Spectroscopic Ellipsometry:

What it is, what it will do, and what it won’t do

by

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- Introduction
- Fundamentals
- Anatomy of an ellipsometric spectrum
- Analysis of an ellipsometric spectrum
- What you can do, and what you can’t do

Perspective

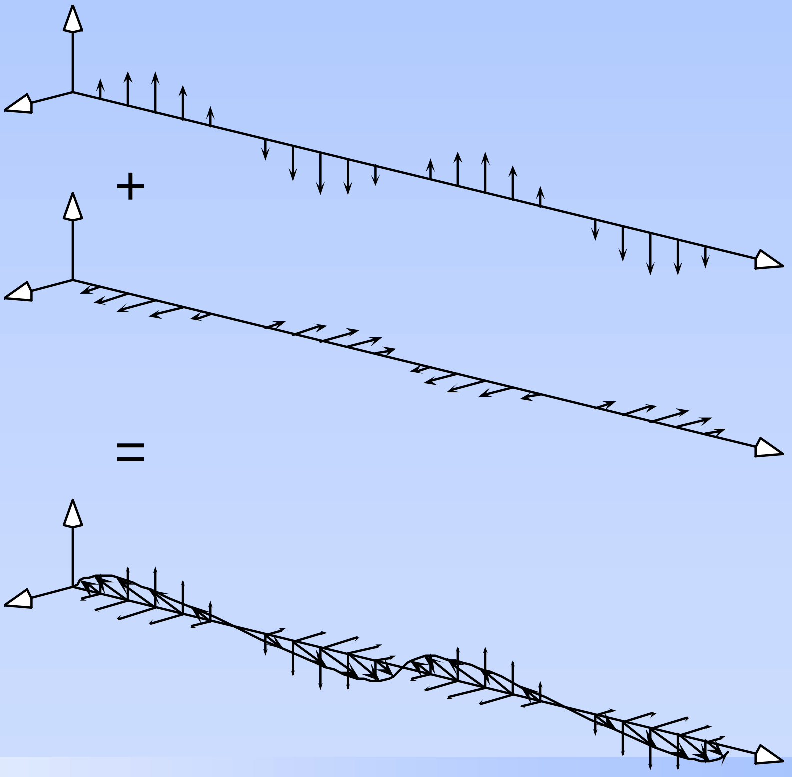
- Spectroscopic Ellipsometry is an optical technique used for analysis and metrology

- A light beam is reflected off of the sample of interest
- The light beam is then analyzed to see what the sample did to the light beam

- We then draw conclusions about the sample
  - thickness
  - optical constants
    - microstructure
- Model based
  - <u>all</u> measurement techniques are model based

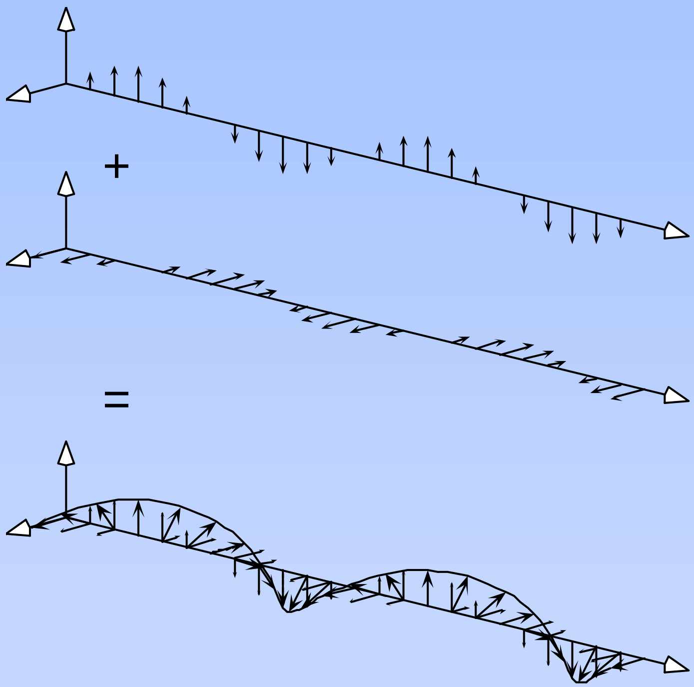
Polarized Light

- The Name
  - “Ellipsometry” comes from “elliptically polarized light”
  - better name would be “polarimetry”



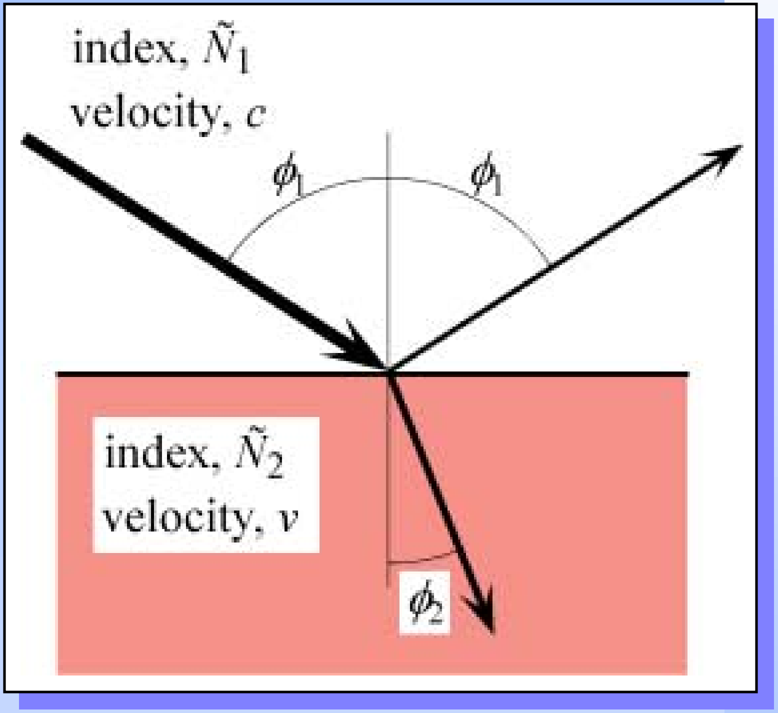
- Linearly Polarized
  - combining two light beams in phase, gives *linearly polarized light*

Polarized Light (continued)



- Elliptically Polarized
  - combining two light beams <u>out of phase</u>, gives *elliptically polarized light*
- Two ways
  - pass through a retarder
  - reflect off a surface
    - absorbing material
    - substrate with film

Laws of **Reflection and Refraction**



- Reflection

$$\phi_{\mathrm{i}} = \phi_{\mathrm{r}}$$

- Refraction (Snell's law)
  - for dielectric, i.e. *k* = 0

$$n_1 \sin \phi_1 = n_2 \sin \phi_2$$

  - in general

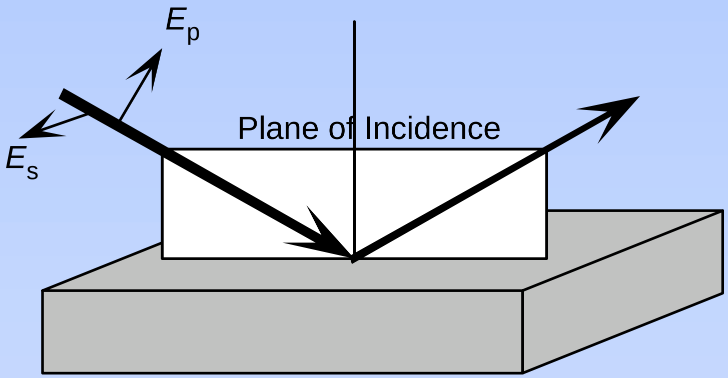
$$\tilde{N}_1 \sin \phi_1 = \tilde{N}_2 \sin \phi_2$$

  - sine function is complex
  - corresponding complex cosine function

$$\sin^2 \phi_2 + \cos^2 \phi_2 = 1$$

Reflections (orientation)

- Electric Field Vector
- Plane-of-Incidence
    - incoming
    - normal
    - outgoing
- s-waves and p-waves
    - “senkrecht” and “parallel”



Equations of Fresnel

- Fresnel reflection coefficients, r_{12}^{p} r_{12}^{s}
  - complex numbers
- ratio of <u>Amplitude</u> of outgoing to incoming
- different for p-waves and s-waves

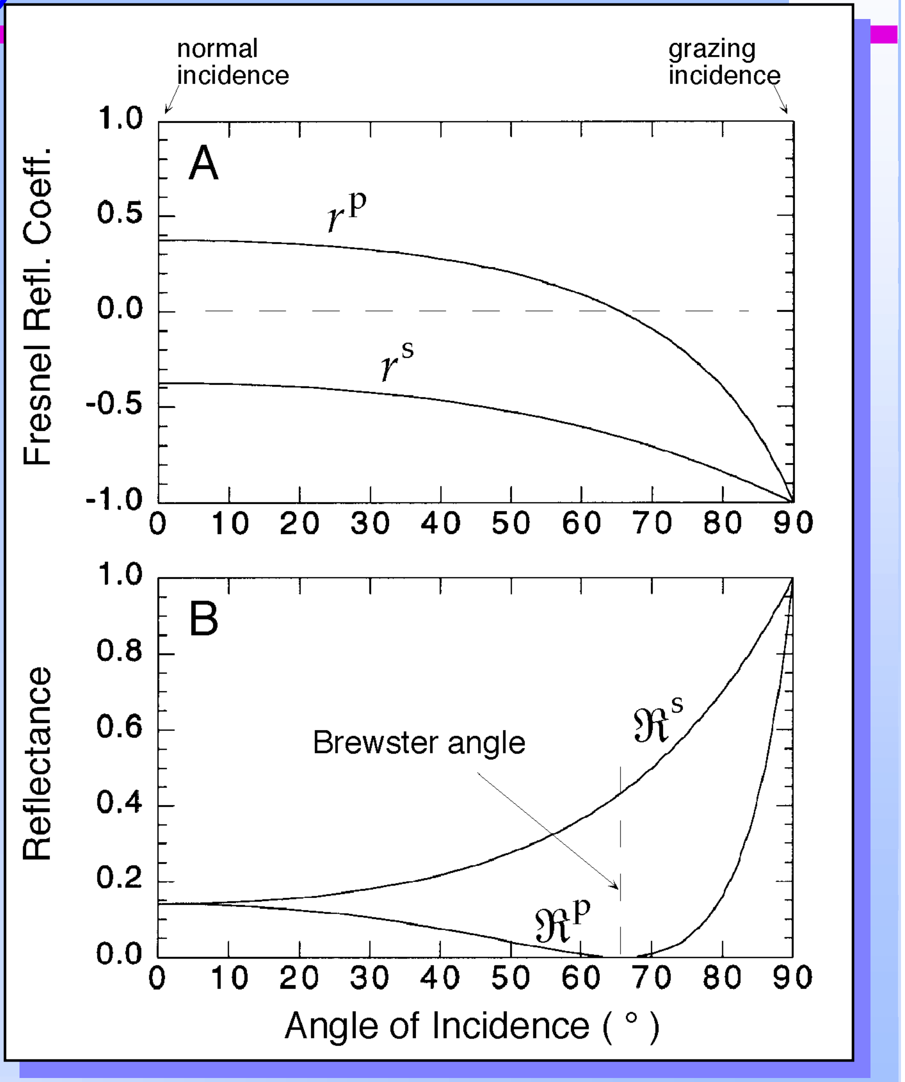
$$r_{12}^{\mathrm{p}} = \frac{\tilde{N}_2 \cos\phi_1 - \tilde{N}_1 \cos\phi_2}{\tilde{N}_2 \cos\phi_1 + \tilde{N}_1 \cos\phi_2} \qquad r_{12}^{\mathrm{s}} = \frac{\tilde{N}_1 \cos\phi_1 - \tilde{N}_2 \cos\phi_2}{\tilde{N}_1 \cos\phi_1 + \tilde{N}_2 \cos\phi_2}$$

- Reflectance $\Re$
  - ratio of <u>Intensity</u>
  - square of Amplitude
  - for a single interface

$$\Re^{p} = \left| r_{12}^{p} \right|^2 \qquad \Re^{s} = \left| r_{12}^{s} \right|^2$$

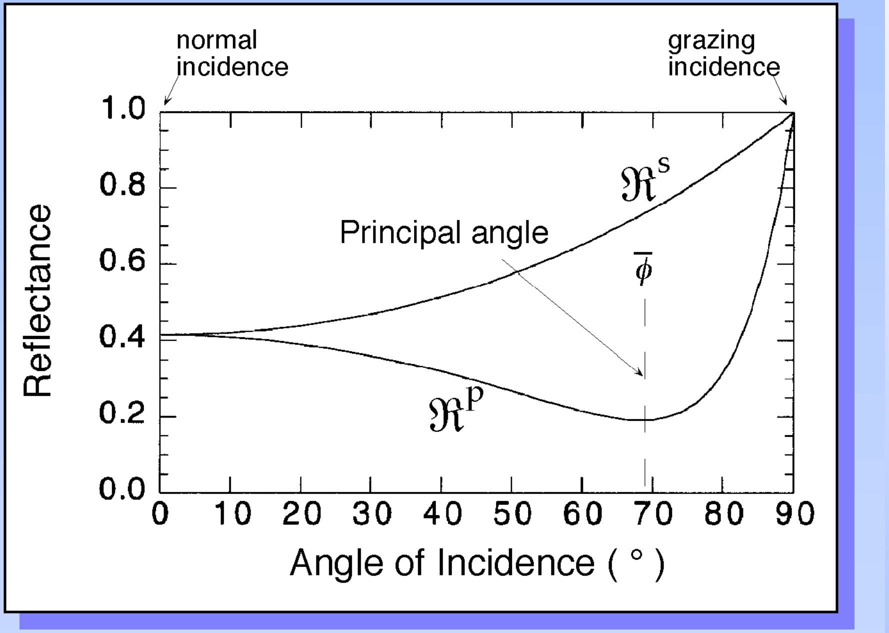
Brewster Angle (for dielectrics)

- r^s always negative and non-zero
- r^p passes through zero
- $\Re^p$ goes to zero
- The Brewster Angle
  - sometimes called the principal angle, polarizing angle
- Reflected light is s-polarized
- ramifications
  - $\tan \phi_B = \dfrac{n_2}{n_1}$
  - $\cos \phi_2 = \sin \phi_B$



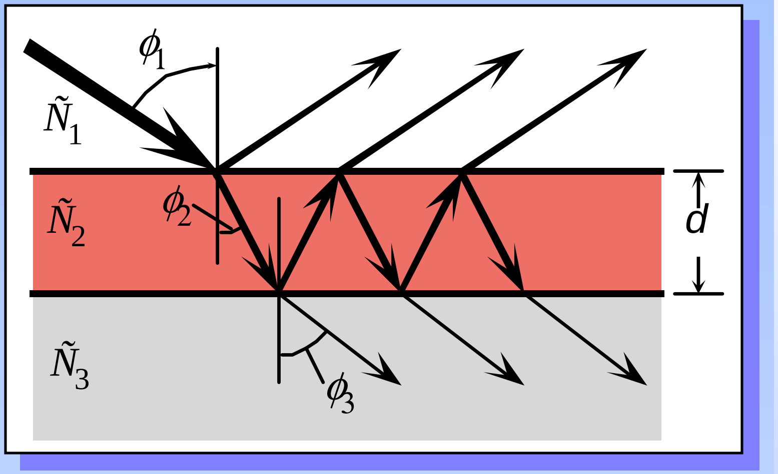
"Brewster" Angle, for metals

- if k is non-zero, r^{s} and r^{p} are complex
- cannot plot r^{s} and r^{p} vs angle of incidence
- However, we can still plot the Reflectance
- $\Re^{p}$ has a minimum, although not zero
- Actually called the "principal angle"



Reflections with Films

- Ellipsometry,
  - Amplitude, phase of outgoing vs incoming
- Reflectometry
  - Intensity of outgoing vs incoming
- Total Reflection Coefficient
  - corresponds to Fresnel Coefficients
  - complex number



$$R^{\mathrm{p}} = \frac{r_{12}^{\mathrm{p}} + r_{23}^{\mathrm{p}} \exp(-\mathrm{j}2\beta)}{1 + r_{12}^{\mathrm{p}} r_{23}^{\mathrm{p}} \exp(-\mathrm{j}2\beta)} \qquad R^{\mathrm{s}} = \frac{r_{12}^{\mathrm{s}} + r_{23}^{\mathrm{s}} \exp(-\mathrm{j}2\beta)}{1 + r_{12}^{\mathrm{s}} r_{23}^{\mathrm{s}} \exp(-\mathrm{j}2\beta)}$$

- β is phase change from top to bottom of film

$$\beta = 2\pi\left(\frac{d}{\lambda}\right)\tilde{N}_2 \cos\phi_2$$

Ellipsometry and Reflectometry definitions

- Reflectance $\Re^{p} = \left|R^{p}\right|^{2}$ $\Re^{s} = \left|R^{s}\right|^{2}$
- Delta, the phase difference induced by the reflection
  - if δ_1 is the phase difference before, and δ_2 the phase difference after the reflection then $\Delta = \delta_1 - \delta_2$
  - ranges from zero to 360º (or -180 to +180º)
- Psi, the ratio of the amplitude diminutions
  - ranges from zero to 90º

$$\tan \Psi = \frac{\left|R^{p}\right|}{\left|R^{s}\right|}$$

- The Fundamental Equation of Ellipsometry

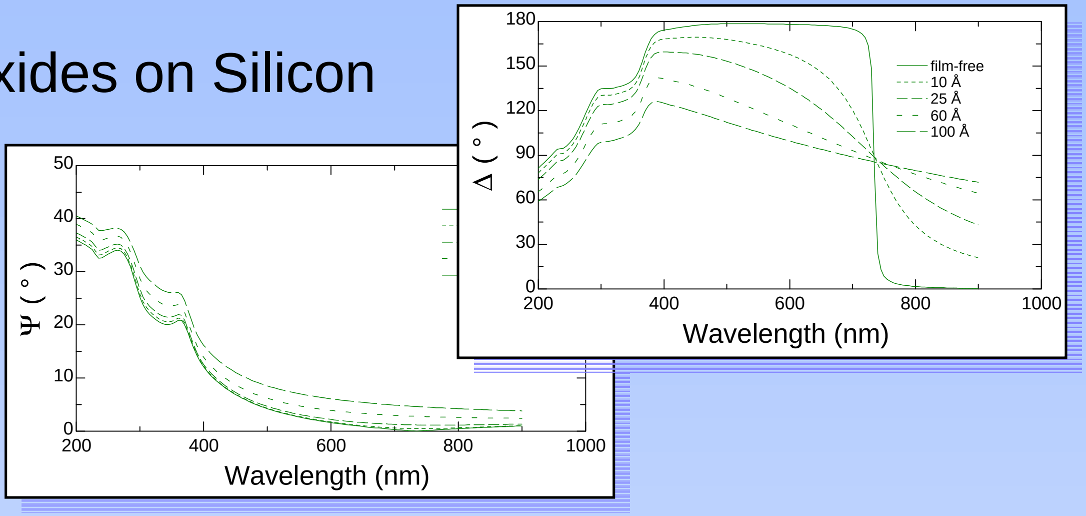
$$\rho = \frac{R^{p}}{R^{s}} \qquad \rho = \tan \Psi \, e^{j\Delta} \qquad \tan \Psi \, e^{j\Delta} = \frac{R^{p}}{R^{s}}$$

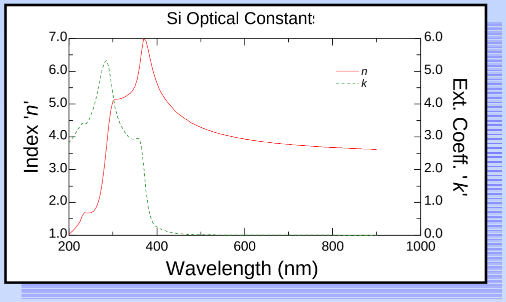
More Perspective

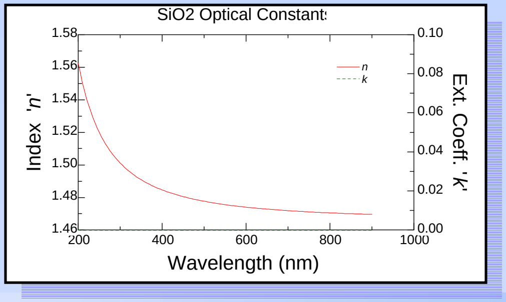
- Ellipsometers measure Δ and Ψ (sometimes only cos Δ)
  - Properties of the probing beam
- Quantities such as thickness and index of refraction are calculated quantities, based on a model.
  - Properties of the sample
- Values of Δ and Ψ are always correct
- Whether thickness and index are correct depend on the model
- Both precision and accuracy for Δ and Ψ
- Precision for thickness
- Accuracy,   ???

Examples

- Thin oxides on Silicon

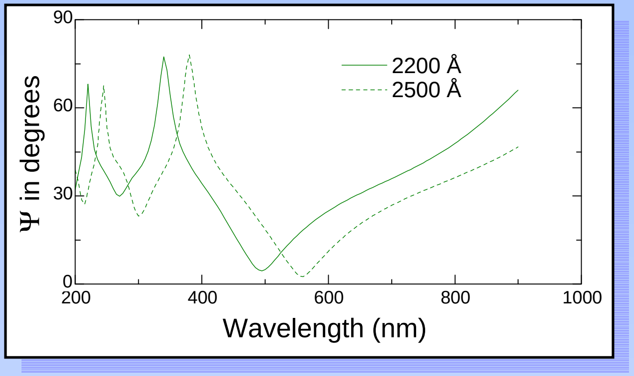


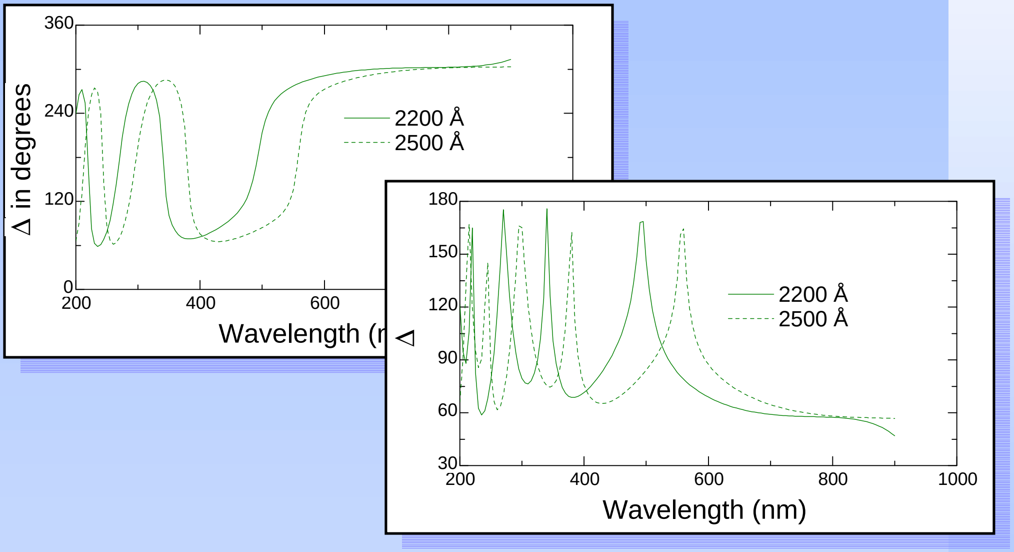


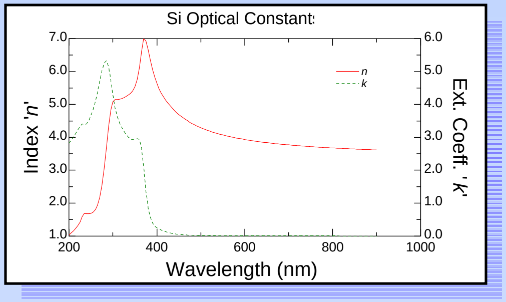


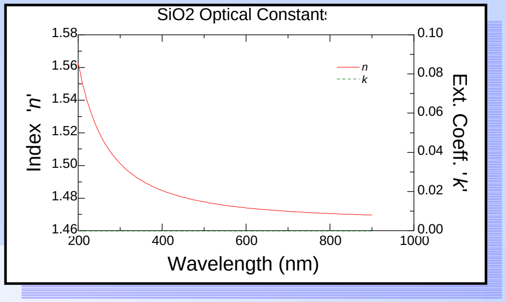
Examples

- Thicker oxide on Silicon





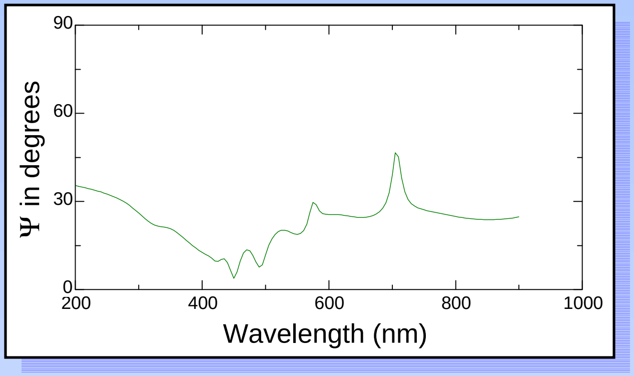


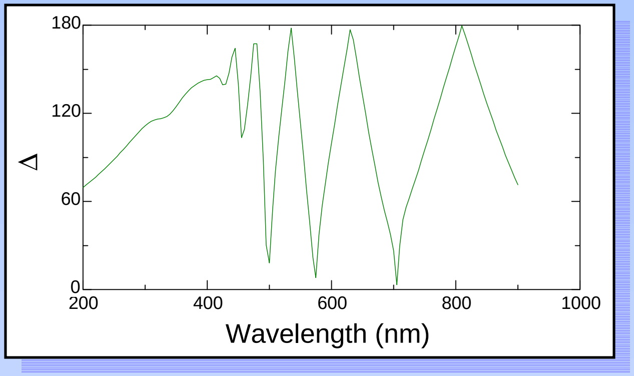


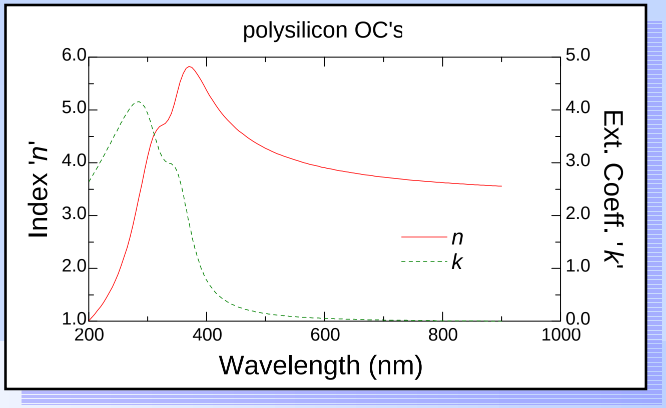
Examples

- Polysilicon on oxide on silicon

3	srough	25 Å
2	polysilicon	3000 Å
1	sio2	1000 Å
0	si	1 mm



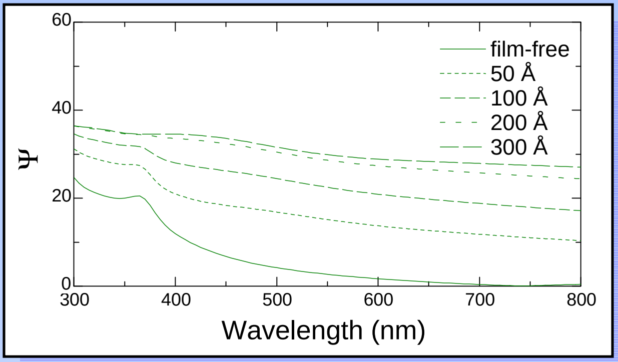


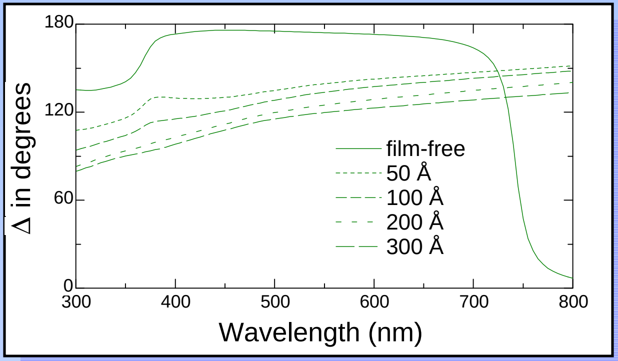


Examples

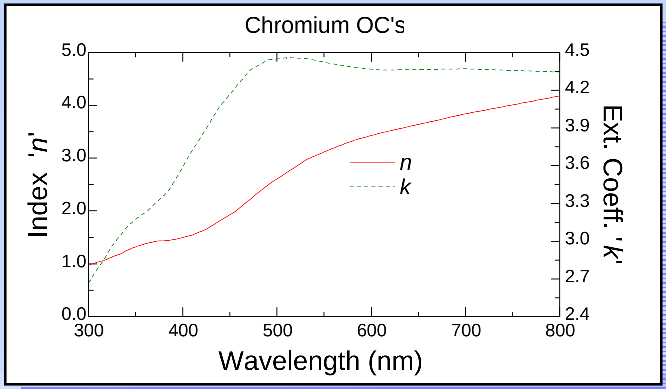
- Thin chromium on silicon

1	cr	300 Å
0	si	1 mm





- caveats

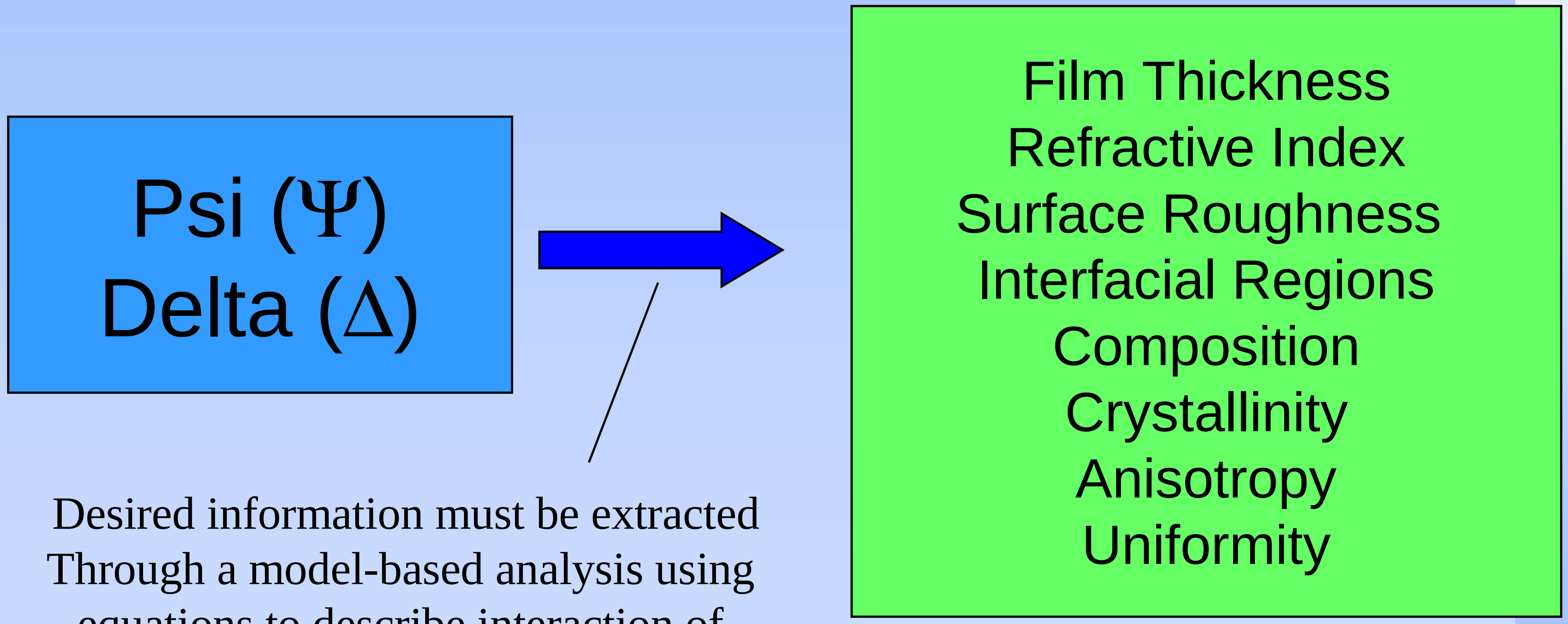


Determining Film properties from SE spectra

- Except for substrates, we cannot do a direct calculation

What Ellipsometry Measures:

What we are interested in:

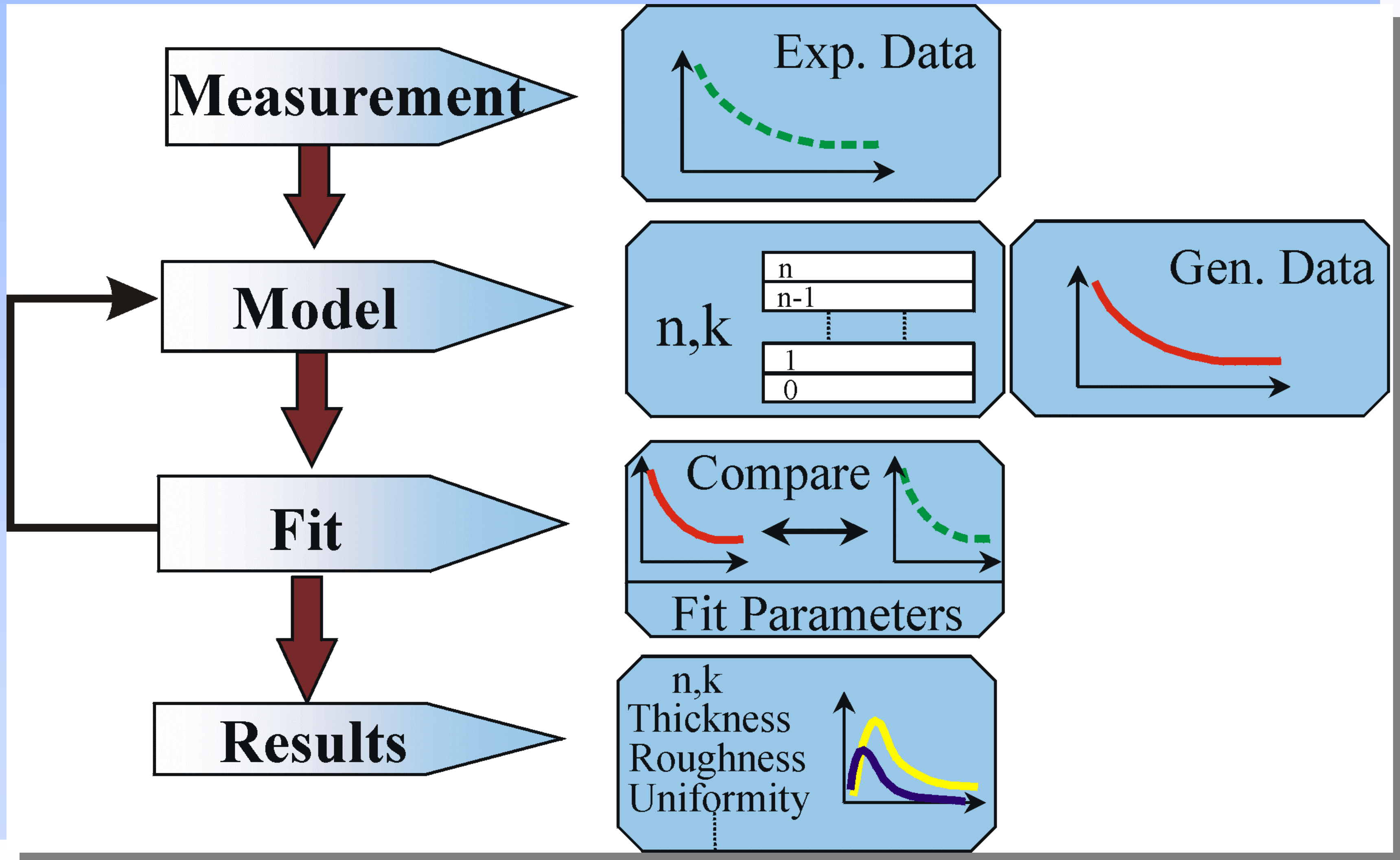


Psi (Ψ)
Delta (Δ)

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

Desired information must be extracted
Through a model-based analysis using
equations to describe interaction of
light and materials

How we analyze data:



Measurement

Exp. Data

Model

n,k

n
n-1
1
0

Gen. Data

Fit

Compare

Fit Parameters

Results

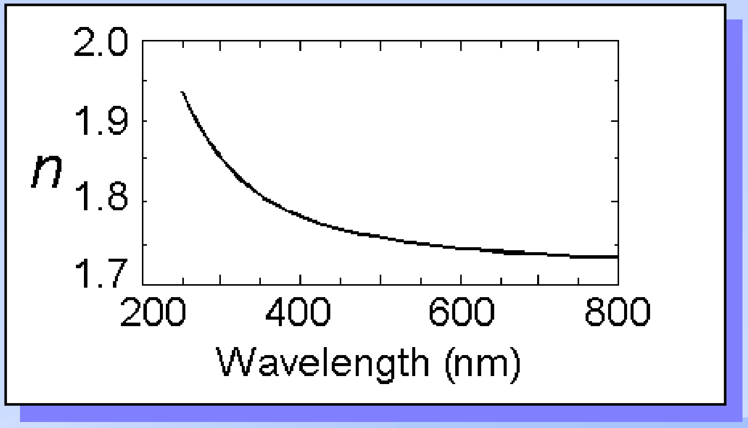
n,k
Thickness
Roughness
Uniformity

Building the model

- Optical Constants
  - Tabulated list
    - when OC’s are very well known
    - single-crystal
    - thermal oxide of Si, LPCVD nitride
  - Dispersion Equation
    - Cauchy equation
      - dielectrics, primarily
      - empirical
      - not K-K consistent

1	cauchy	0 Å
0	si	1 mm

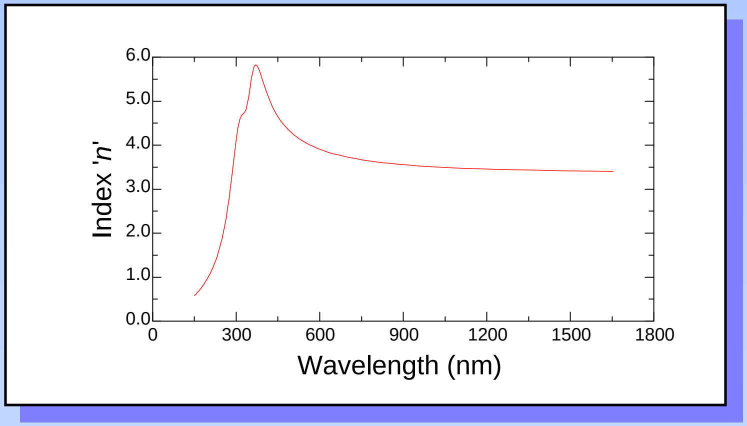
$$n(\lambda) = A_n + {}^{B_n}\!/_{\lambda^2} + {}^{C_n}\!/_{\lambda^4}$$

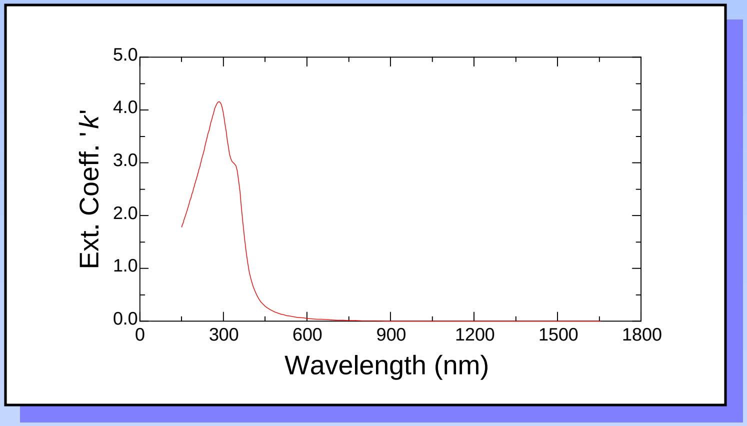


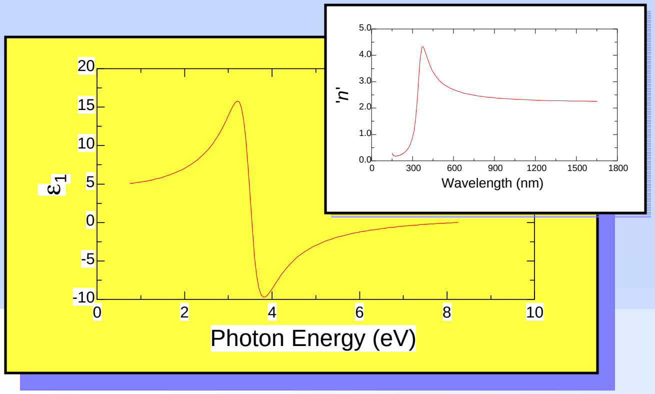
Building the model

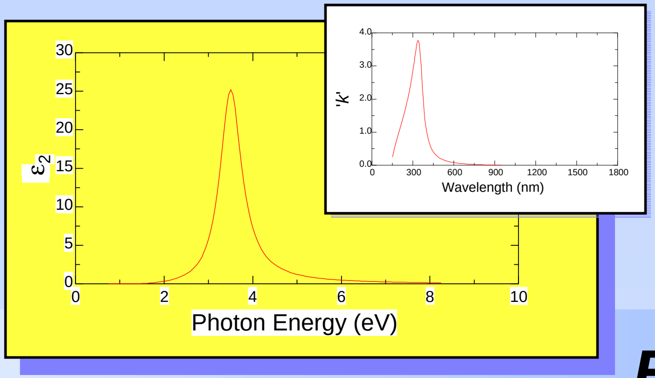
- Optical Constants
  - Dispersion Equation
    - Oscillator equation

2	polysilicon	0 Å
1	sio2	1000 Å
0	si	1 mm



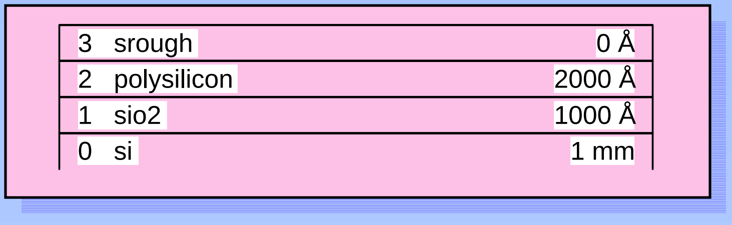






Building the model

- Optical Constants
    - Mixture
        - EMA, effective medium approximation



3 srough 0 Å
2 polysilicon 2000 Å
1 sio2 1000 Å
0 si 1 mm

    - Graded Layers
    - Anisotropic Layers
    - Superlattice

Building the model

- Seed Values
    - Thickness
        - process engineer’s guess
        - analyst's guess
        - trial-and-error
            - till it looks good
    - Cauchy coefficients
        - A_n between ~ 1.4 and 2.2
        - higher for poly or a_Si
    - Oscillators
        - tough
        - “GenOsc” formalism

A wise old sage once said:

> “The best way to solve a problem is to have solved one just like it yesterday.”

The regression process

- Don’t turn all the variables loose to begin with
  - e.g. for a Cauchy
    - thickness first
    - then A_n and thickness
    - then include B_n
    - add in extinction coefficient
- For a stack
  - don’t try to determine thicknesses and OC’s simultaneously
    - creative deposition
- “done” is a relative term
  - does it make sense

A wise old sage once said:

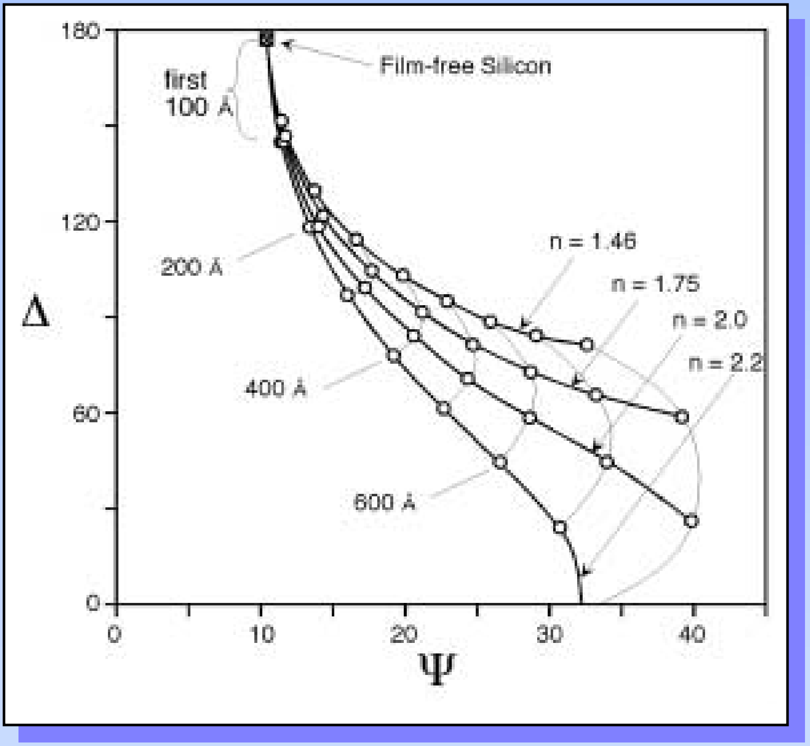
> “You *can* have it all, you just can’t have it all at once.”

Requirements

- plane parallel interfaces
  - roughness
- film must be uniform
  - graded layers
  - anisotropic layers
- multilayers
  - need to know something about OC’s
- coherence
  - patterned wafers
  - non-uniform thickness
  - macroscopic roughness
- helps if the film-of-interest is on top
- optical contrast
  - polymer on glass

Optical Constants of Very Thin Films

- consider a single wavelength (632.8 nm) at 70°
- oxynitride on silicon
- Delta/Psi trajectories

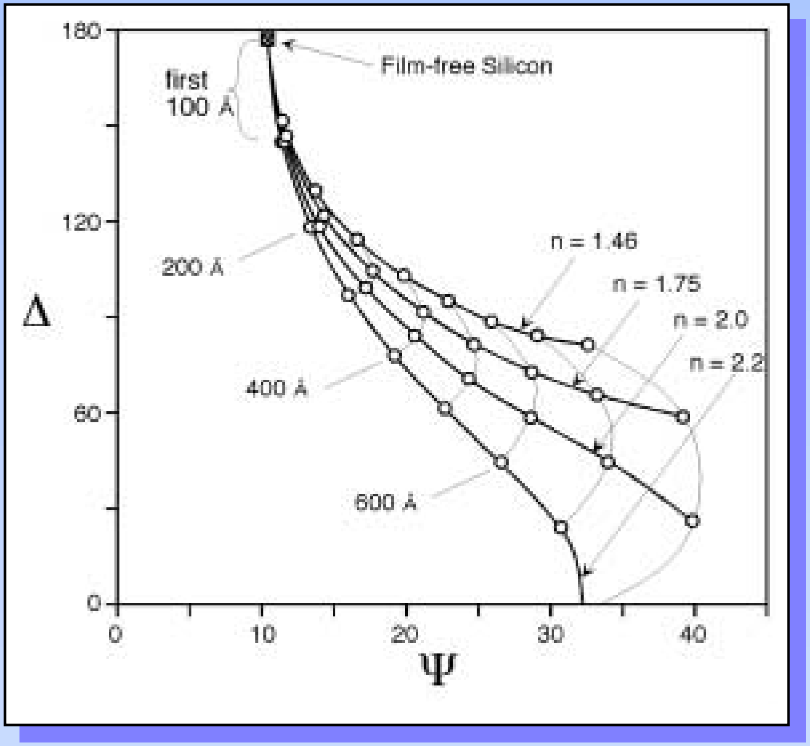


- below 100Å, very difficult to determine index, *n*
  - distinguishing one material from another
  - determining thicknesses in a stack
    - e.g., ONO
- however, if you’re willing to assume *n*, can determine thickness of very thin film
  - classic experiment of Archer
  - how far can you be off?

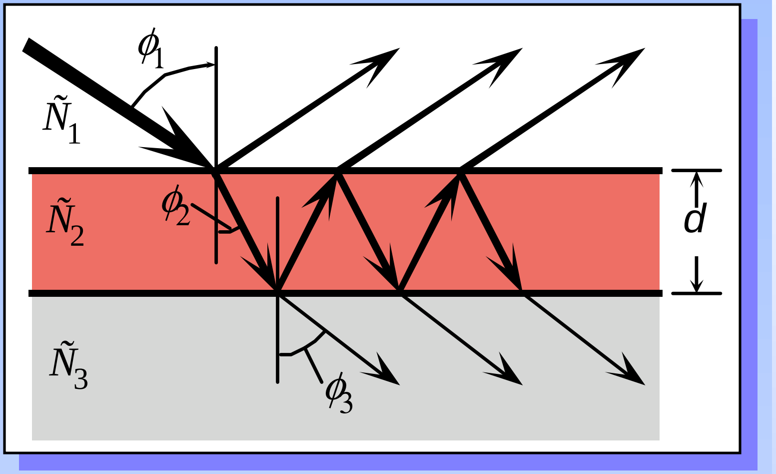
Optical Constants of Very Thin Films

making it better → directions

- DUV or VUV
  - shorter wavelengths
  - extinction coefficient often nonzero
- IR
  - absorption bands are different for different materials



Optical Constants of Very Thin Films



Fundamental Limitation

- Our ability to make films with:
  - plane parallel interfaces
  - uniformity

Acknowledgements

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- Motorola
- J. A. Woollam Co., Inc.
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