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

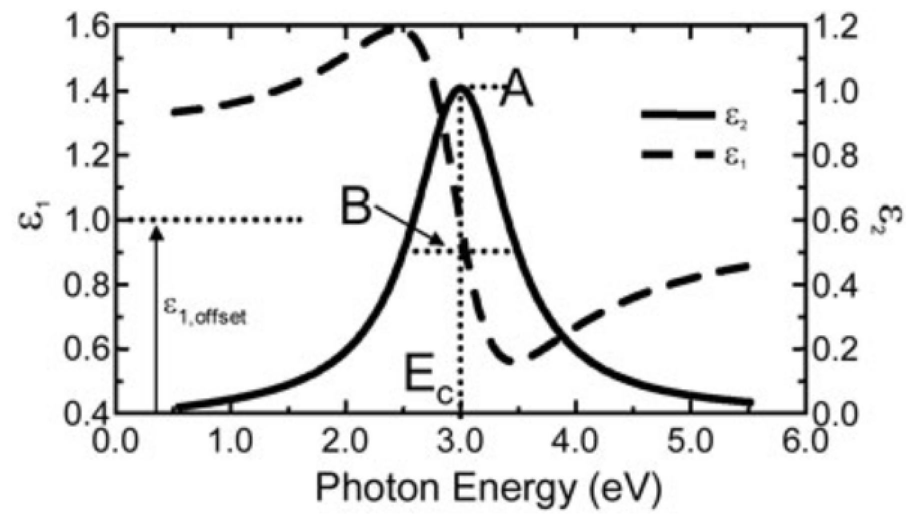
$$\alpha = \frac{4\pi k}{\lambda}$$

α: absorption coefficient

Kramers Kronig Relation

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

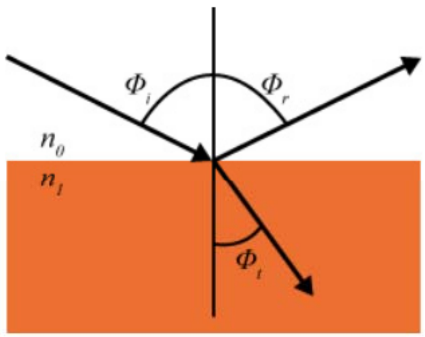
$$\varepsilon_2(\omega) = \frac{-1}{\pi} P \int_{-\infty}^{\infty} \frac{\varepsilon_1(\omega')}{\omega' - \omega} d\omega'$$



- Refractive index arises from absorption
- Real and imaginary parts are linked

Snell’s Law and Fresnel Equations

$$n_0 \sin(\Phi_i) = n_1 \sin(\Phi_t)$$



$$r_s = \left(\frac{E_{0r}}{E_{0i}}\right)_s = \frac{n_i \cos(\Phi_i) - n_t \cos(\Phi_t)}{n_i \cos(\Phi_i) + n_t \cos(\Phi_t)}$$

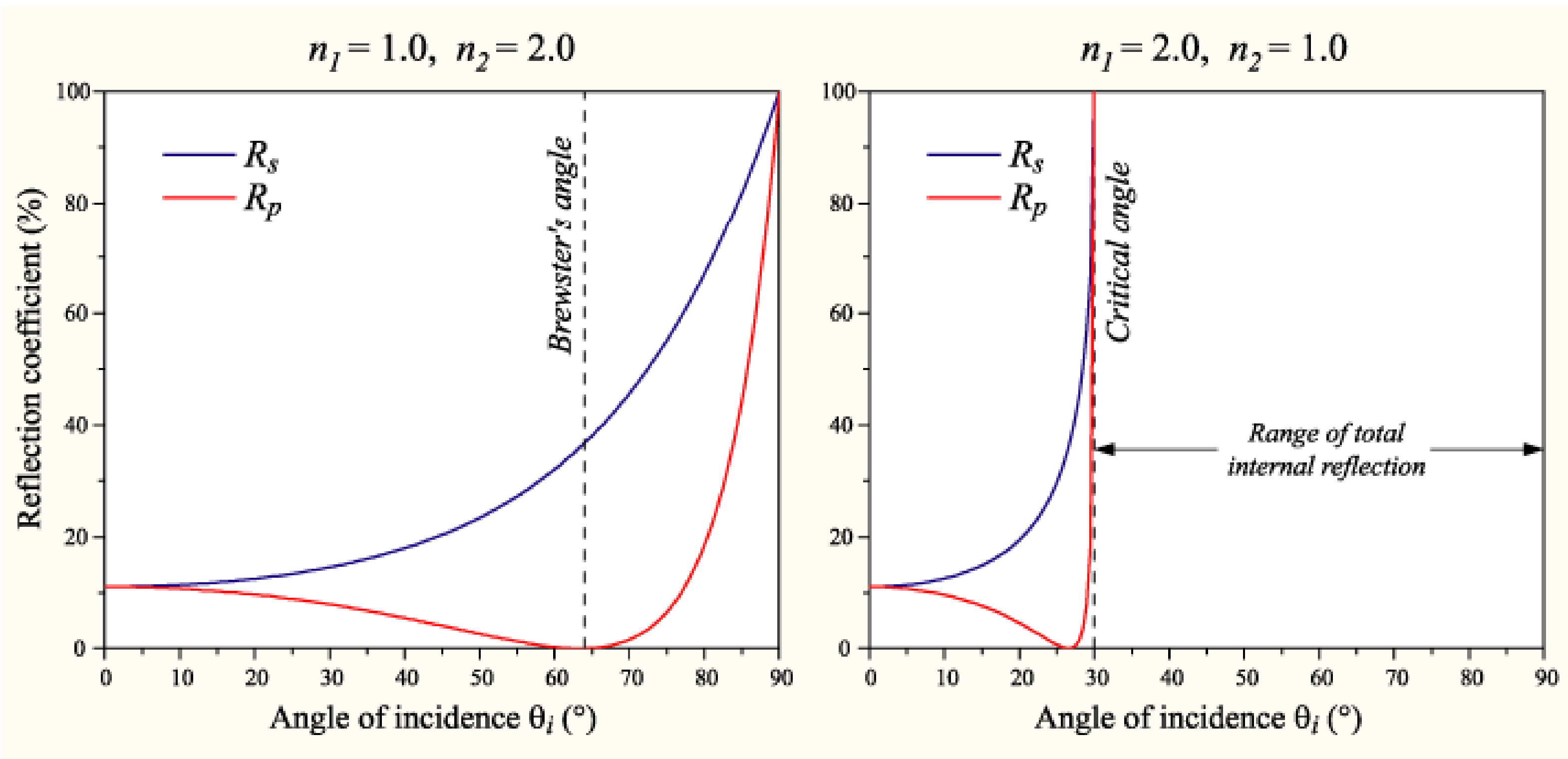
$$r_p = \left(\frac{E_{0r}}{E_{0i}}\right)_p = \frac{n_t \cos(\Phi_i) - n_i \cos(\Phi_t)}{n_i \cos(\Phi_t) + n_t \cos(\Phi_i)}$$

$$t_s = \left(\frac{E_{0t}}{E_{0i}}\right)_s = \frac{2 n_i \cos(\Phi_i)}{n_i \cos(\Phi_i) + n_t \cos(\Phi_t)}$$

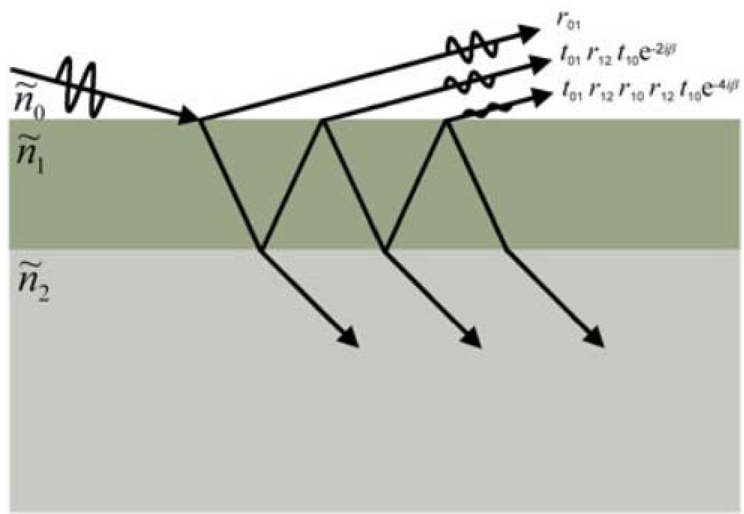
$$t_p = \left(\frac{E_{0t}}{E_{0i}}\right)_p = \frac{2 n_i \cos(\Phi_i)}{n_i \cos(\Phi_t) + n_t \cos(\Phi_i)}$$

- 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 $\perp$

Fresnel Equations Graphed

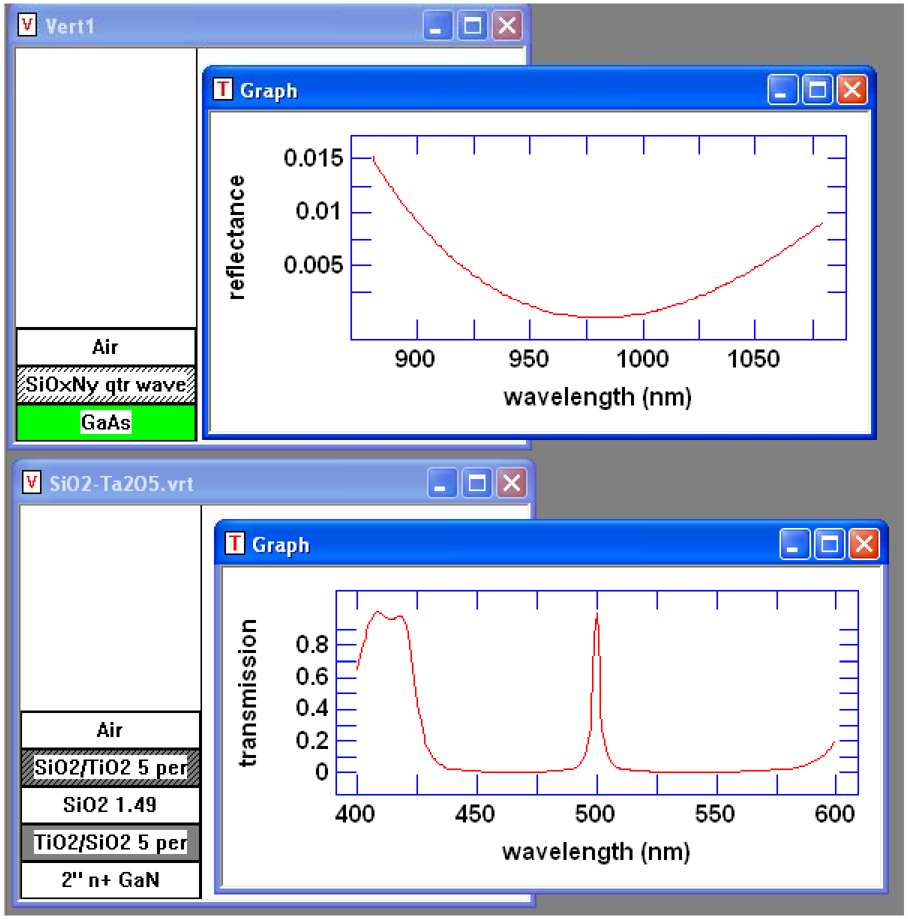


Multilayers



- 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

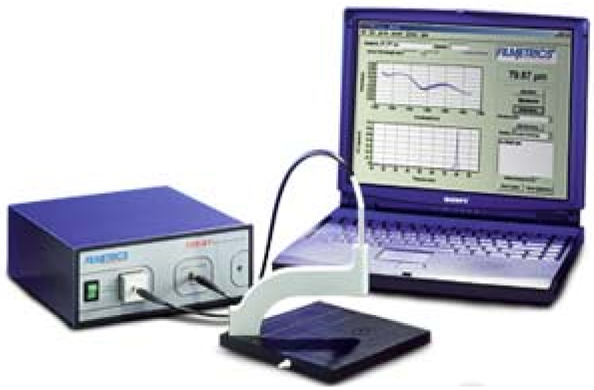
Spectral Reflectance Modeling

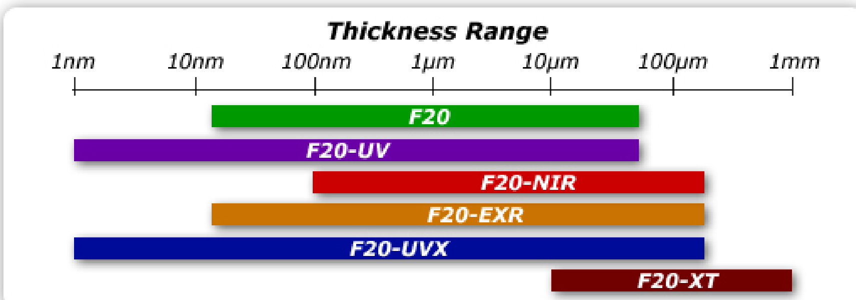


Spectral Reflectometry

- 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 Reflectometery



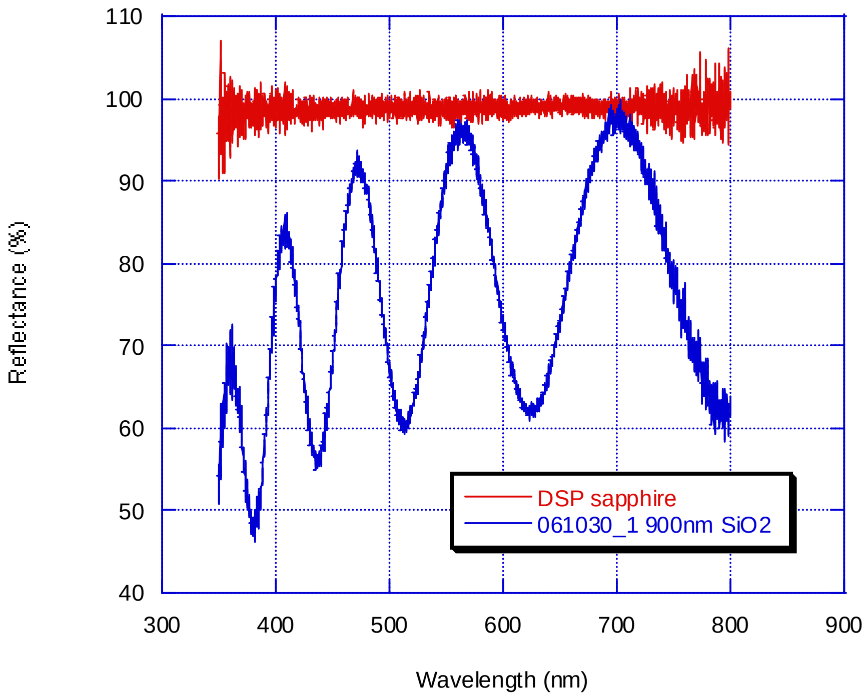


Model	Thickness Range*	Wavelength Range
F20	15nm - 70µm	380-1050nm
F20-UV	1nm - 70µm	200-1100nm
F20-NIR	100nm - 250µm	950-1700nm
F20-EXR	15nm - 250µm	380-1700nm
F20-UVX	1nm - 250µm	200-1700nm
F20-XT	10µm - 1mm	1590-1650nm

*See F20 datasheet for details

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

900 nm SiO2 on Sapphire



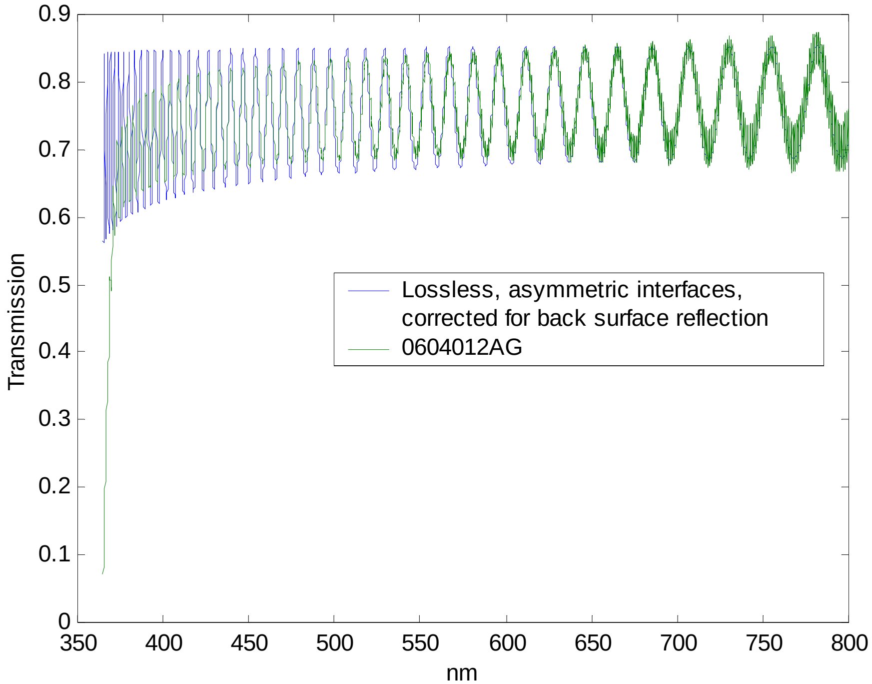
- Peaks are at nd = mλ/2
- DSP sapphire as reference
- Drop in peak value indicates loss
- Quick loss estimate:

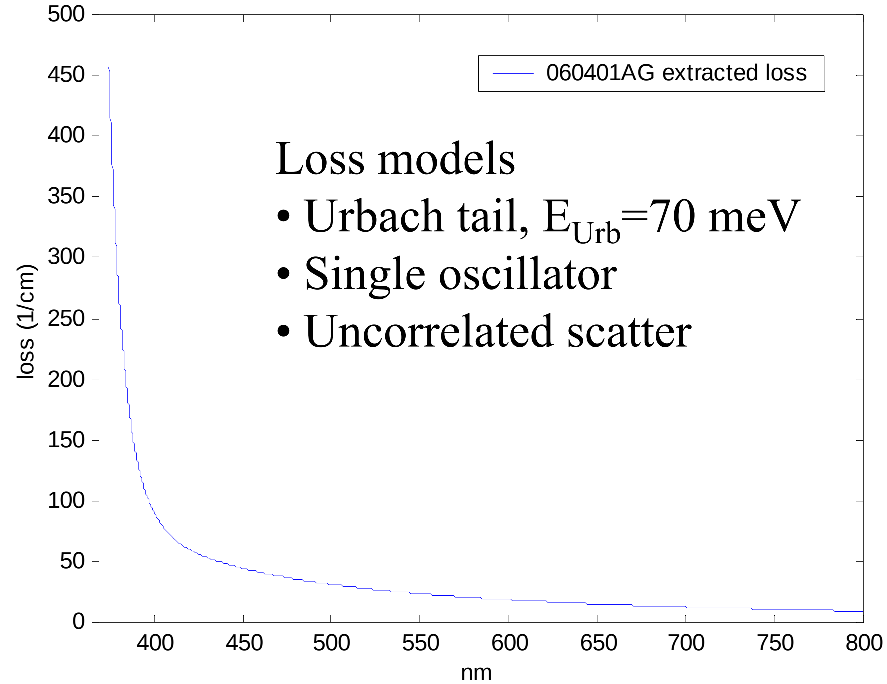
  T=exp(-2αd) = 0.85 at 400nm

  α(400 nm) $\cong$ 900 cm^{-1}

  bad scattering

GaN Template Loss from Spectral Transmission

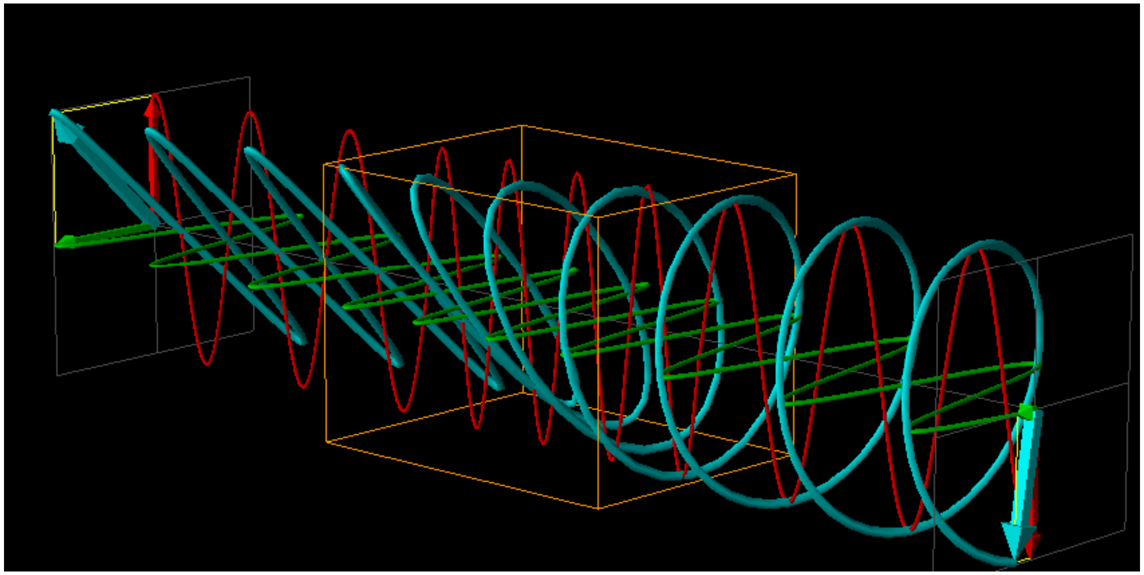




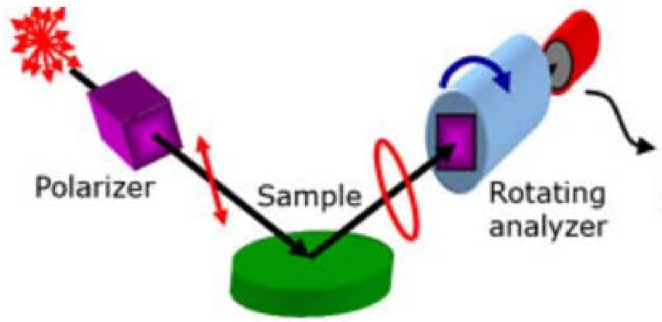
• Careful model fitting reveals thickness, real index, and loss

Ellipsometry

Analyze the change in ellipticity of light to understand the material



Ellipsometry



Complex reflectance ratio, ρ

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

- 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 ρ

Model Fitting

- In general, ρ cannot be inverted to obtain optical constants
- Build model and fit to data

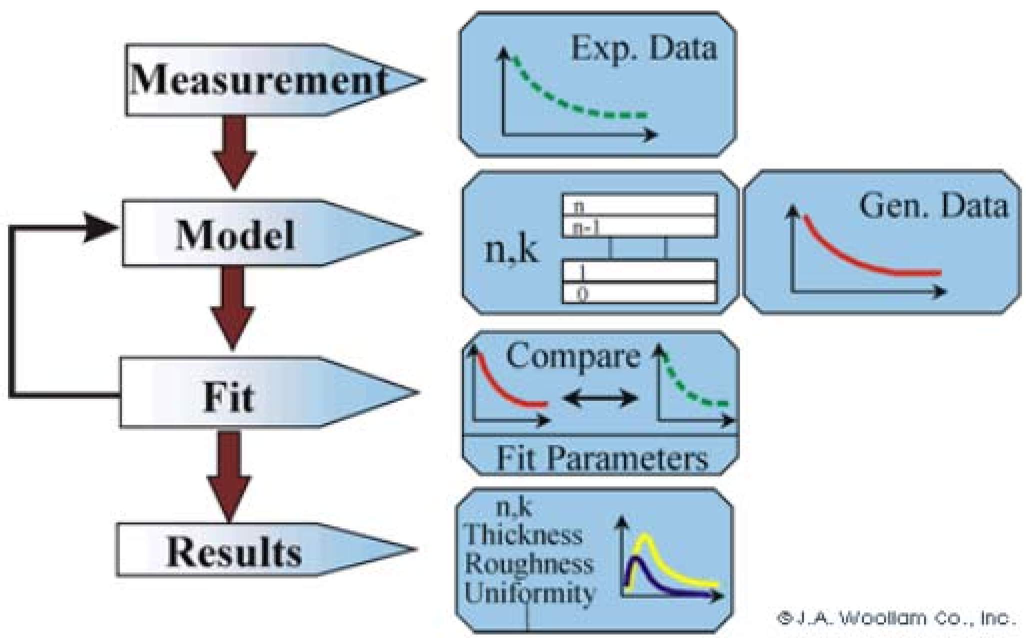


Figure 10 Flowchart for ellipsometry data analysis.

Common Material Models

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

- Cauchy: Purely empirical, diverges at short λ

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

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

$$\varepsilon_{1,\text{offset}} + \frac{AE_c}{E_c^2 - E^2 - \mathrm{i}BE}$$

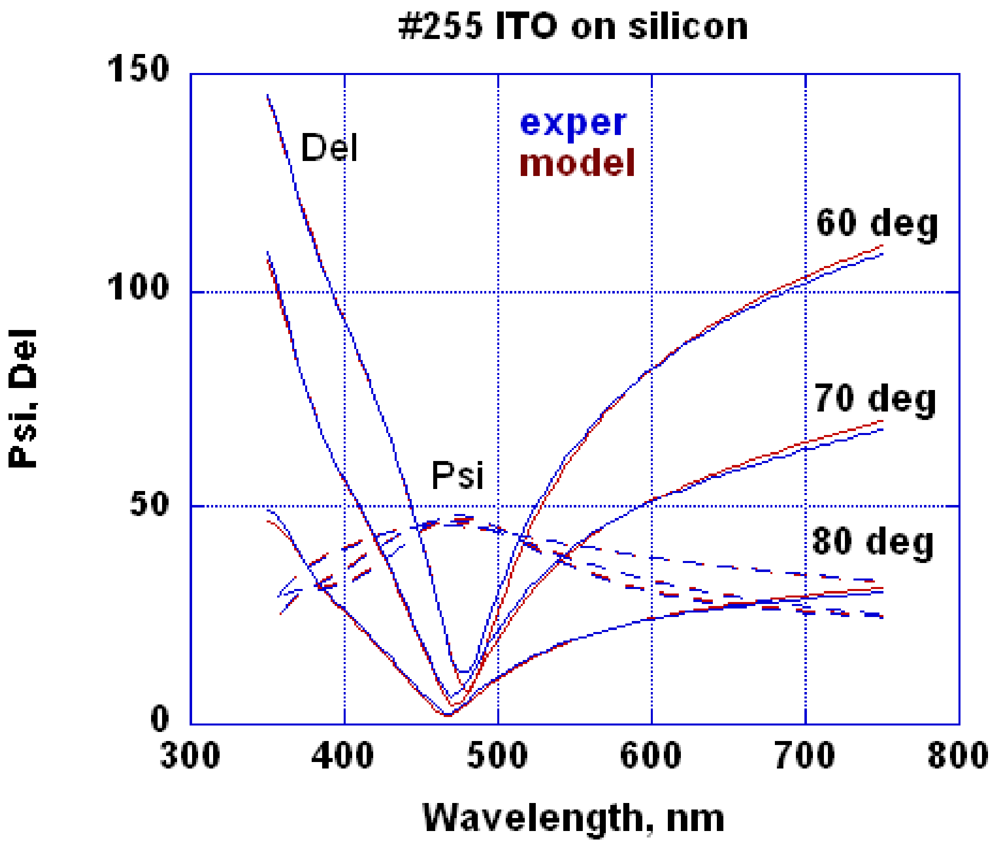
- Lorentz Oscillator: Some physical basis and reasonable response above band edge

Complications in Ellipsometry

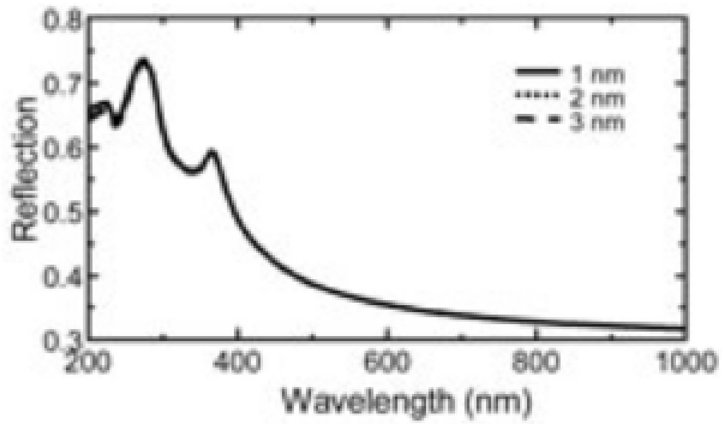
- Ψ and Δ are periodic in $\lambda/2$: need an estimate of thickness or index
- Reflections from back surface of transparent substrate
- Scattering from surface roughness or buried layers
- Birefringence
- Free carrier absorption
- (Sound familiar, Nitride folks?)

- Collect more data and build more sophisticated model

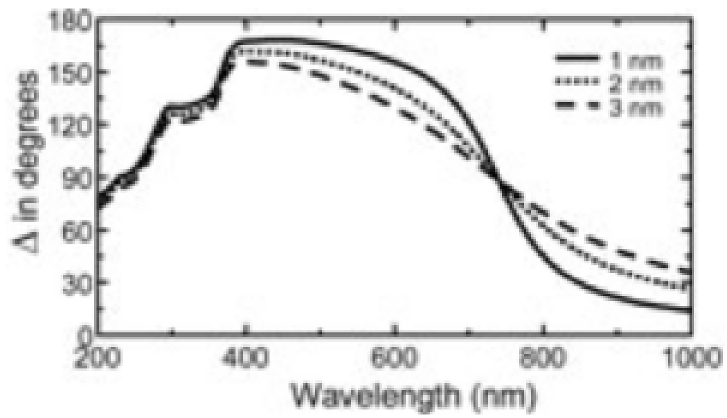
Variable Angle Spectroscopic Ellipsometery



Thickness Sensitivity



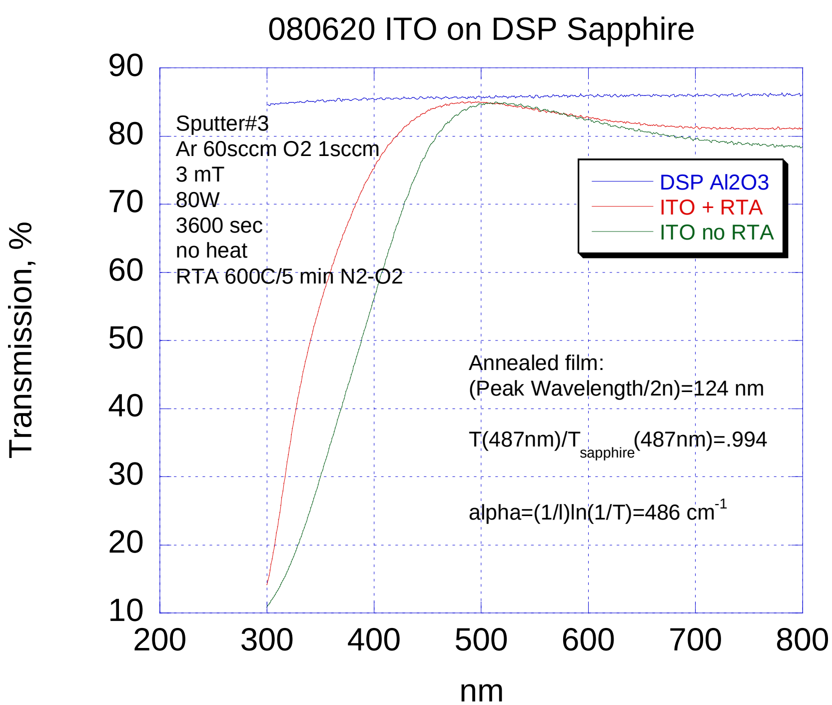
Power Reflectivity

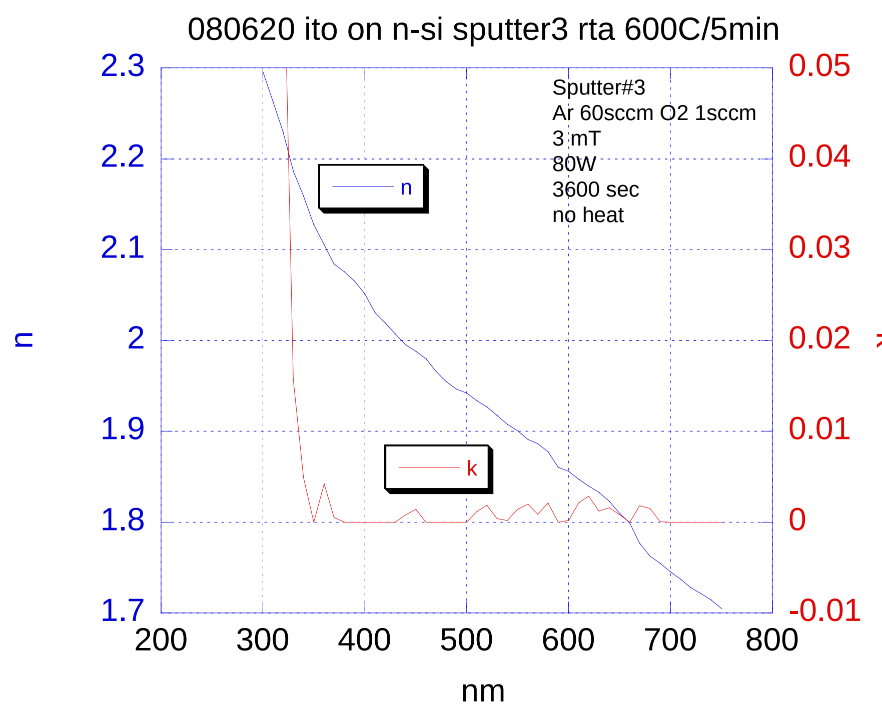


Phase, Δ

- 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





$k(500\text{nm}) = 1\text{E-}3$

$\alpha(500\text{nm}) = 314\ \text{cm}^{-1}$

Credits

- www.jawoollam.com
- www.wikipedia.com
- www.filmetrics.com