing optics / thick substrate.
   - Wedged substrate.

3. Index-match backside to scatter/absorb light.
   - Translucent Scotch tape for glass.
Spatial Separation

Only collect Front Surface reflection

Surface of interest
Surface Roughness

- Ellipsometry is very sensitive to surface conditions
  - (effectively lower-index surface film)

- Modeled by mixing optical constants of material with 50% air/voids (n=1)
  - Effective Medium Approximation (EMA)

- Model as srough.mat
  - Note that srough layer may include roughness, lower-index surface layer, & contamination

<table>
<thead>
<tr>
<th></th>
<th>srough</th>
<th>2.160 nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>cauchy</td>
<td>1 mm</td>
</tr>
</tbody>
</table>
Surface Roughness Effects (transparent substrate)

- Delta deviates from 0°, 180°
- Shorter wavelengths are more sensitive

Experimental Data

<table>
<thead>
<tr>
<th>Wavelength (nm)</th>
<th>0</th>
<th>300</th>
<th>600</th>
<th>900</th>
<th>1200</th>
<th>1500</th>
<th>1800</th>
</tr>
</thead>
<tbody>
<tr>
<td>Δ in degrees</td>
<td>0</td>
<td>30</td>
<td>60</td>
<td>90</td>
<td>120</td>
<td>150</td>
<td>180</td>
</tr>
</tbody>
</table>

Exp E 55°
Exp E 65°
Exp E 75°
Example 1: uncoated glass.dat

- Open data
- Add layer of Cauchy.mat into model substrate
- Turn on Cauchy A, B, and C and Fit (to match Psi)
- Add surface roughness (srough.mat) and Fit (to match Delta)
View Optical Constants

- Right-Click on Graph Window. Then Data > Current Layer (Opt. Const.)

- Make sure > is pointing to the layer of interest. (use arrow keys to adjust)

What should the optical constants look like?
Normal Dispersion

- Without absorption: Increasing index with decreasing $\lambda$
- Desired outcome with Cauchy layer is positive Cauchy coefficients
Unphysical Dispersion

- Decreasing index with decreasing $\lambda$
  - Anything other than increasing index with decreasing $\lambda$
    - Negative $B$ usually unphysical
    - Negative $C$ sometimes unphysical
      - all negative $C$ values are acceptable IF the results are still physical (probably insensitive to $C$)
Which results are physical?

\[ n(\lambda) = A + \frac{B}{\lambda^2} + \frac{C}{\lambda^4} \]

A: 
- \( A = 1.555 \)
- \( B = -0.00177 \)
- \( C = 0.01640 \)

B: 
- \( A = 1.643 \)
- \( B = 0.009 \)
- \( C = -4.8600 \times 10^{-5} \)

C: 
- \( A = 1.520 \)
- \( B = 0.015 \)
- \( C = -0.001 \)

D: 
- \( A = 1.643 \)
- \( B = -0.04009 \)
- \( C = 0.009 \)
- Model data set using same procedure as Example 1.
- Verify result has Normal Dispersion.
- Is roughness required?

<table>
<thead>
<tr>
<th></th>
<th>MSE</th>
<th>Roughness (nm)</th>
<th>A</th>
<th>B</th>
<th>C</th>
</tr>
</thead>
<tbody>
<tr>
<td>example2</td>
<td>1.635</td>
<td>3.085</td>
<td>1.5003</td>
<td>0.007497</td>
<td>0</td>
</tr>
<tr>
<td>example3</td>
<td>1.086</td>
<td>0.043</td>
<td>1.4469</td>
<td>0.00303</td>
<td>4.96E-05</td>
</tr>
</tbody>
</table>
Typical examples (VIS/NIR) include:

» Optical coating materials
  • SiO2, TiO2, Ta2O5, MgF2…

» Some Nitrides
  • Si3N4, AlN…

» Organic Films
  • Photoresists, PMMA, spin-on polymers…
Data Features

- Multiple reflections cause interference pattern – oscillations in data.
- Pattern affected by thickness and index.

<table>
<thead>
<tr>
<th>nm</th>
<th>eV</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 300</td>
<td>0 2</td>
</tr>
<tr>
<td>600 1200</td>
<td>4 6</td>
</tr>
<tr>
<td>900 1500</td>
<td>8</td>
</tr>
<tr>
<td>1800</td>
<td>0 30</td>
</tr>
</tbody>
</table>

Wavelength (nm) | Photon Energy (eV) | Y in degrees |
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0 300 600 900 1200 1500 1800</td>
<td>0 2 4 6 8</td>
<td>0 5 10 15 20 25 30</td>
</tr>
</tbody>
</table>

Transparent - oscillations
Thickness Effects

- # of oscillations ~ thickness
- Thicker films = more interference oscillations

![Graph showing thickness effects with different wavelengths and Psi values.](image)
Index Effects

- Psi magnitude ~ index Δ between film/substrate
- Greater contrast = greater amplitude
- Index also affects # of oscillation peaks
Open data
Add Si_JAW.mat into model substrate
Add Cauchy.mat
Turn on Cauchy A, B, C and Thickness
Adjust Thickness to match # oscillations
Adjust A to match Psi amplitude
Fit
Verify normal dispersion (view Cauchy layer optical constants)
Start Value Matters

- "local" minima
- "global" minimum

Diagram showing changes in "Psi" with respect to energy for different angles and film thickness.
Normal Fit

Marquardt-Levenberg algorithm used to quickly determine the minimum (BEST FIT)

Start Values Matter!…What if nominal values are not known?

How to get good start values?

- Global fit – Searches a ‘grid’ of starting points for the best match
- Particularly useful to avoid local MSE minimums
  - Complicated models with many parameters
  - Thick films
Global Fit in WVASE

- Select model parameters
  - Check parameter “fit box” in model layer.
  - Actual values of fit parameters do not matter.

- Define range and step for each parameter
  - “Edit Parms” from “Fit” Window.
EditParmsforGlobalFit

1. Highlighta fit parameter
2. Set minimum, maximum and number of guesses
3. ‘Change Parm Coupling’ to update the changes
4. Repeat until all fit parameters have defined ranges and number of guesses
5. Perform “global” fit
Global Fit Guidelines

- Use ~50 guesses per 1 micron thickness range
- Use ~10-20 guesses for Index range of 1 (An)
- Avoid global fitting dispersion (Bn, Cn)
- Try to keep total number of guesses under 1000
- Helpful with bi-layer films.
- Open Experimental data
- Add Si_JAW.mat into model substrate
- Add Cauchy.mat
- Turn on Cauchy A, B, C and thickness
- Global fit for **Thickness**
- Global fit for **A** parameter
- Fit
- Verify normal dispersion (view Cauchy layer optical constants)

Remember to hit ‘Change Parm Coupling’ after entering each parameter!
Saving Environment Files

Environment File includes data, model, fit result, & material files!
Environment Files

- Saves a copy of data, model, and fit results – all in one file with *.env extension.
- Useful when:
  - Final result is reached.
  - Before you are trying something that may jeopardize your fit.
  - When sending your data/results to other WVASE users (i.e. sending to J.A. Woollam Company).
Examples 5, 6, 7 & 8

- Example5_HfO2_on_Si.dat  Example7_Ta2O5_on_Si.dat
- Example6_MgF2_on_Si.dat  Example8_SiN_on_Si.dat

- Fit all 4 data sets
- Use Global Fit? Use Mouse Scroll Wheel?
- Verify Normal Dispersion
- Save Environment file when finished.
Saving a Material File

- Right-click on layer
- Then ‘Save’
Saving a Material File

Saving Optical Constants of a layer

Two formats:

- **Parameterized (YES)**
  - Will save dispersion parameters, such as Cauchy A, B and C.
  - Can extrapolate and interpolate using dispersion equation.

- **Tabulated (NO)**
  - Will save a table of n and k in the measured wavelength range.
  - Linear extrapolation or interpolation based on two points.

Both are *.mat files!
Saving a Model

**Model:**
Layered structure with results and fit parameters.

TIP: Save material files FIRST to retain layer names.
Evaluating Results

✓ Compare experimental and generated data
✓ Are the results physically meaningful?
  – Normal dispersion
  – Positive thickness values, reasonable index values, etc
  – K-K consistency

▪ How low is MSE? Can it be lowered by increasing model complexity?

▪ Check other mathematical “goodness of fit” indicators
  – Correlation matrix
  – Error bars
Common Complexities

- Surface Roughness
- Index Grading
- Backside Reflections*

*Covered later this week
Surface Roughness

- Ellipsometry very sensitive to surface conditions
  - (effectively lower-index surface film)

- Modeled by mixing optical constants of material with 50% air/voids (n=1)
  - Effective Medium Approximation (EMA)

- Simple to model, just add srough.mat
  - But may include roughness, lower-index surface layer, & contamination
Surface Roughness Effects (Films)

Not obvious for transparent films

Transparent oscillations

Rough Surface – shifts in data
Index Grading

- Optical properties can vary with depth into a film.
- Modeled by dividing film into ‘slices’ where optical constants can vary between each.

Right-click layer to Grade Layer
Index Grading Effects

- Oscillations too narrow or too wide

![Diagram showing graded TiO₂ and BK7 layers compared to un-graded TiO₂ and BK7 layers.](image)
Index Grading Slices

- Each step represents a ‘Slice’.
- Number of slices can be changed in the model.
- Adding slices may not improve MSE.
Example9_SiC_on_Si.dat

- Use Si_jaw.mat for substrate
- Use Cauchy.mat to model SiC
- Add roughness
- Remove roughness, add grading
- Add both roughness and grading
- Compare MSE and Results from each step.
- Which answer is correct?
Example 9 Results

Ideal Model (MSE=14.3)  Rough & Graded (MSE=5.1)

Grading increases sensitivity to surface roughness…
better contrast with high index at surface
- Make sure to use correct substrate!
  - sic_palik.mat in Semiconductor Folder

- Try Roughness, Grading, Both? … What is best model?
SimpleGradedIndex Optical Constants

<table>
<thead>
<tr>
<th>Wavelength (nm)</th>
<th>Index of Refraction 'n'</th>
<th>Extinction Coefficient 'k'</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>2.25</td>
<td>0.00</td>
</tr>
<tr>
<td>600</td>
<td>2.30</td>
<td>0.02</td>
</tr>
<tr>
<td>900</td>
<td>2.35</td>
<td>0.04</td>
</tr>
<tr>
<td>1200</td>
<td>2.40</td>
<td>0.06</td>
</tr>
<tr>
<td>1500</td>
<td>2.45</td>
<td>0.08</td>
</tr>
<tr>
<td>1800</td>
<td>2.50</td>
<td>0.10</td>
</tr>
</tbody>
</table>

Fit

- MSE: 1.059
- An.1: 2.2654 ± 0.000136
- Bn.1: 0.020151 ± 0.000175
- Cn.1: 0.0031555 ± 3.63e-005
- Angle0: 55.008 ± 0.00267
- Thick.2: 204.010 ± 0.0211
- Variation.2: 0.32156 ± 0.00799
- Thick.3: 1.716 ± 0.00895
Summary

Methods to Analyze and Report Results for Transparent Materials:

- **Dispersion Equations**
  - Cauchy for Transparent Substrates and Films

- **Normal Dispersion**
  - Increasing index w/ decreasing λ (for transparent materials/regions)

- **Starting Values Matter**
  - Use Mouse Scroll & Global Fit

- **Common Complexities**
  - Avoiding backside reflections
  - Surface Roughness and Index Grading
Additional Content
Thickness Effects of Films on Glass

- Thickness ~ # of oscillations
- Thicker films = more interference oscillations
Index Effects (Glass substrate)

- Index $\Delta$ between film/substrate $\sim \Psi$ magnitude
- greater contrast $=$ greater amplitude
- Index also affects # of oscillation peaks
- Watch for index-matched films ($n \sim 1.5$)
- Is film index higher or lower than substrate?
Example11_transparent_film_on_glass.dat

- Use 7059_C.MAT as substrate
- Use Cauchy.mat for film
- Try with & without roughness
Absorption Tails

- Cauchy.mat also includes 3 parameters for modeling absorption tails
- This is the only exception for modeling absorption with Cauchy layer
- Limited shape (exponential), UV only
Absorption Tails - Parameters

- **k Amplitude**
  - Often the only fit parameter needed (of these 3)
  - Controls amplitude of the exponential tail

- **Exponent**
  - Controls shape of the tail
  - Default value often ok (if not, another model may be best)

- **Band Edge**
  - Specifies point at which $k = k \text{ Amp}$
  - Typically set to shortest $\lambda$ (not critical)
Could restrict $\lambda$ range...
Fit for k amp.
Fit for exponent?
Compare results for Cauchy with and without Urbach tail.