Reflectometry and Ellipsometry

• Optical constants of bulk materials and thin films important for
  • HR, AR coatings
  • DBRs
  • Waveguide design
  • Gain, loss calculations
• Measure by Ellipsometry, Reflectometry, or prism coupling
Optical Constants

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

Complex dielectric function or index of refraction

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

\[ \varepsilon_2 = 2k \]

k: extinction coefficient

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

\(\alpha\): absorption coefficient
Kramers Kronig Relation

$$\varepsilon_1(\omega) = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\varepsilon_2(\omega')}{\omega' - \omega} \, d\omega'$$

$$\varepsilon_2(\omega) = \frac{-1}{\pi} P \int_{-\infty}^{\infty} \frac{\varepsilon_1(\omega')}{\omega' - \omega} \, d\omega'$$

- Refractive index arises from absorption
- Real and imaginary parts are linked
Snell’s Law and Fresnel Equations

- Govern magnitude and phase of reflection or transmission
- Complex: magnitude and phase
- “plane of incidence” defined by incident and reflected beams
- “p-polarization” in the plane of incidence; “s- or n-pol” is ⊥
Fresnel Equations Graphed
Multilayers

- Net amplitude reflection is sum of individual complex reflections
- Reflection and transmission “sample” complex refractive indexes
- Transmission matrix formalism to keep track of all reflections
Spectral Reflectance Modeling
Spectral Reflectometry

- Usually a broadband source: W-halogen or arc lamp
- Usually near normal incidence
- Monochromator before sample, or spectrometer after sample
- Measure $R(\lambda)$ and fit model to data
- Requires reference mirror for spectrometer calibration
- Best for films thick enough to produce significant change in $R$
Pocket Spectrometer Based Reflectometry

- Fast and cheap
- Great for films > 1 micron
- Useable below 100 nm, for well characterized films

**Thickness Range**

<table>
<thead>
<tr>
<th>Model</th>
<th>Thickness Range</th>
<th>Wavelength Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>F20</td>
<td>15nm - 70μm</td>
<td>380-1050nm</td>
</tr>
<tr>
<td>F20-UV</td>
<td>1nm - 70μm</td>
<td>200-1100nm</td>
</tr>
<tr>
<td>F20-NIR</td>
<td>100nm - 250μm</td>
<td>950-1700nm</td>
</tr>
<tr>
<td>F20-EXR</td>
<td>15nm - 250μm</td>
<td>380-1700nm</td>
</tr>
<tr>
<td>F20-UVX</td>
<td>1nm - 250μm</td>
<td>300-1200nm</td>
</tr>
<tr>
<td>F20-XT</td>
<td>10μm - 1mm</td>
<td>1590-1850nm</td>
</tr>
</tbody>
</table>

*See F20 datasheet for details*
900 nm SiO2 on Sapphire

- Peaks are at $nd = m\lambda/2$
- DSP sapphire as reference
- Drop in peak value indicates loss
- Quick loss estimate:
  \[ T = \exp(-2\alpha d) = 0.85 \text{ at } 400\text{nm} \]
  \[ \alpha(400 \text{ nm}) \cong 900 \text{ cm}^{-1} \]
  bad scattering
GaN Template Loss from Spectral Transmission

Loss models
- Urbach tail, $E_{\text{Urb}} = 70$ meV
- Single oscillator
- Uncorrelated scatter

- Careful model fitting reveals thickness, real index, and loss
Ellipsometry

Analyze the change in ellipticity of light to understand the material
Ellipsometry

Complex reflectance ratio, $\rho$

$$\rho = \frac{\tilde{r}_p}{\tilde{r}_s} = \tan(\Psi) \exp(i\Delta)$$

- Illuminate with linear polarization at an angle to surface
- Choose angle of incidence and polarization for max sensitivity
- Measure ellipticity of reflected beam, then calculate $\rho$
Model Fitting

• In general, \( \rho \) cannot be inverted to obtain optical constants

• Build model and fit to data

\[ \text{Figure 10} \] flowchart for ellipsometry data analysis.
Common Material Models

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

- Cauchy: Purely empirical, diverges at short \( \lambda \)

\[ \varepsilon_1 = \frac{A\lambda^2 \lambda_0^2}{(\lambda^2 - \lambda_0^2)} \]

- Sellmeir: K-K consistent, but diverges at band edge

\[ \varepsilon_{1, \text{offset}} + \frac{A E_c}{E_c^2 - E^2 - iBE} \]

- Lorentz Oscillator: Some physical basis and reasonable response above band edge
Complications in Ellipsometry

• $\Psi$ and $\Delta$ are periodic in $\lambda/2$: need an estimate of thickness or index
• Reflections from back surface of transparent substrate
• Scattering from surface roughness or buried layers
• Birefringence
• Free carrier absorption
• (Sound familiar, Nitride folks?)

• Collect more data and build more sophisticated model
Variable Angle Spectroscopic Ellipsometry

#255 ITO on silicon

Psi, Del

Wavelength, nm

Psi, Del

60 deg

70 deg

80 deg

exper model
Thickness Sensitivity

• Δ can be measured precisely, and is sensitive to small film changes
• Measures thickness to 0.1nm; n to 0.005; k to 1E-3 (α≈250 cm⁻¹)
ITO from Sputter#3

080620 ITO on DSP Sapphire

Transmission, %

200 300 400 500 600 700 800 nm

Annealed film:
(Peak Wavelength/2n)=124 nm
T(487nm)/T_{sapphire}(487nm)=.994
alpha=(1/l)ln(1/T)=486 cm⁻¹

080620 ito on n-si sputter3 rta 600C/5min

k(500nm) = 1E-3
\alpha(500nm) = 314 cm⁻¹
Credits

- www.jowoollam.com
- www.wikipedia.com
- www.filmetrics.com