Optical Characterization
By Spectroscopic Ellipsometry.

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J.A. Woollam Co., Inc.
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Morning Overview

- Spectroscopic Ellipsometry:
  - Part 2: Standard Applications.
  - Break
  - Part 3: Grading and Anisotropy.
  - Part 4: Infrared and In-Situ Ellipsometry.
1. Wavelength (Å, nm, or microns)

2. Photon Energy (eV).

\[ E_{eV} = \frac{12400}{\lambda_{\AA}}, \quad E_{eV} = \frac{1240}{\lambda_{nm}}, \quad E_{eV} = \frac{1.240}{\lambda_{\mu m}} \]

3. Wavenumber (cm\(^{-1}\)). Used Mid to Far IR.

\[ cm^{-1} = \frac{10000}{\lambda_{\mu m}} \]
Light Polarization

- “Shape” of the beam as it propagates towards our eyes. (Looking down z-axis).

- Polarization state defined by orientation & phase of the E-field vector
Linearly Polarized Light

Orthogonal $E_x$ & $E_y$ propagating in same direction.

- Component waves are *in phase* with each other.
- Result: *linearly polarized* wave.
  - the 'plane of vibration' depends on relative amplitudes of $E_x$ & $E_y$
Circularly Polarized Light

Orthogonal \( E_x \) & \( E_y \):
- \( 90^\circ \) out-of-phase \& equal in amplitude with each other
- Result: circularly polarized wave
Elliptically Polarized Light

Orthogonal $E_x$ & $E_y$:

- Arbitrary phase & amplitude with each other
- Result: Elliptically polarized wave
  - linear and circular are subsets of elliptical polarization
  - Most general description of polarization state is elliptical.
Intensity and Polarization

- **Intensity** = “Size” of the Ellipse. \( I \propto E^2 \)
  - One Number Describes Wave Amplitude.

- **Polarization** = “Shape” of Beam.
  - 2 numbers required: ellipse Orientation and Ellipticity.
  - Independent of ellipse size. Independent of intensity.

 ![Intensity vs. Polarization Diagram](image-url)
Ellipsometry Overview

1. linearly polarized light ...

2. reflect off sample ...

3. elliptically polarized light !

- Measure the **change in polarization** of light reflected from surface.

Horizontal (s-) and Vertical (p-) components present.

\[ \rho = \tan(\psi) e^{i\Delta} = \frac{\tilde{R}_p}{\tilde{R}_s} \]
Ellipsometers

- Every Ellipsometer contains the same basic components

- SE also needs wavelength selection.
Optical components needed for any ellipsometer:

- Light Source(s)
- Two Polarizers (Polarizer & Analyzer)
- Compensator (Optional, but desirable)
- Detector(s)
Ellipsometer Types

- Rotating Analyzer (RAE)
- Rotating Polarizer (RPE)
- Rotating Compensator (RCE)
- Polarization Modulation (PME)
- Null Ellipsometer
Ellipsometry Advantages

- **Measures ratio of two values!!!**
  - highly accurate & reproducible (even at low light levels).
  - no reference necessary.
- Measures a 'phase' quantity, ‘Δ’
  - very sensitive, especially to ultrathin films (<10 nm).
- **Spectroscopic** Ellipsometry (SE)
  - increased sensitivity to multiple layer film stacks.
  - measures data at wavelengths of interest...193, 633 nm, 1550 nm, bandgaps, etc.
- **Variable Angle Spectroscopic** Angle (VASE)
  - new information (different path length) with each angle optimizes sensitivity.
**CONCLUSIONS:**

- Light is reflected or transmitted from a sample.
- The polarization state of incoming light is known.
- The polarization state of reflected/transmitted light is measured.
- An accurate ellipsometer can determine $\Psi$ and $\Delta$ from the sample.
Optical Properties: Basic Theory

Interaction of Light With Materials:

**Goal:** Provide a basic background on:

- Propagation of light in materials.
- Optical constants:
  - Dielectrics
  - Metals
  - Semiconductors
- Optical Absorption.
  - Mechanical Analogies.
  - Absorption Coefficient
- Brewster’s Angle.
  - Optimum Angles for ellipsometry.
- Coated Samples with many reflections.
  - Fresnel Coefficients. Interference effects.
Polarization Changes

- Reflections occur from:
  - Uncoated “Bulk” Substrates.
  - Thin film Samples (Coatings).

- Reflections caused by:
  - DIFFERENCES in Refractive Index at interfaces...
  - Air to glass, Glass to Silicon, etc.

\[ R = \frac{(n_0 - n_1)^2}{(n_0 + n_1)^2} \]

For Uncoated Substrate
At Normal Incidence.

- Need to further understand Refractive index.
Refractive Index: What is it?

- **Refractive Index** = Optical “Density”
  - Impediment to propagation of light.
  - Speed in vacuum: \( c = 3 \times 10^8 \text{ m/s} \).
  - Wave speed in material = \( c/n \)

- **Analogy:**
  - Walking along the beach (easy).
  - Wading through water (harder).

- \( n_{\text{(air)}} = 1.00; \) Reference Value.
- \( n_{\text{(glass)}} = 1.50 \)
- \( n_{\text{(water)}} = 1.33 \)
Light

- Velocity and wavelength vary in different materials.

\[ v = \frac{c}{n} \]

- Energy of photon: \( E(eV) = h\nu \approx \frac{1,240}{\lambda(nm)} \)

- Frequency, \( \nu \) of wave remains constant!
  (Conservation of Energy.)

\[ \nu = \frac{v}{\lambda} \]
Refractive Index

- Determines Wave speed.
  
  \[ \nu = \frac{c}{n} \]

- Determines Angle of Propagation.
  - Snell’s Law of Refraction:
    \[ n_1 \sin \theta_1 = n_2 \sin \theta_2 \]
  
  - Pencil in glass of water appears “Broken”.

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Absorption and Extinction

Absorption With Depth

- For absorbing bulk materials:
  = deeper propagation.
  = more energy loss.
  = complete extinction.

\[ I(z) = I_0 e^{-\alpha z} \]
\[ \alpha = \frac{4\pi k}{\lambda} \]

- As absorbing films become thicker:
  = longer propagation path in film.
  = wave spends longer time in film.
  = more absorption by material.
  = more extinction of wave.
Absorption Coefficient

Absorption with Depth:
- Exponential Absorption with depth, z, or film thickness.
  
  \[ I(z) = I_{\text{max}} e^{-\alpha z} \]

- Exponential Decay of wave.

Absorption Coefficient, \( \alpha \):

\[ \alpha(\lambda) = \frac{4\pi k(\lambda)}{\lambda} \]

- Units: 1/(length) (1/nm, 1/microns, 1/Å, etc.)
Complex Refractive Index.

- Both n and k are needed to describe real materials.
- \( n = "\text{Refractive Index}" \)
  - Gives wave speed = \( c/n \).
  - Gives direction of propagation = refraction angle.
  - Snell’s Law
- \( k = "\text{Extinction Coefficient}" \)
  - Loss of energy in wave. Intensity is “Extinguished.”
- Both n and k vary with wavelength.
  - Index Dispersion: One reason for doing Spectroscopic ellipsometry.
- Together called “Complex Refractive Index”:
  \[ \tilde{n}(\lambda) = n(\lambda) + ik(\lambda) \]
Optical Constants: Definitions

Complex Refractive Index:
\[ \tilde{n}(\lambda) = n(\lambda) + ik(\lambda) \]
- Describes what material does to light wave.
  - Slows down, wavelength changes, refraction, extinction.

Alternatively...

Complex Dielectric Function:
\[ \varepsilon(\lambda) = \varepsilon_1(\lambda) + i\varepsilon_2(\lambda) \]
- Describes what wave does to material.
  - \( \varepsilon_1 = \) volume polarization term ➔ Oscillating charges = Dipoles.
  - \( \varepsilon_2 = \) volume absorption ➔ Carrier generation.
Complex Dielectric Function

- Dielectric function describes material’s response to electro-magnetic radiation
- Refractive index describes changes to light wave caused by interaction with materials
  - is the complex square root of the dielectric function

\[ n + ik = \sqrt{\varepsilon} = \sqrt{\varepsilon_1 + i\varepsilon_2} \]
Optical Constants: Conversions

Converting dielectric function & refractive index.

At each wavelength:

\[ \varepsilon = \varepsilon_1 + i \varepsilon_2 = (n + ik)^2 \]

\[ \varepsilon_1 = n^2 - k^2 \]
\[ \varepsilon_2 = 2nk \]

\[ n = \sqrt{\frac{\varepsilon_1 + \sqrt{(\varepsilon_1^2 + \varepsilon_2^2)}}{2}} \]
\[ k = \sqrt{\frac{-\varepsilon_1 + \sqrt{(\varepsilon_1^2 + \varepsilon_2^2)}}{2}} \]

WVASE32 will do these conversions automatically!
Optical Absorption

- Absorption can also occur: \( k > 0 \).

- **Four causes of Absorption:**
  - 1. Free electrons absorb wave energy.
    - Metals, Semiconductors \( \rightarrow \) Conductivity.
  - 2. Electrons bound to atoms in material.
    - Dielectrics. \( \rightarrow \) Oscillating electron clouds. Heat Losses.
  - 3. Electrons broken free from bound states.
    - Bound electrons become free electrons.
    - Occur at higher energies in visible and UV.
  - 4. Vibrations of atoms or molecules.
    - Infrared spectroscopy. \( \lambda = 2 \) microns and longer.

- Consider each type separately.
Optical Constants

Different regions represent different absorptions.

Rutile TiO$_2$, UV to IR Spectral Range

Lattice Vibrations

Transparent

Electronic Transitions

\[ \varepsilon_1 \]

\[ \varepsilon_2 \]

Photon Energy (eV)

IR

Visible

UV

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Metals: Refractive Index

- **Metals**: Have more electrons than needed for bonding. (Covalent Bonds = Sharing of electrons).
- **“Extra” electrons** not shared are set “free” by the atoms. Travel freely in the material. **Absorb Light**.

- Free electrons give:
  - Electrical Conduction.
  - Optical absorption.

- Applied field of light wave causes electrons to move! Wave energy lost as heat.
Dielectrics: Refractive Index

- Oscillating electron charge cloud.

- Electrons can move easily. Very light.
- Heavy atomic cores move hardly at all.
- Displaced charge = Electric Dipoles.
Dielectrics: Refractive Index

- Oscillations Take Time!
  - Wave must start charge cloud moving. “Push” electrons out of way.
  - Moving charge cloud will re-emit wave. \( \rightarrow \) No energy lost!!
  - Re-emitted wave is “Delayed” in phase.

\[ n = \frac{\text{speed in air}}{\text{speed in material}} \]

- Analogy: \( \rightarrow \) Walking in water.
  - You must push water out of the way.
  - You become slowed down.

\[ \rightarrow \text{WAVE HAS BEEN SLOWED!!} \]

Reference Wave: In Phase \( \rightarrow \) Out of Phase
Dielectrics: Refractive Index

- Transparent at visible & near infrared wavelengths.
- Absorption occurs in UV (Sometimes deep UV).
- High index materials absorb at longer wavelengths.
- Low index materials transparent into UV or VUV.

**Low Index**
- Low Index Films: MgF2, SiO2, and Al2O3

**High Index**
- Hi Index Films: Ta2O5 and Nb2O5

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Dielectrics: Refractive Index

- **Oscillating Charge Cloud** = Mechanical Oscillator.

- **Mechanical Oscillators:**
  - Mass on Spring.
  - Simple Pendulum = Playground Swing.

- Mechanical Oscillators have:
  - **RESONANT FREQUENCY!!!**
  - Oscillators can be driven **Below, At, or Above** the Resonant Frequency. 3 different cases.
Dielectrics: Refractive Index

Case 1: Below Resonance

- Index increases with frequency (shorter $\lambda$).
- Energy more efficiently coupled to oscillators.

![Graph showing dielectric optical constants with wavelengths ranging from 200 to 1400 nm and indices of refraction and extinction coefficients plotted.]

- Material is Transparent.
- Dipoles give energy back to wave.

  Index increases toward shorter $\lambda$: 
  - Trying to walk faster through water.
Dielectrics: Refractive Index

Case 2: Resonance

- Maximum amplitude of Electron clouds.
- Neighboring clouds begin to interact with each other.

Absorption due to e-cloud “bumping”.

Energy taken from Dipoles, given to k.

Dielectric Optical Constants: At Resonance

Wavelength (nm) | Index of refraction $n$ | Extinction Coefficient $k$
--- | --- | ---
200 | 1.70 | 0.00
300 | 1.80 | 0.00
400 | 1.90 | 0.00
500 | 2.00 | 0.00
600 | 2.10 | 0.00

Electron Clouds Bump. Lose energy as heat.
Index Dispersion

- Optical constants vary with wavelength:
  \[ \hat{n}(\lambda) = n(\lambda) + ik(\lambda) \]

- Real and imaginary optical properties are not independent (Kramers-Kronig consistent).

Normal Dispersion: (transparent wavelengths)
No absorption present \((k=0)\),
Index decreases as wavelength increases

Anomalous Dispersion: (absorbing wavelengths)
Absorption in material causes wavelength-dependent changes in index as described by K-K consistency
Dielectrics: Refractive Index

- Multiple resonant absorptions often occur.
- Organic AR Coating.

AZ BARLi ARC Optical Constants

<table>
<thead>
<tr>
<th>Wavelength in nm</th>
<th>Index of Refraction (n)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.2</td>
</tr>
<tr>
<td>200</td>
<td>2.2</td>
</tr>
<tr>
<td>400</td>
<td>1.8</td>
</tr>
<tr>
<td>600</td>
<td>1.6</td>
</tr>
<tr>
<td>800</td>
<td>1.4</td>
</tr>
<tr>
<td>1000</td>
<td>1.2</td>
</tr>
<tr>
<td>1200</td>
<td>1.0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Wavelength in nm</th>
<th>Extinction Coefficient (k)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.0</td>
</tr>
<tr>
<td>200</td>
<td>0.2</td>
</tr>
<tr>
<td>400</td>
<td>0.4</td>
</tr>
<tr>
<td>600</td>
<td>0.6</td>
</tr>
<tr>
<td>800</td>
<td>0.8</td>
</tr>
<tr>
<td>1000</td>
<td>1.0</td>
</tr>
<tr>
<td>1200</td>
<td>1.0</td>
</tr>
</tbody>
</table>

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Semiconductors: Refractive Index

- **Sharp absorption features = “Critical Points”**.
  - Valence to conduction band transitions.
  - Bound charge becomes free charge...ionization. $E > E_g$.

### Silicon 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>0</td>
<td>1.0</td>
<td>0.0</td>
</tr>
<tr>
<td>300</td>
<td>6.0</td>
<td>5.0</td>
</tr>
<tr>
<td>600</td>
<td>5.0</td>
<td>4.0</td>
</tr>
<tr>
<td>900</td>
<td>4.0</td>
<td>3.0</td>
</tr>
<tr>
<td>1200</td>
<td>3.0</td>
<td>2.0</td>
</tr>
<tr>
<td>1500</td>
<td>2.0</td>
<td>1.0</td>
</tr>
<tr>
<td>1800</td>
<td>1.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

Sharp Absorptions
- In UV
- Normal Dispersion
- At longer wavelengths
Semiconductors: Refractive Index

- Compare Crystalline and Amorphous Silicon.
  - Sharp critical point transitions seen in crystalline Silicon.
  - No critical points seen in amorphous materials.

![Graphs showing the comparison between Crystalline and Amorphous Silicon](image-url)
Semiconductors: Refractive Index

Polycrystalline Silicon: Optical constants change with crystallinity.
Infrared Absorption: Molecular Vibration

Electric Field with slow frequency (IR) can vibrate molecules (stretch or bend)

- CH\textsubscript{2} stretch (symmetric)
- CH\textsubscript{2} stretch (asymmetric)
- N-H stretch
- C=O stretch

![Infrared Absorption Graph](image-url)
Optical Absorption

Review:
4 major types studied.

- **Metals.**
  - Free Carrier Absorption.

- **Dielectrics.**
  - Resonant Absorption.

- **Semiconductors.**
  - Resonant absorption below band gap.
  - Bound to free electron transitions at band gap $E_g$ and above.
  - Free carriers above band gap...Interband transitions.

- **Infrared Wavelengths.**
  - Vibrational absorption of molecules.
Dispersion Equations

- Mathematical representations of optical constants as a function of wavelength
- **Advantages:**
  - Easily adjust optical constants with only a few "free" parameters.
  - No noise
  - Easier to interpolate or extrapolate
  - Often maintain K-K consistency
- **Transparent Types:**
  - Cauchy and Sellmeier
Normal Dispersion: Cauchy Model

- Used to describe index of refraction ($n$) of transparent materials ($k=0$).
- Three parameters ($A$, $B$, $C$) describe index versus wavelength ($\lambda$).

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

$\lambda$ sets index range

$B$ and $C$ give dispersion shape

Index of refraction $n$ versus Wavelength (nm)
All Oscillator models have 3 parameters in common:

- 1. Amplitude (Amp) or “Strength”
- 2. Broadening (Br)…”Width”
- 3. Center energy (E_c) or wavelength…”position”
Anomalous Dispersion: Oscillator Models

- Oscillator models: Variety of Functions Available!
  - Lorentz, Gaussian, Harmonic, Tauc-Lorentz, etc.
  - Built-in Kramers-Kronig Consistency!

![Graph showing Real(Dielectric Constant), ε₁ and Imag(Dielectric Constant), ε₂ as functions of Wavelength (nm). Brackets indicate Br and Amp, with Ec as a critical point.]
Multiple Absorptions: Ensemble Model

- Dielectric function can be modeled as a sum or ensemble of various oscillators
  - Different Oscillator can be used for each absorption region
  - Oscillators are summed together.
  \[ \tilde{\varepsilon}(\omega) = \varepsilon_{\text{offset}} + \sum_n \text{Osc}_{\text{type}}(\text{Amp}, \omega_n, \gamma_n, \ldots) \]
  - Remains KK-consistent.

[Graph showing imaginary part of dielectric constant versus photon energy with different oscillator types: Drude, Gaussian, Tauc-Lorentz, Ito, PBP]
Fitting More than 1 Oscillator. Genosc.mat Layer

1) Model absorptions - multiple Tauc-Lorentz or Gaussian Oscillators.
2) Example of an Organic shown in Figure below (before $\varepsilon_2$ fit).
Example: Brewer DUV 30 Polymer

- Use 14 Gaussian oscillators to fit point by point results.
- Data fit 130-1700 nm.
Example: Brewer DUV 30

Compare Point by point with Oscillator Model fits.

DUV 30 Optical Constants

- Refractive Index $n$
- Extinction Coefficient $k$

Wavelength (nm):
- 0, 300, 600, 900, 1200, 1500, 1800

Photon Energy (eV):
- 0, 2, 4, 6, 8, 10

DUV 30, point by point vs. DUV 30-Gaussian Oscillators
Example: Brewer DUV 30

Data Fit 130-1700 nm.

Oscillator Model Fit.

<table>
<thead>
<tr>
<th>1</th>
<th>duv30-14 oscillators</th>
<th>609.64 Å</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>si_vuv</td>
<td>1 mm</td>
</tr>
</tbody>
</table>

Generated and Experimental

![Generated and Experimental](image)

Model Fit
- Exp E 65°
- Exp E 70°
- Exp E 75°

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Dispersion Relationships

- Mathematical representations of optical constants as a function of wavelength..."Oscillator Models"

- Advantages:
  - Add flexibility beyond tabulated optical constants.
  - Use much smaller set of “free” parameters.
  - Often maintain K-K consistency.
  - No noise.
  - Easier to interpolate or extrapolate.

- Types:
  - Cauchy, Sellmeier (Transparent Region).
  - Lorentz, Gaussian, Tauc-Lorentz (Absorbing Region).
Thin Film Interference

- Each reflected wave has phase and amplitude.
Thick versus Thin

- Thicker films have more interference oscillations.
- Oscillations provide information about $\Delta n$ and thickness.
Data Acquisition

- Wavelengths (Range and Number)?
  - Wavelengths of interest?
  - Where is film transparent?
  - Film thickness?
  - Sharp features in data?

- Angles?
  - What are Substrate and Films?
  - Single or Multilayers?
  - Complex materials?
Wavelengths?

- Resolve data features.

<table>
<thead>
<tr>
<th>Film Thickness</th>
<th>Steps (eV)</th>
<th>Steps (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt;200 nm</td>
<td>0.1 eV</td>
<td>20 nm</td>
</tr>
<tr>
<td>200 - 500 nm</td>
<td>0.05 eV</td>
<td>10 nm</td>
</tr>
<tr>
<td>500 nm - 1 μm</td>
<td>0.025 eV</td>
<td>5 nm</td>
</tr>
<tr>
<td>1 - 3 μm</td>
<td>0.01 eV</td>
<td>2 nm</td>
</tr>
<tr>
<td>&gt;3 μm</td>
<td></td>
<td>2 nm, Long wavelengths</td>
</tr>
</tbody>
</table>

Experimental Data

Data every 2nm

2.5 μm Oxide
**Typical Angles**

**Typical Angle Combinations:**

- Thin films on Si: $65^\circ$, $75^\circ$
- Thick films on Si: $60^\circ$, $75^\circ$
  or $55^\circ$, $65^\circ$, $75^\circ$
- n-matched films on glass: $55^\circ$, $56.5^\circ$, $58^\circ$
- Other films on glass: $50^\circ$, $60^\circ$, $70^\circ$
- Films on metals: $65^\circ$, $75^\circ$
- Anisotropic & Graded films: $55^\circ$, $65^\circ$, $75^\circ$
  or $45^\circ$, $60^\circ$, $75^\circ$

**Spot size vs. angle**

<table>
<thead>
<tr>
<th>Angle of Incidence</th>
<th>(spot-length)/(beam-dia.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25°</td>
<td>1.1</td>
</tr>
<tr>
<td>35°</td>
<td>1.2</td>
</tr>
<tr>
<td>45°</td>
<td>1.4</td>
</tr>
<tr>
<td>55°</td>
<td>1.7</td>
</tr>
<tr>
<td>65°</td>
<td>2.4</td>
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<td>75°</td>
<td>3.9</td>
</tr>
<tr>
<td>80°</td>
<td>5.8</td>
</tr>
<tr>
<td>85°</td>
<td>11.5</td>
</tr>
</tbody>
</table>
Data Analysis

What Ellipsometry Measures:

Psi ($\Psi$)
Delta ($\Delta$)

What we are Interested in:

Film Thickness
Refractive Index
Surface Roughness
Interfacial Regions
Composition
Crystallinity
Anisotropy
Uniformity
...

Model-based analysis usually required to extract quantities of interest!!
2. Build Model

- Layered structure that describes sample that light interacted with.
- Need thickness and optical constants for all layers.

![Diagram](image)
3. Generated data

- Calculate $\Psi(\lambda, \phi)/\Delta(\lambda, \phi)$ values of model

- Compare to Experimental data
  - Visually & Mathematically.

- Adjust unknown (fit) parameters to get close to solution.
Mean Squared Error

- How do we compare results?
- **Mean Squared Error (MSE)** used to quantify the difference between experimental and model-generated data.

\[
MSE = \sqrt{\frac{1}{2N - M} \sum_{i=1}^{N} \left[ \left( \frac{\Psi_{i}^{\text{mod}} - \Psi_{i}^{\text{exp}}}{\sigma_{\Psi,i}^{\text{exp}}} \right)^2 + \left( \frac{\Delta_{i}^{\text{mod}} - \Delta_{i}^{\text{exp}}}{\sigma_{\Delta,i}^{\text{exp}}} \right)^2 \right]}
\]

- A smaller MSE implies a better fit.
- MSE may be weighted by the error bars of each measurement, so noisy data are less influence.
4. Data Fit

- The Marquardt-Levenberg* algorithm is used to quickly find the minimum MSE.
- Good starting values may be important.

Data Fit Types

- All vary “fit” parameters to find best agreement with Experimental Data

**Normal Fit**
- Works with **ALL** selected data simultaneously.

**Global Fit**
- **Searches Grid** of starting values.

**Point-by-Point Fit**
- **Fit on wavelength-by-wavelength basis.**
Evaluate Results

- Find the **simplest optical model** that fits Experimental Data.
- Visually compare experimental and generated data.
- How low is MSE? Can it be reduced?
- Are fit parameters physical?
- Check mathematical “goodness of fit” indicators
  - Correlation matrix, 90% confidence limits.
Morning Overview

- Spectroscopic Ellipsometry:
  - Part 2: Standard Applications.
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  - Part 4: Infrared and In-Situ Ellipsometry.
Data Analysis Strategies

Substrates
- Opaque Substrates.
- Semiconductor substrates.
- Transparent substrates.

Films
- Transparent thin films.
- Absorbing thin films.
- Dispersion Models.
Substrate Optical Constants

- **Substrate**

- **Dielectrics**

- **Semiconductors**

- **Metals**

Index of Refraction, $N$

- **Silicon**
  - Index, $n$
  - Extinction Coefficient, $k$

- **Aluminum**
  - Index of refraction, $n$
  - Extinction Coefficient, $k$
Opaque Substrates

Two Categories:

- **“Bulk” Samples** → No overlayers.
  - Polished metal.

- **Metal films**: Optically thick.
  - Small 1/\(a\) penetration depth.
  - \(~800\,\text{Å}\) or more metal becomes opaque.
  - \(~400\,\text{Å}\) in reflection mode since 2 passes needed.
Opaque Substrates

Bulk Materials and Optically Thick Films

- Two experimental parameters measured: $\Psi$ and $\Delta$.
- Two unknowns to be determined: $n$ and $k$ at each wavelength.

Fit Strategy:
- “Invert” psi and delta for $n$ and $k$.
  - Normal fit from reference values if material is known (e.g. bulk aluminum).
  - Point by point fit from pseudo optical constants if unknown.

Examples: Optically thick Gold (Au, Al, Pt, etc).

For Practice: WVASE32 Software manual.
Example: Optically Thick Aluminum

Simple Point-by-Point fit for $n$ and $k$.

Optical Constants

Generated and Experimental

Optical Constants

Generated and Experimental

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Semiconductor Substrates

- Bulk semiconductor optical constants are well known.
  - Crystalline structure insures repeatable optical/electrical properties.

- Semiconductors have high index.
  - Great index contrast with low index native oxides or coatings!
  - High index contrast gives extra sensitivity to thickness and index.

- VERY Smooth.

- Doping not important at visible wavelengths.
  - Use any doping value and crystalline orientation.
  - Doping IS important in the MID-IR, however (5 micron or longer).

- Fit Strategy:
  - Use published index values.
  - Fit for oxide thickness.

- Example: Thin SiO<sub>2</sub>/Si.

- For Practice: Ellipsometer Calibration Wafer.

Transparent Substrates

Two Categories:

1. Uncoated Glass.
2. Rigid bulk Plastic.

• **VERY** Transparent (k=0 or very small).
  - Large to infinite 1/a penetration depth.
  - Back surface reflections may be present.

• 3 ways to handle back surface reflection:
  - Separate front and back beams (thick samples).
  - Roughen back side (grinder, sandpaper, small sandblaster).
  - Model with WVASE32 back surface reflection correction.
Transparent Substrates

- **Examples:** 1 mm thick 7059, 1737, or float glass.

- **Fit Strategy:**
  - One unknown to be determined \( n(\lambda) \).
  - Only need one experimental parameter \( \Psi(\lambda) \).

- **Fit psi for index at each wavelength.**
  - Cauchy fit, or
  - Normal fit.
  - **Tip:** Reflectance will be very low near Brewster’s angle...so acquire data above Brewster’s angle.
    - Use 60°-80° for best psi data, delta will be near zero.
    - Effectively a psi only fit.

- **For Practice:** WVASE32 Software manual.
Cauchy

- Describes index \( n \) of transparent materials \( (k=0) \). “Normal Dispersion”.

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

\[\text{A sets amplitude}\]

\[\text{B and C give dispersion shape}\]

- Wavelength (nm)

- Index of refraction \( n \)

<table>
<thead>
<tr>
<th>Wavelength (nm)</th>
<th>Index of refraction ( n )</th>
</tr>
</thead>
<tbody>
<tr>
<td>200</td>
<td>1.44</td>
</tr>
<tr>
<td>400</td>
<td>1.47</td>
</tr>
<tr>
<td>600</td>
<td>1.50</td>
</tr>
<tr>
<td>800</td>
<td>1.53</td>
</tr>
<tr>
<td>1000</td>
<td>1.56</td>
</tr>
<tr>
<td>1200</td>
<td>1.59</td>
</tr>
</tbody>
</table>

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**Transparent Substrates**

- **Obtain Error Bars on index.**
  - Perform both Cauchy and normal fits.
  - Compare them!...great way to obtain error bars at each wavelength.
  - Cauchy gives smooth average.
  - Normal fit gives measured error.

![Graph showing index of refraction 'n' vs Wavelength (nm) for Glass Optical Constants: Comparison](image_url)
Transparent Substrates

How to obtain small k-values.

- $k(\lambda)$ can be as small as $10^{-6}$ (0.000001) for transparent glasses!
  - NOT seen in reflection mode. (no path length.)
  - Increase path length with transmission data.
  - EASY to see small k-values with transmission data.

**Graphs:**

- **Wavelength (nm)**: 0, 300, 600, 900, 1200, 1500, 1800
- **Transmission (0.0, 0.2, 0.4, 0.6, 0.8, 1.0)**
- **Model Fit** and Experimental data

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Transparent Substrates

How to obtain small $k$-values.

- $k(\lambda)$ can be as small as $10^{-6}$ (0.000001) for transparent glasses!
Transparent Substrates

Soda-Lime Glass

5 mm thick Soda-Lime glass:

- VERY important to know substrate absorption if fitting transmission data for thin films.
Transparent Films

- Sensitivity comes from **INDEX DIFFERENCE** between layers = Stronger reflections.
- High index difference gives greater sensitivity:
  - Smaller error bars on thickness and index, OR
  - More layers!...Hi-Lo stack → optical filters.
- Fit refractive index with Cauchy equation.
- Tip: For greatest sensitivity, maximize the index difference between adjacent layers.

For Practice: WVASE32 Software manual.
Absorbing Films

- Thin Film Data Analysis
  - Organic and Polymer Thin Films.
    - Resists, AR coatings, pellicles.
  - Semiconductor Thin Films.
    - Point-by-Point versus Dispersion Models.
    - Alloy ratio models.
    - Surface oxides and roughness.
    - Dispersion Models.
  - Metal and Opaque Thin Films.
    - Thin metal on glass? …Add transmission data.
    - Thin metal film on thick SiO$_2$ on Silicon.
UV Absorbing Films

- Transparent films with onset of absorption in UV: Si$_3$N$_4$, SiON, Resists, Organics, etc.

![Diagram of UV absorbing films with index of refraction (n) and extinction coefficient (k) curves](image1)

![Experimental Data graph showing wavelength vs. index of refraction and extinction coefficient](image2)
UV Absorbing Films

Divide analysis into 2 parts:

- **Step 1: Transparent Region.**
  - Range select data where film is transparent ($k=0$)
    - typically longer wavelengths.
  - Two unknowns $\rightarrow n(\lambda)$ & thickness.
  - Two measured parameters $\rightarrow \Psi(\lambda)$ & $\Delta(\lambda)$.
  - Cauchy fit $n(\lambda)$ & thickness

- **Step 2: Absorbing Region.**
  - Fix thickness from Step 1.
  - Fit $n/k$ on a wavelength-by-wavelength basis.
  - “Point by Point Fit.”
Step 1: Cauchy fit

- Cauchy fit at long wavelengths determines thickness

Cauchy only valid in transparent region
Advantages

- Small features in n/k are identified.
- QUICK!
- EASY!
Point-by-Point Fits

- **Advantages**
  - QUICK!
  - EASY!
  - Capture small features.

- **Disadvantages**
  - Not necessarily KK consistent. Noise can be present.
Zinc Sulfide on Silicon

- Fit to Cauchy model over limited spectral range (0.73 to 3eV)
- Include surface layer, optical constants obtained from separate sample that had been annealed.
- Add index grading.
- Point-by-point fit $n$ and $k$ over entire spectral range.
- Small glitches in Pt-by-Pt optical constants. Can use them to set up dispersion model.

Small glitches are not physical.
Setting up Dispersion Model

Using questionable Pt-by-Pt optical constants to set up parameterized dispersion model.

- Generate data from “bulk” Pt-by-Pt optical constants.
- Set up oscillators fitting to $\langle \varepsilon_2 \rangle$.
- Fit pole magnitudes and positions to $\langle \varepsilon_1 \rangle$.
- Replace Pt-by-Pt optical constants with dispersion model.
- Make small adjustments fitting to experimental data.
Absorbing Thin Films: Dispersion Models

- **Advantages:**
  - Correct surface layer optical constants not as critical.
  - Fit to all the data simultaneously.
    - Sensitive to all parameters at once. Regions of spectrum are more sensitive to certain parameters that others are not.
  - More Flexibility.

- **Disadvantages:**
  - Setting up dispersion model can be rigorous.
  - Can miss small details in optical constants.
Procedure for Absorbing Films

1. Cauchy Fit
   - transparent region only
2. Pt-by-Pt Fit – all wavelengths
   - fix thickness
   - Save tabulated n & k values
   - Replace Cauchy with Genosc
3. Match n,k using Genosc
   - Load tabulated file from pt-by-pt fit into Reference
   - fit reference – first e2, then e1
4. Fit Ψ & Δ data using new Genosc model
Compound Semiconductor Films

Alloy Semiconductors:

- AlGaAs, InGaAs, HgCdTe, etc.
- Use alloy material files. Fit for alloy ratio.
  - Critical points shifted automatically with alloy fraction!

For Practice: WVASE32 Software manual.
  - Example #10, page 13-71. GaAs/AlGaAs/GaAs wafer.
Alloy Ratio Model: $\text{Al}_x\text{Ga}_{1-x}\text{As}$ Multilayer

- Superlattice model allows coupling layers together.
- Fit alloy ratios and thicknesses.
- Many fit parameters but do not appear to be correlated.

Different alloy ratios produce different optical constants. Alloy ratios models allow adjustment of optical constants with a single parameter ($x$).

<table>
<thead>
<tr>
<th>Layer</th>
<th>Optical Constant ($\lambda$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>9 GaAs Oxide</td>
<td>19.9 Å</td>
</tr>
<tr>
<td>8 GaAs</td>
<td>3348.1 Å</td>
</tr>
<tr>
<td>7 AlGaAs $x=0.365$ (Coupled to 5)</td>
<td>995.6 Å</td>
</tr>
<tr>
<td>6 GaAs</td>
<td>849.3 Å</td>
</tr>
<tr>
<td>5 AlGaAs $x=0.365$</td>
<td>995.6 Å</td>
</tr>
<tr>
<td>4 GaAs</td>
<td>852.9 Å</td>
</tr>
<tr>
<td>3 AlGaAs $x=0.274$</td>
<td>866.5 Å</td>
</tr>
<tr>
<td>2 GaAs</td>
<td>843.3 Å</td>
</tr>
<tr>
<td>1 AlGaAs $x=0.168$</td>
<td>742.5 Å</td>
</tr>
<tr>
<td>0 GaAs Substrate</td>
<td>1 mm</td>
</tr>
</tbody>
</table>

Thin Metal Films on Glass

- Semitransparent Ag on Quartz substrate
  - Adding Transmission intensity data breaks correlation between optical constants and thickness.
  - Ag optical constants can be fit at each measured wavelength, or modeled with summation of Drude and several Lorentz oscillators.

For Practice: WVASE32 Software manual.
  - Example #7, page 13-51. Thin Silver on Fused Silica.
Thin Metal Film on Glass

Results: 300 Å Silver on Fused Silica.

<table>
<thead>
<tr>
<th>0</th>
<th>siO2</th>
<th>1 mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>ag</td>
<td>341.7 Å</td>
</tr>
<tr>
<td>2</td>
<td>srough</td>
<td>7.4 Å</td>
</tr>
</tbody>
</table>

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<th>0</th>
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<td>2</td>
<td>srough</td>
<td>7.4 Å</td>
</tr>
</tbody>
</table>

- Wavelength (nm): 300, 600, 900, 1200, 1500, 1800
- Ψ in degrees: 10, 20, 30, 40, 50
- Δ in degrees: 0, 30, 60, 90, 120, 150, 180

- Model Fit
- Exp E 65°
- Exp E 70°
- Exp E 75°
Thin Metal Over Thick Oxide

- TiN on thick SiO$_2$ on Silicon.
  - SiO$_2$ introduces interference oscillations in data.
  - TiN dampens and phase shifts these oscillations, extent depends on thickness of TiN film.
  - Data acquired at a wide angle spread to ensure largely different path lengths.

Oscillations damped with increasing TiN thickness.

For Practice: WVASE32 Software manual.
- Example #12, page 13-83. TiN on SiO$_2$ on Silicon.
Thin Metal on Thick Oxide

- Results: TiN on SiO₂ on Silicon.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>tin_I</td>
<td>55.128 nm</td>
</tr>
<tr>
<td>sio2_jaw</td>
<td>627.46 nm</td>
</tr>
<tr>
<td>si_jaw</td>
<td>1 mm</td>
</tr>
</tbody>
</table>

Generated and Experimental

tin_I Optical Constants

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Break!!