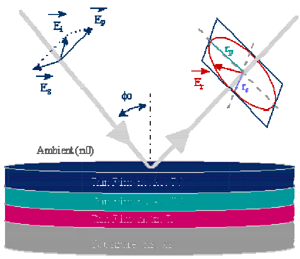
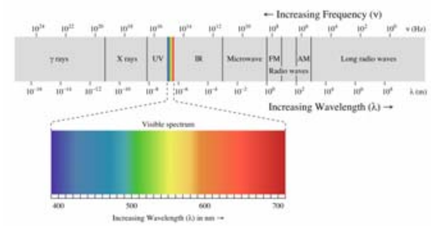
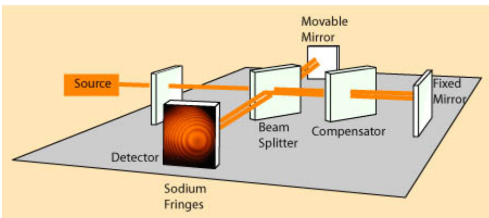



# Phys 774: Ellipsometry

Fall 2007



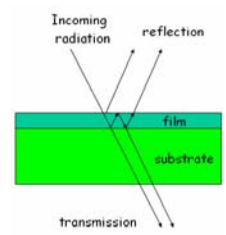



## Dielectric function

- Optical vibrations (phonons)
- Free electrons (plasma)
- Electronic transitions (valence → conduction band)
- Dielectric function and refractive index are generally complex:

$\varepsilon_r = \varepsilon_r' + i\varepsilon_r''$ ; ; $\varepsilon_r' = n_R^2 - n_I^2$ ; $\varepsilon_r'' = 2n_R n_I$

absorption coefficient $\alpha = 2k_0 n_I$ $n_I$ - extinction coefficient




$$\chi_1(\omega) = \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} d\omega' \frac{\chi_2(\omega')}{\omega' - \omega}$$

and

$$\chi_2(\omega) = -\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} d\omega' \frac{\chi_1(\omega')}{\omega' - \omega}.$$

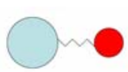
$$\mathcal{R} = \left|\frac{1 - \tilde{N}_{\text{complex}}}{1 + \tilde{N}_{\text{complex}}}\right|^2 = \frac{(1-\tilde{n})^2 + \tilde{k}^2}{(1+\tilde{n})^2 + \tilde{k}^2}$$

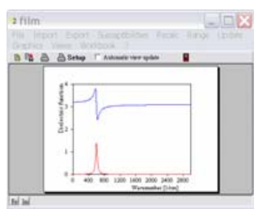


## Dielectric function contributions

$$\varepsilon(\omega) = 1 + \chi_{Ph}(\omega) + \chi_{FC}(\omega) + \chi_E(\omega) = \varepsilon_\infty + \chi_{Ph}(\omega) + \chi_{FC}(\omega)$$

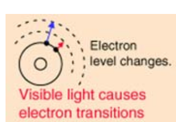
$$\chi_{ph}(\omega) = \sum_j \left( \frac{S_j^{\,2}}{\omega_{TO_j}^2 - \omega^2 + i\omega\gamma_j} \right)$$





$$\chi_{FC}(\omega) = \frac{\Omega_p^{\,2}}{-\omega^2 + i\omega\gamma} \qquad \Omega_p^{\,2} = \frac{ne^2}{\varepsilon_0 m^*}$$

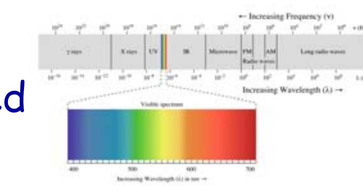
$$\chi_E(\omega) = \sum_j \frac{P_j^{\,2}}{\omega_{0j}^2 - \omega^2 + i\omega\gamma_j}$$






## Spectroscopic Measurements in IR

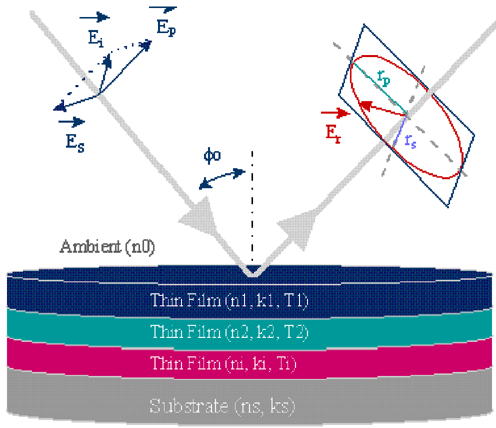
Fourier Transform Infra-Red Spectroscopy



ELLIPSOMETRY $30 - 10000\ \text{cm}^{-1}$

- Technique that determines the change in polarization state of light reflected from a sample.
- Typically used for characterizing thin films, strongly correlated materials.
- Used in a wide range of industrial applications.
- Non contact, non destructive method.

## Principles and goals of Ellipsometry




$$\rho = \frac{r_p}{r_s}$$

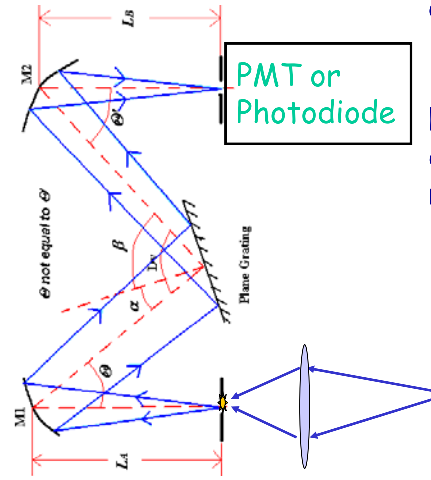
$\phi_0$ variable

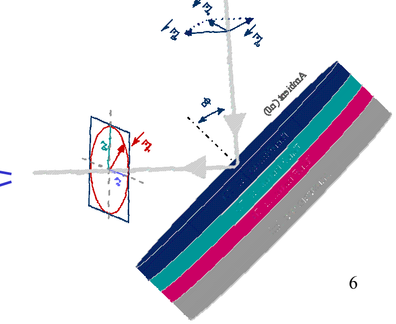
Ellipsometry:

Linear polarized light is incident on the sample under an angle $\phi_0$ and polarization of the reflected light is measured.



## Ellipsometry and Grating Spectrometers



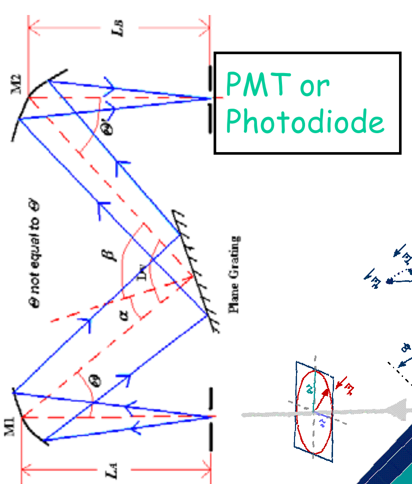



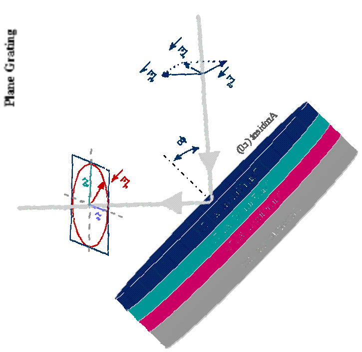
Disadvantages:
Cannot use lenses due to Depolarization effects

Normalization is difficult due to complicated response of the grating



## Ellipsometry and Grating Spectrometers



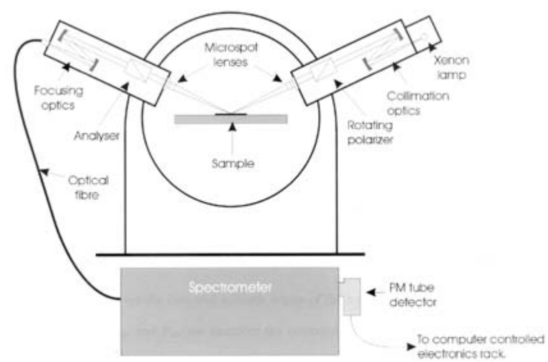
Disadvantages here ?

Resolution decreases if we cannot illuminate all groves of the grating

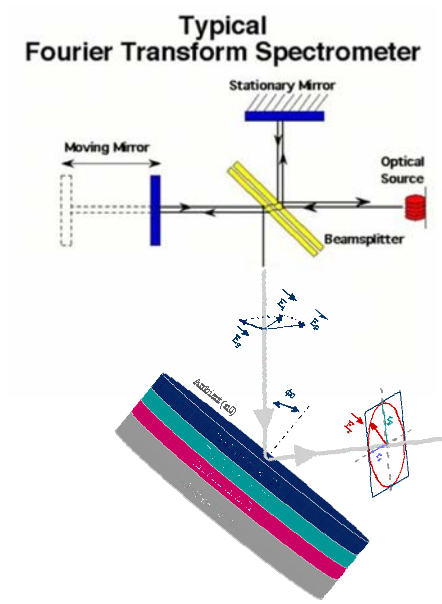


# Spectroscopic Ellipsometer SOPRA GESP5

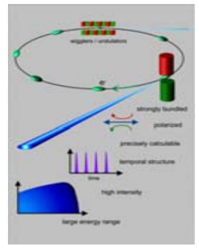
- SOPRA variable angle spectroscopic ellipsometer GESP5

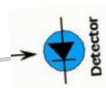


# FT-IR Ellipsometry




Advantages:
1. Multiplexing
2. Throughput (no slits needed)






IR-bolometer



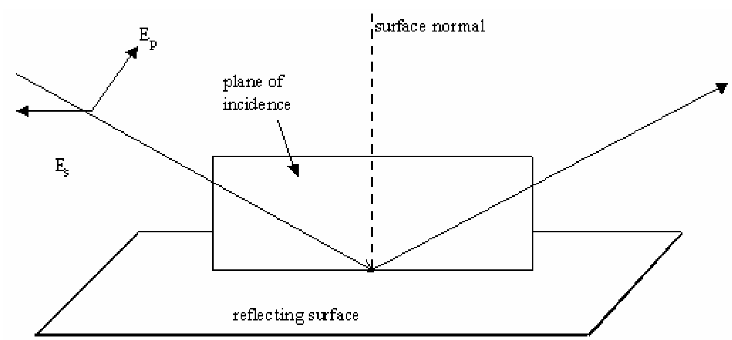
# Types of Ellipsometer

- Ellipsometers may be single wavelength or spectroscopic
- They may operate as rotating element or as nulling ellipsometers
- They may be single point or imaging



# Plane of Incidence

- Plane of incidence of light is the plane containing the normal to the sample surface and the incident direction of light.
- The *s*-plane is perpendicular to the plane of incidence.
- The *p*-plane is parallel to the plane of incidence.





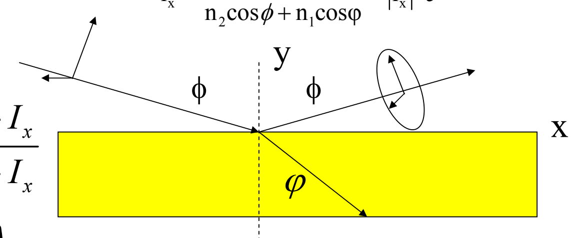

# Fresnel's Equations

- Fresnel's equations give the complex amplitude of the reflected light

$$r_y = \frac{n_1\cos\phi - n_2\cos\varphi}{n_1\cos\phi + n_2\cos\varphi} = |r_y| \cdot e^{i\delta_y}$$

$$r_x = \frac{n_2\cos\phi - n_1\cos\varphi}{n_2\cos\phi + n_1\cos\varphi} = |r_x| \cdot e^{i\delta_x}$$

$$Polarization \equiv P = \frac{I_y - I_x}{I_y + I_x}$$




Jones Formalism

$$E^{Jones}{}_{linear} = E_0 \begin{bmatrix} \cos\alpha \\ \sin\alpha \end{bmatrix}$$

$$E^{Jones}{}_{circular} = E_0 \begin{bmatrix} 1 \\ i \end{bmatrix}$$

Optical elements (polarizers, mirrors, etc)

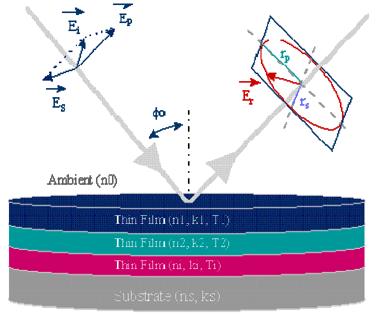
$$J^{Jones} = \begin{bmatrix} J_{11} & J_{12} \\ J_{21} & J_{22} \end{bmatrix} \qquad \begin{bmatrix} E_x \\ E_y \end{bmatrix} = \begin{bmatrix} J_{11} & J_{12} \\ J_{21} & J_{22} \end{bmatrix} \cdot \begin{bmatrix} E_{0x} \\ E_{0y} \end{bmatrix}$$

# Ellipsometric Equations

$$\varepsilon = \sin^2\phi_0 + \sin\phi_0 \cdot \tan^2\phi_0 \cdot \left[\frac{1-\rho}{1+\rho}\right]$$

$$\rho = \frac{r_p}{r_s} = \tan\Psi \cdot e^{i\Delta}$$

$\phi_0$ variable, $\tan\Psi = \left|\frac{r_p}{r_s}\right|$, $\Delta = \delta_p - \delta_s$




$\varepsilon$ is a function of frequency (energy)
in real experiment we need to connect
$\rho$ with the polarizer angles of the instrument
using, e.g., Jones matrices

Pseudo-dielectric function, which coincides with
"dielectric function" for uniform and isotropic bulk materials
Anisotropy can be measured directly by changing $\phi_0$



# What does an ellipsometer measure?

- The polarization change of light reflected from a sample in terms of two parameters Δ and Ψ
- These values are related to the ratio of the Fresnel reflection coefficients for *p*- and *s*- polarized light

$$\frac{r_p}{r_s} = \tan\Psi \cdot e^{i\Delta}$$

- This ratio is complex
- tanΨ measures the ratio of the modulus of the amplitude reflection ratio
- The phase difference between *p*- and *s*-polarised reflected light is given by Δ



# What can ellipsometry tell us about samples?

- Taken on there own values of Δ and Ψ tell us little about a sample.
- We take the measured values of Δ and Ψ, typically as a function of wavelength and angle of incidence (Variable Angle Spectroscopic Ellipsometry).
- An optical model is then built using as much information about the sample as possible

# What cannot be directly determined from ellipsometry measurement?

Multilayer sample structure (it is not a forensic tool)



# Select the model and Optical Functions

The optical model will generally consist of

- The thickness of a film or layer
- The complex refractive index

$$N = n_r - in_i$$

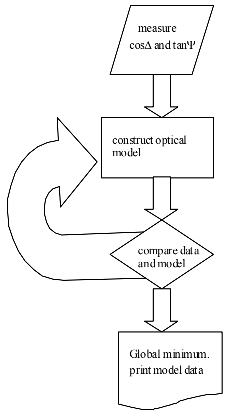
Sometimes, the complex dielectric constant $\varepsilon = \varepsilon_r - i\varepsilon_i$ is given, where

$$N^2 = \varepsilon$$

- For a Mixture of materials use the Effective Medium Approximation

# Extracting data in ellipsometry

- Acquire data of spectral range and angle of incidence required
- Build an optical model that describes sample structure.
- Generate theoretical data from optical model.
- Compare experimental and theoretical data
- Vary model parameters, such as film thickness, until a "best fit" to experimental data is obtained.






# Regression

- Regression algorithms are used to vary unknown parameters and minimize the difference between model and experimental data.
- The Levenberg-Marquardt algorithm is the most widely used.

The algorithm seeks to minimise the function

$$\chi = \sqrt{\frac{1}{2N - M} \sum_{N} \left\{ \left( \tan\psi_{\text{measured}} - \tan\psi_{\text{model}} \right)^2 + \left( \cos\Delta_{\text{measured}} - \cos\Delta_{\text{model}} \right)^2 \right\}}$$

where N is the number of data points at the different measured wavelengths and M the number of model parameters.



# Fit the data
# Regression Analysis

- The data are then compared with the data generated from the theoretical model.
- Unknown parameters in the optical model, such as film thickness or optical constants, are varied to try to produce a "best fit" to experimental data.
- Regression algorithms, such as Levenberg-Marquadt, are used to vary unknown parameters and minimize the difference between experimental and model-generated data.
- Physical parameters are obtained once a good fit is achieved.



# Advantages of Ellipsometry

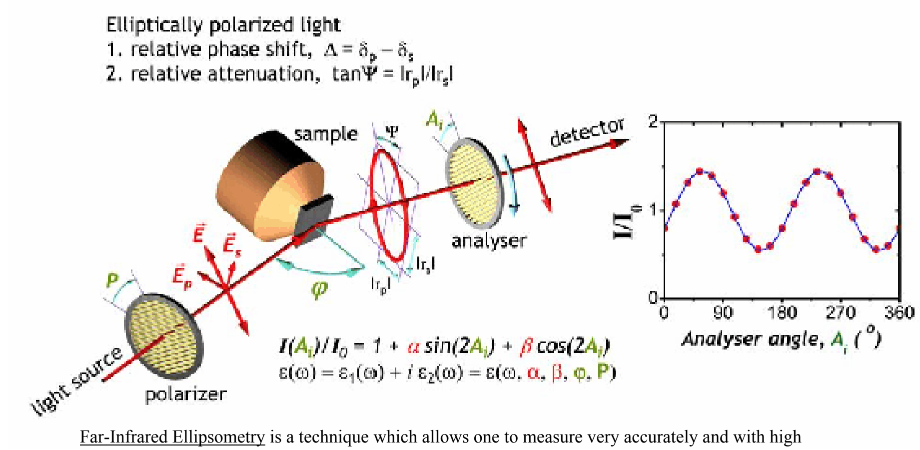
- It measures the ratio of two values so is highly accurate and reproducible, does not need a reference sample, and is not so susceptible to light source fluctuation
- Since it measures phase, it is highly sensitive to the presence of ultra-thin films (down to sub-monolayer coverage).
- It provides two pieces of data at each wavelength. More film properties can be determined.

# Some applications of Ellipsometry:

- Data storage:
  - Characterization of thin films used the manufacturing of storage media
- Display technology:
  - Characterisation of materials used in flat panel displays
- Optical coatings:
  - Study of coatings on filters, beam splitters and other optical components.
- Biology / Chemistry:
  - Study of organic semiconductors, and tissue samples.
- In-situ measurement:
  - Allows real time monitoring of etching and thin film deposition processes.



# What is far-IR Ellipsometry?

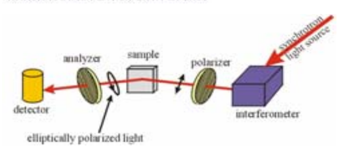



Far-Infrared Ellipsometry is a technique which allows one to measure very accurately and with high reproducibility the complex dielectric function $\varepsilon(\omega) = \varepsilon(\omega)_1 + i\,\varepsilon(\omega)_2$ of oxide thin films and single crystals. It measures the change in polarization of Infrared light upon non-normal reflection on the surface of a sample to be studied. To extend the Ellipsometry technique to the Far-Infrared part of the electromagnetic spectrum, we are going to carry out these experiments at Brookhaven National Laboratory, National Synchrotron Light Source. Synchrotron light provides three orders of magnitude more brilliant light in the Far-Infrared as compared to conventionally available light sources, like mercury arc lamps.

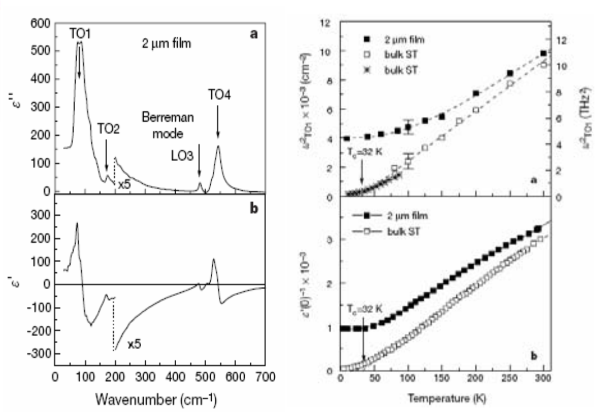


## Example of far-IR spectroscopic Ellipsometry: Hardening of the soft modes in $SrTiO_3$ thin films

NSLS
NATIONAL SYNCHROTRON LIGHT SOURCE



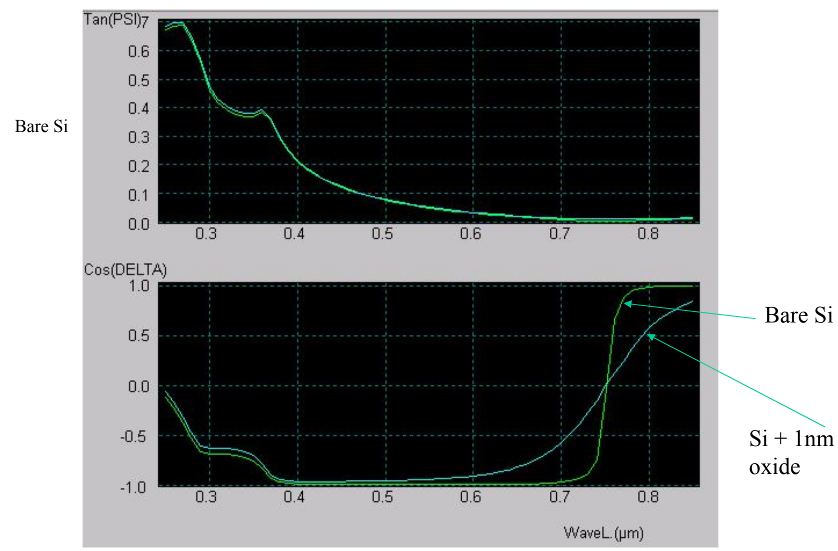

Ellipsometry of $SrTiO_3$ thin films




*A.A. Sirenko, et al., Nature* **404**, 373 (2000)



# Another example: Sensitivity to thin film

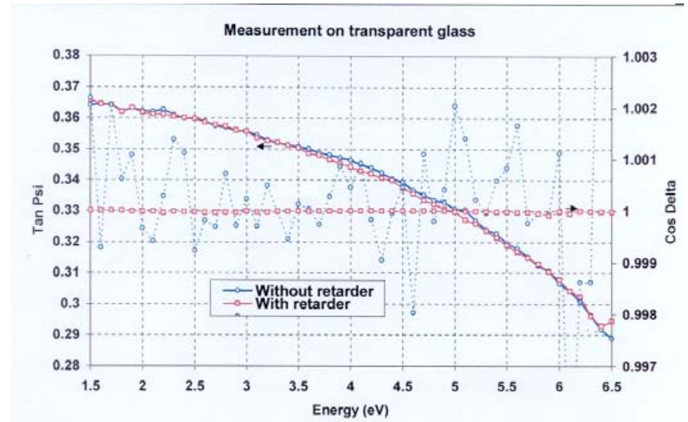


# Problems with transparent samples

- The error in $\Delta$ is proportional to cosec $\Delta$
- For transparent samples, $\Delta \sim 180^0$
- This can be overcome by placing a retarder in front of the light source to introduce a phase shift into the light.
- Alternatively, a rotating compensator ellipsometer could be used

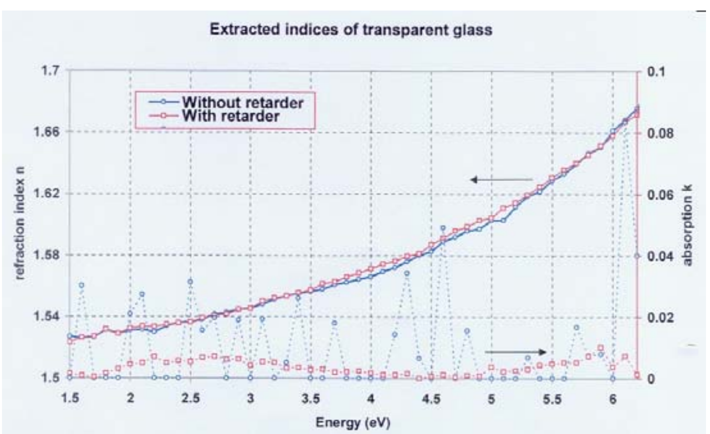


# Problems with transparent samples



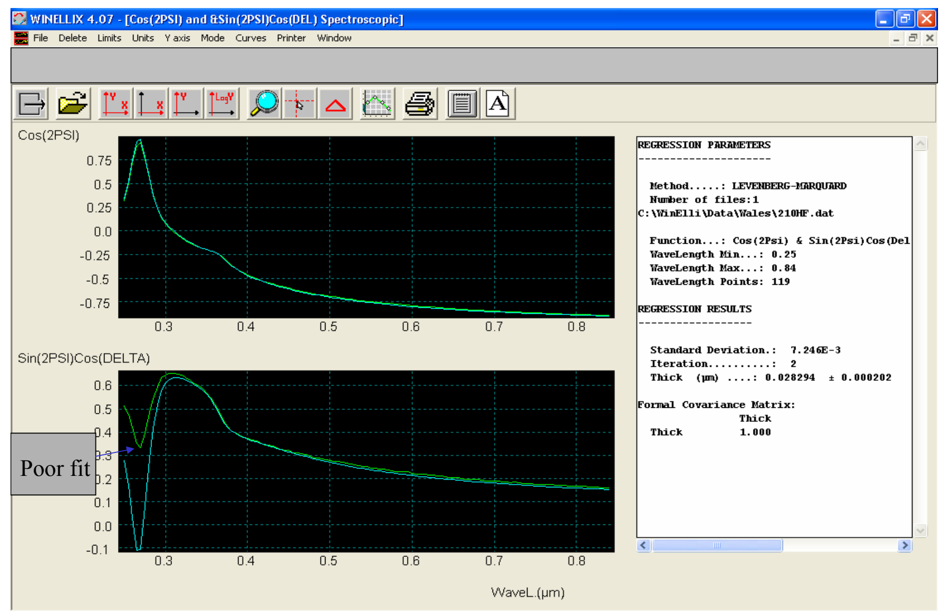



# Problems with transparent samples

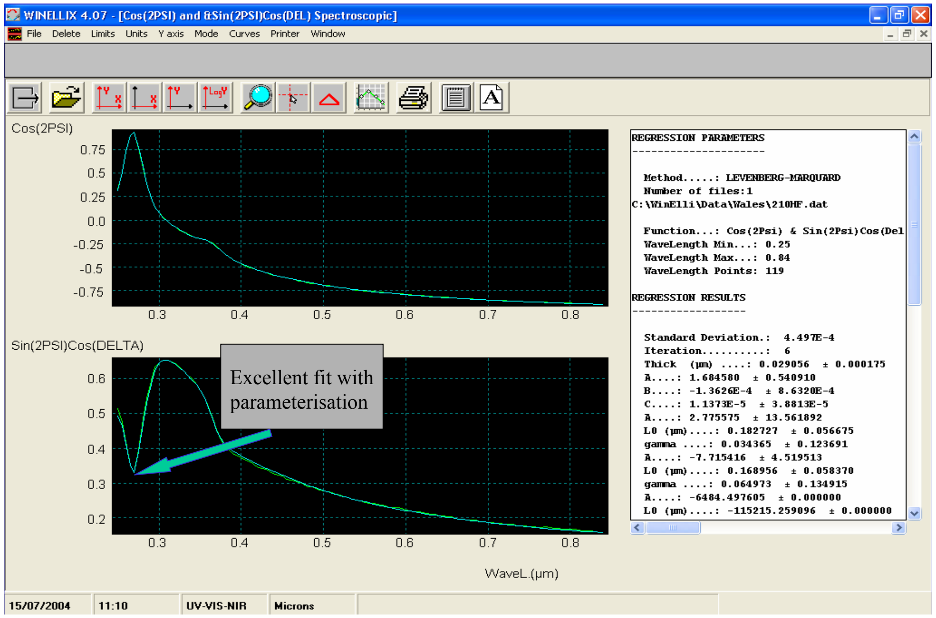




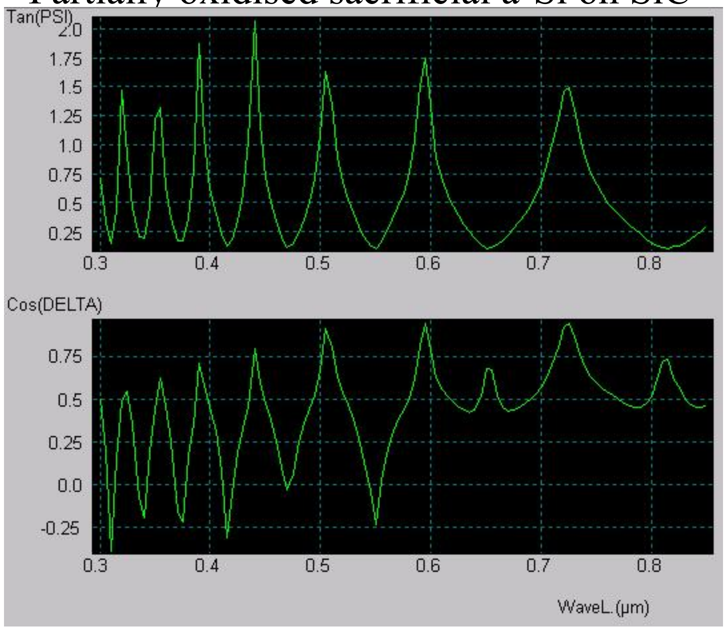

# Hafnium oxide on silicon



# Hafnium oxide on silicon




# Partially oxidised sacrificial a-Si on SiC






# Partially oxidised sacrificial a-Si on 4H-SiC

- Model ($SiO_2$ database – aSi Forouhi)

$SiO_2$ (1.41176 µm)

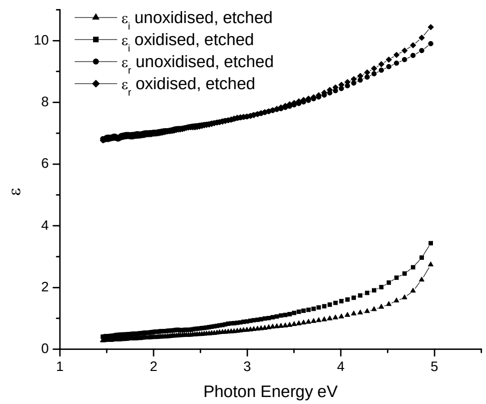
aSi + $SiO_2$ with density gradient (27.92 nm)

aSi (64.7 nm)

SiC substrate



# Ellipsometry of conventionally grown oxide on 4H-SiC



# Very thin films

- For films of thickness about 10 nm or less, there exists a correlation between thickness and refractive index
- Complementary techniques must be used to measure some parameters, usually thickness.
- GIXR employed



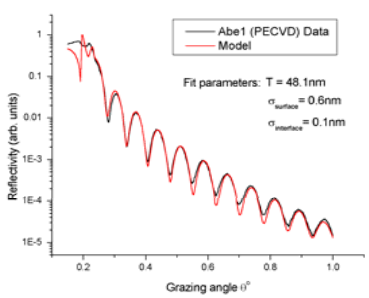
# Grazing Incidence X-ray Reflectometry

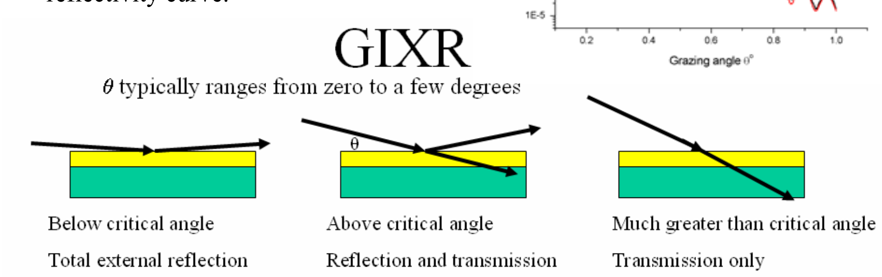
- X-rays used in XRR have wavelengths of the order of 1Å. Since the refractive index of materials at these short wavelengths is slightly less than unity, x-rays are totally externally reflected at angles of incidence typically up to a few tenths of a degree.
- As the incidence angle increases above the critical angle for total reflection, x-rays penetrate the layers of the material.



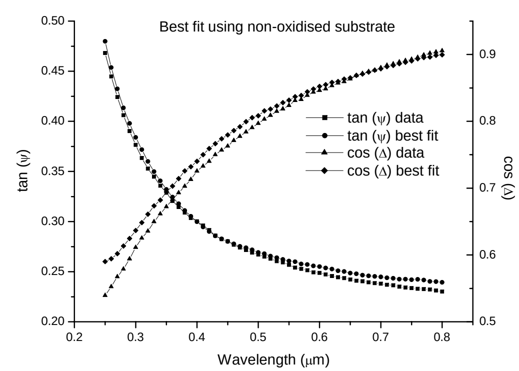
# Grazing Incidence X-ray Reflectometry vs. Ellipsometry

- At the interface between each layer, some of the radiation is reflected to the layer above, while some is transmitted (refracted) to the layer below.
- The wave interference produces a series of fringes in the reflectivity curve.
- Layer densities, thickness and interface roughness can be determined from the reflectivity curve.

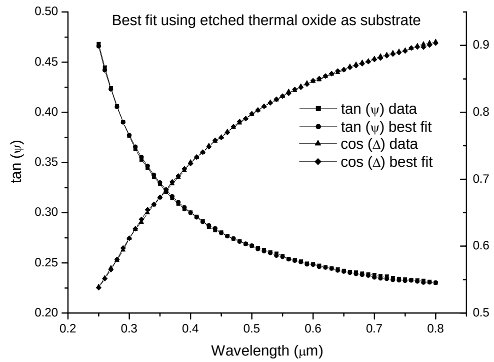



# Ellipsometry of conventionally grown oxide on 4H-SiC



# Ellipsometry of conventionally grown oxide on 4H-SiC






# Another example:

# Comparison of XTEM and Spectroscopic Ellipsometry