ELLIPSOMETRY ELLIPSOMETER AND THIN FILMS

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Outline

- ❖ Principle
- ❖ Instrumentation
- ❖ Modeling
- ❖ General Applications
- ❖ Summary

PRINCIPLE

On Spectroscopic Ellipsometry

Nature of the Light Waves

Light waves are electromagnetic in nature and require four basic field vectors to completely describe them.

- The electric-field strength: ***E***
- The electric-displacement density: ***D***
- The magnetic-field strength: ***H*** and
- The magnetic-flux density: ***B***

Of these four vectors, the electric-field strength is chosen to describe the polarization state of light waves. It is because the force exerted on the electrons by ***E*** is much greater than by the magnetic-filed of the wave when light interacts with matter. Once the polarization of electric-field vector has been determined, the other three vectors can be also determined based on Maxwell's field equations and the associated constitutive material relations.

Mathematic Description of Light Wave

For simplification, we consider a linearly polarized plane wave which propagates along the positive z direction and vibrates in the x-plane. The electric field of the wave can be written as:

$$c^2 \frac{\partial^2 E_x}{\partial z^2} = \varepsilon \frac{\partial^2 E_x}{\partial t^2} + 4\pi\sigma \frac{\partial E_x}{\partial t} \quad \Rightarrow \quad E_x = E_0 \exp\left[i\omega \left(t - \frac{z\tilde{N}}{c} \right) \right]$$

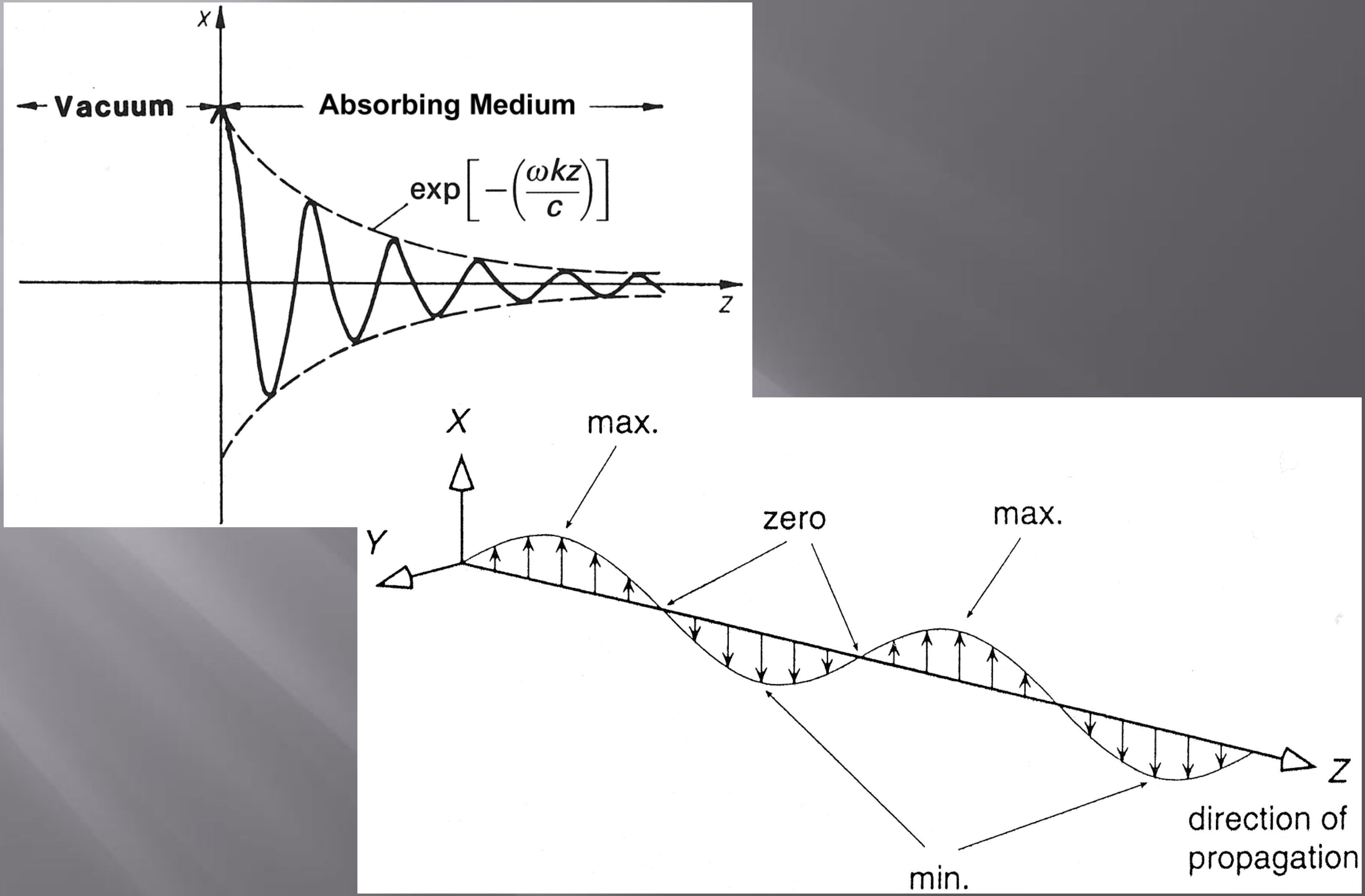
where E_x is the x-component of the electric-field strength; ε is the dielectric constant; σ is the conductivity. ω ($=2\pi\nu$) is the angular frequency, E_0 is the maximal value of the electric field strength.

$\tilde{N}$ is the complex index of refraction

$$\tilde{N} = n - ik$$

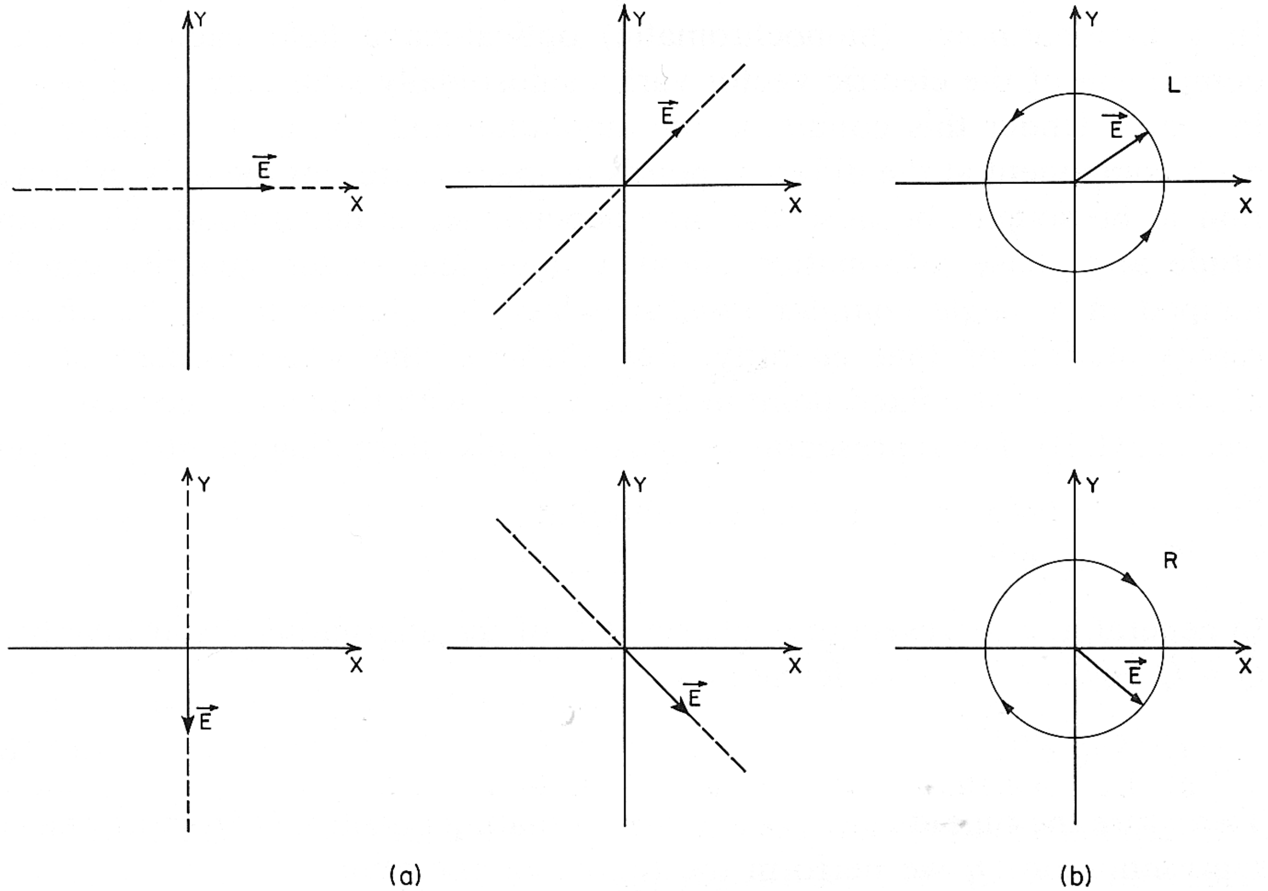
$$\Rightarrow \quad E_x = E_0 \exp\left[i\omega \left(t - \frac{z(n-ik)}{c} \right) \right] \quad \Rightarrow \quad E_x = E_0 \underbrace{\exp\left[-\frac{\omega k}{c} z \right]}_{\text{Damped Term}} \cdot \underbrace{\exp\left[i\omega \left(t - \frac{zn}{c} \right) \right]}_{\text{Undamped Term}}$$

Light Wave Propagation



Rolf E. Hummel: Electronic Properties of Materials, Springer-Verlag, 2nd Edition, 1997

Linearly and Circularly Polarized Light

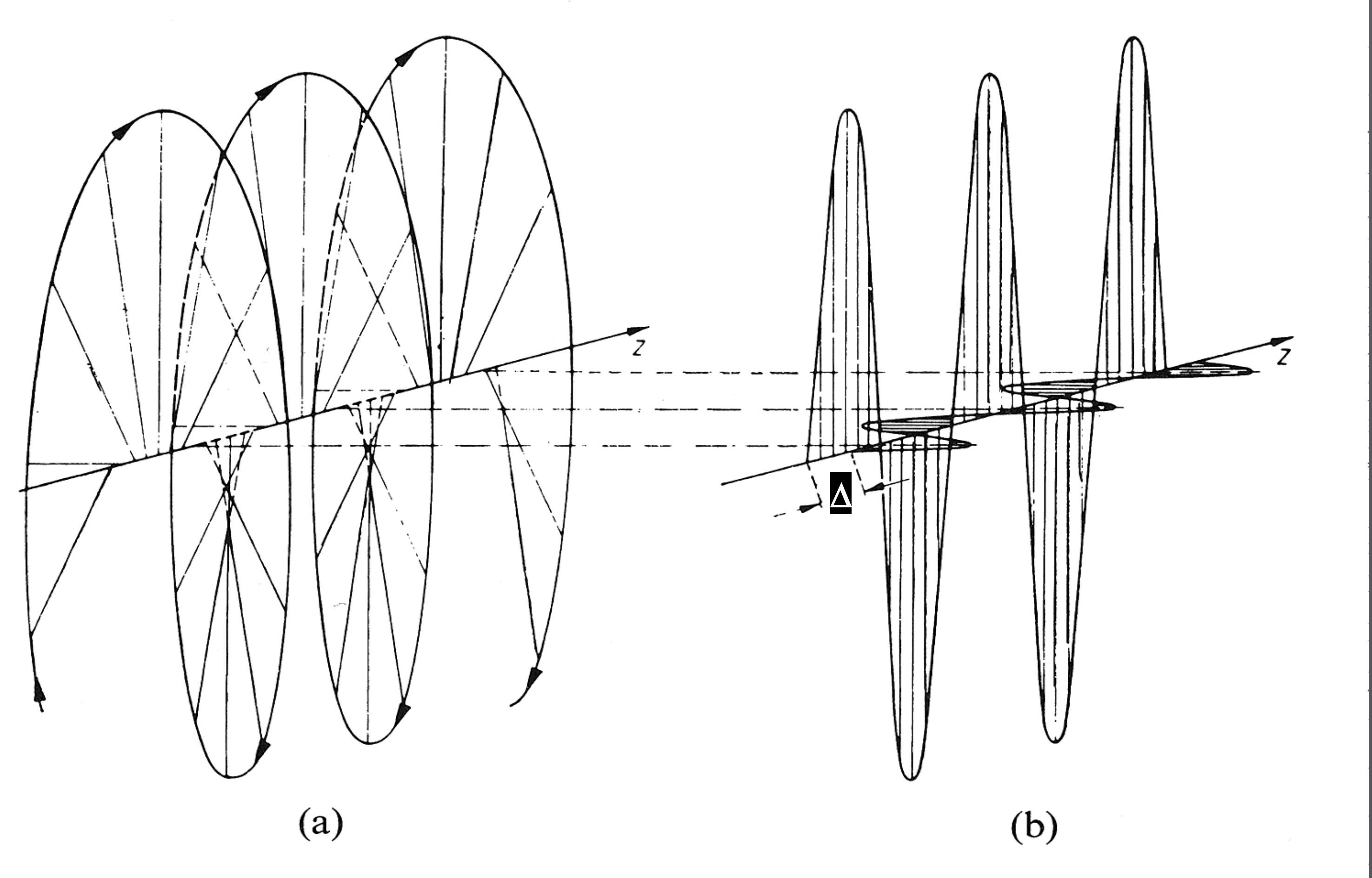


The special cases of linear (a) and circular (b) polarization. In (a), the dashed line indicates the locus of the terminus of the electric vector *E*. In (b), L and R represent the left- and right-circular polarizations, respectively.

R.M.A Azzam & N.M. Bashara: Ellipsometry and Polarized Light, Elsevier Sci., New York, 1999

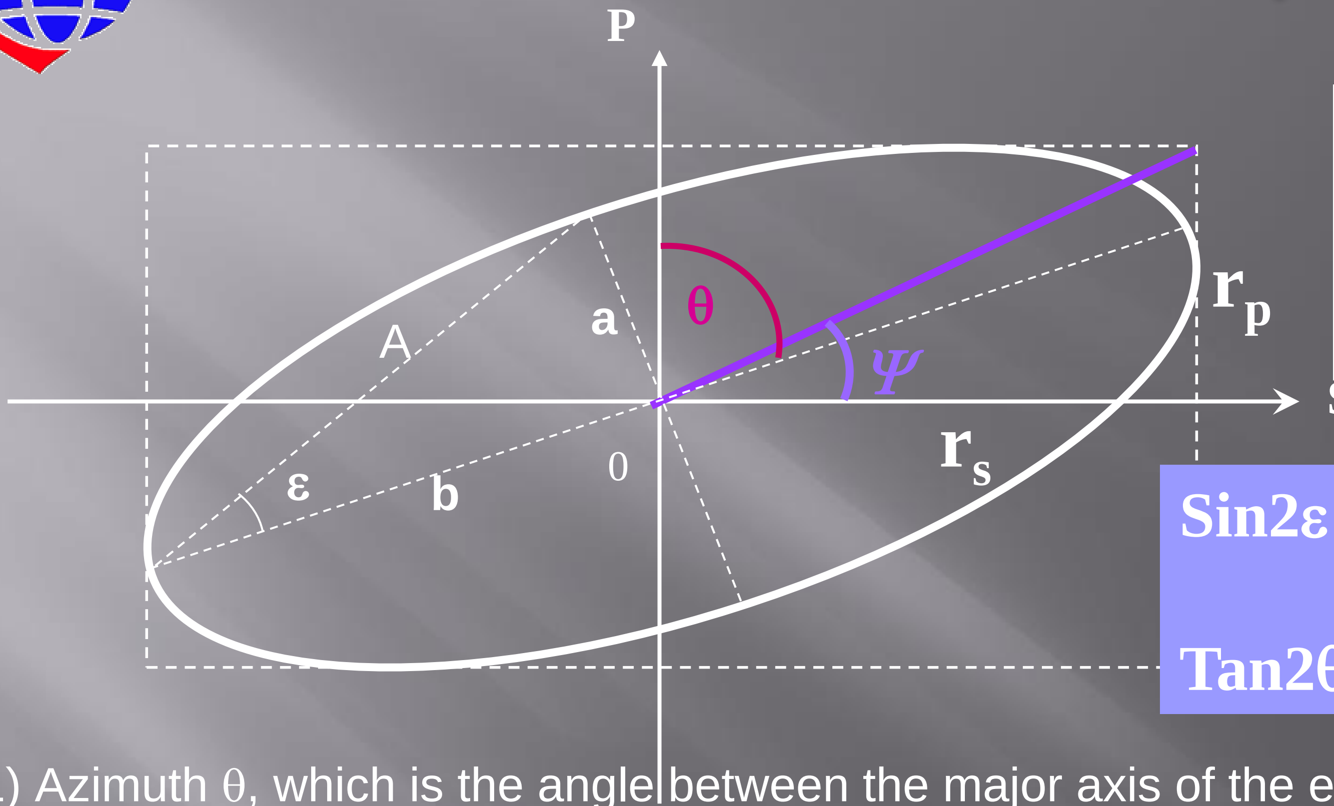
Elliptically Polarized Light

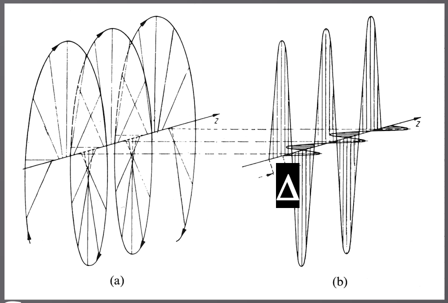
---- The extremity of its electric field vector describes an ellipse



(a) Elliptically polarized light; (b) decomposition of elliptically polarized light into two
(b) mutually perpendicular plane polarized waves P and S with a phase difference, Delta;
R.W. Pohl, Optik und Atomphysik, Springer-Verlag, Berlin, 1958

Parameters to Describe the Ellipse





Sin2ε = Sin2ψSinΔ

Tan2θ = Tan2ψCosΔ

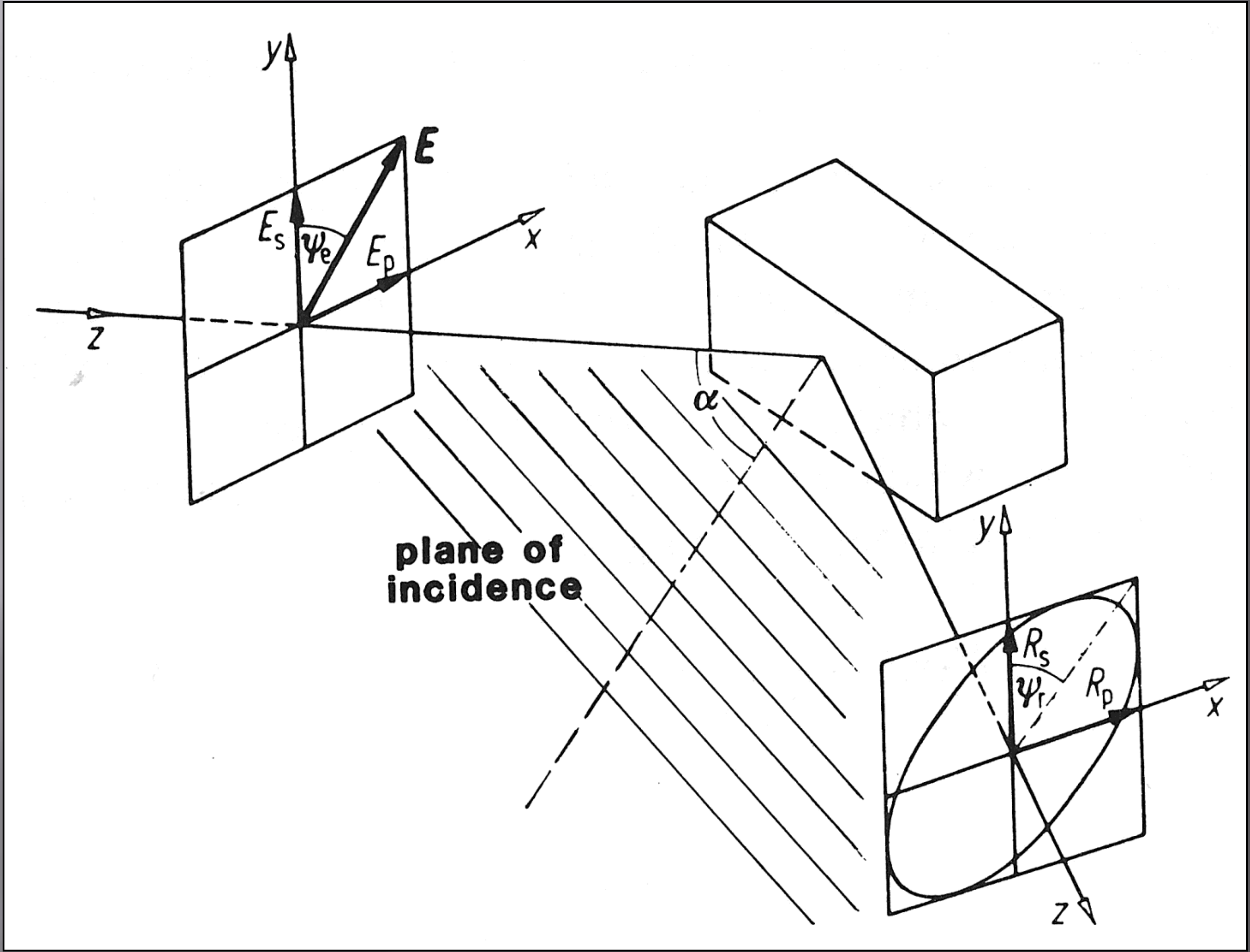
(1) Azimuth θ, which is the angle between the major axis of the ellipse and the positive direction of the P. It defines the orientation of the ellipse ($-90^o \leq \theta < 90^o$).

(2) Ellipticity e, which is the ratio of the length of the semi-minor axis and that of its semi-major axis. e = a/b = Tan(ε)

(3) Amplitude A, which is a measure of the strength of elliptical vibration. Its square is proportional to the energy density of the wave. $A = (a^2 + b^2)^{1/2}$

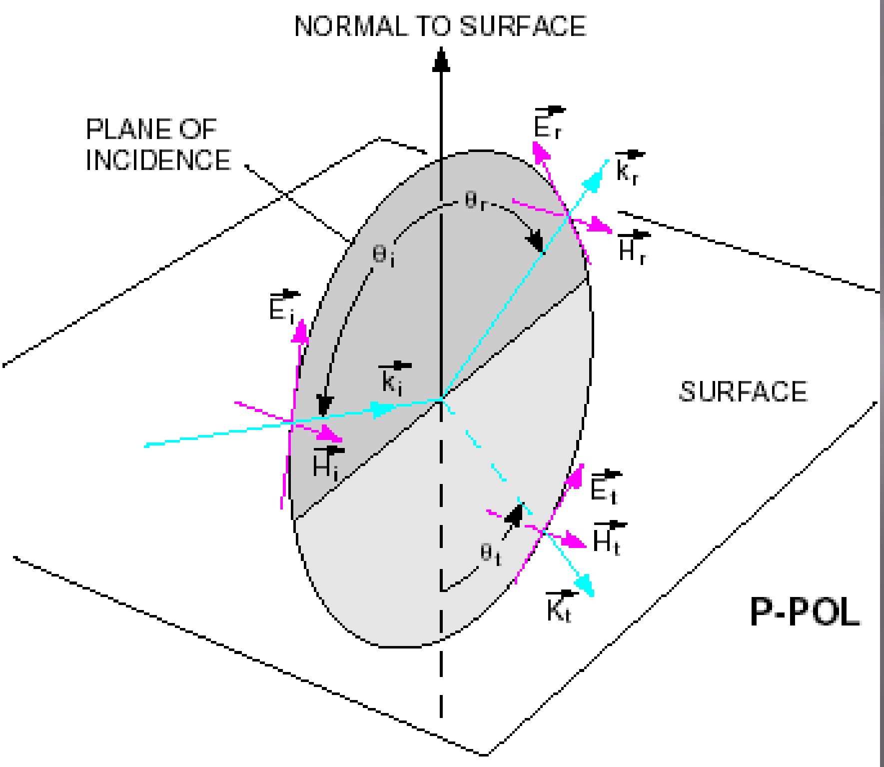
(4) Handedness, which is used to describe wave propagation sense. Right handed – clockwise; Left handed – counter-clockwise when looking into the beam.

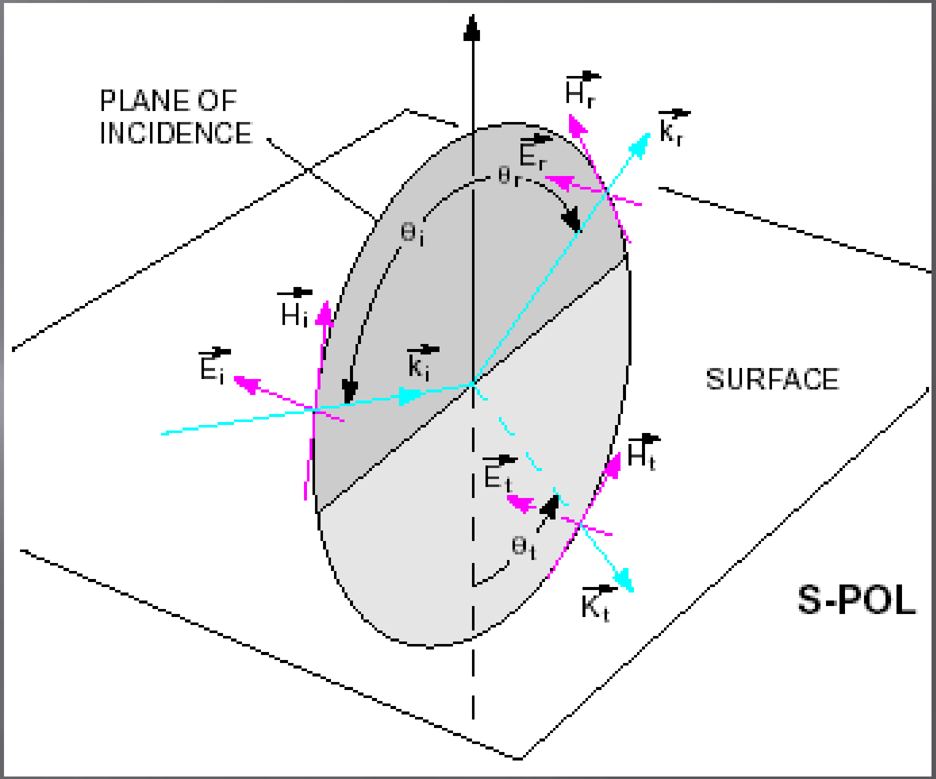
Plane of Incidence

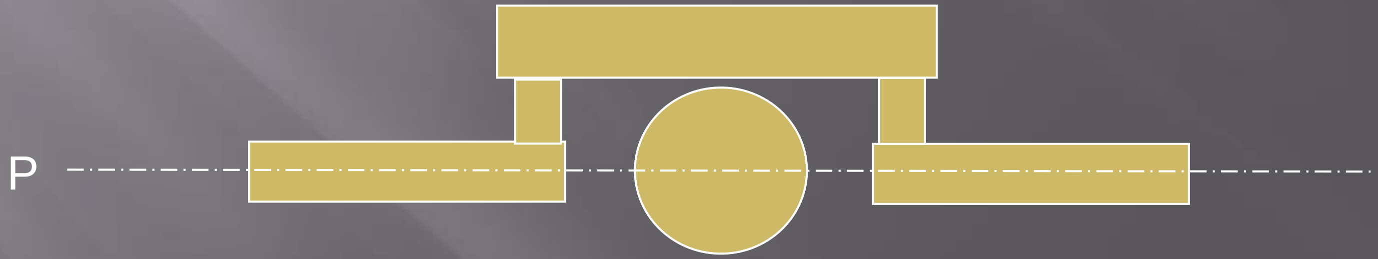


Rolf E. Hummel: Electronic Properties of Materials, Springer-Verlag, 2nd Edition, 1997

P-polarization / S-polarization

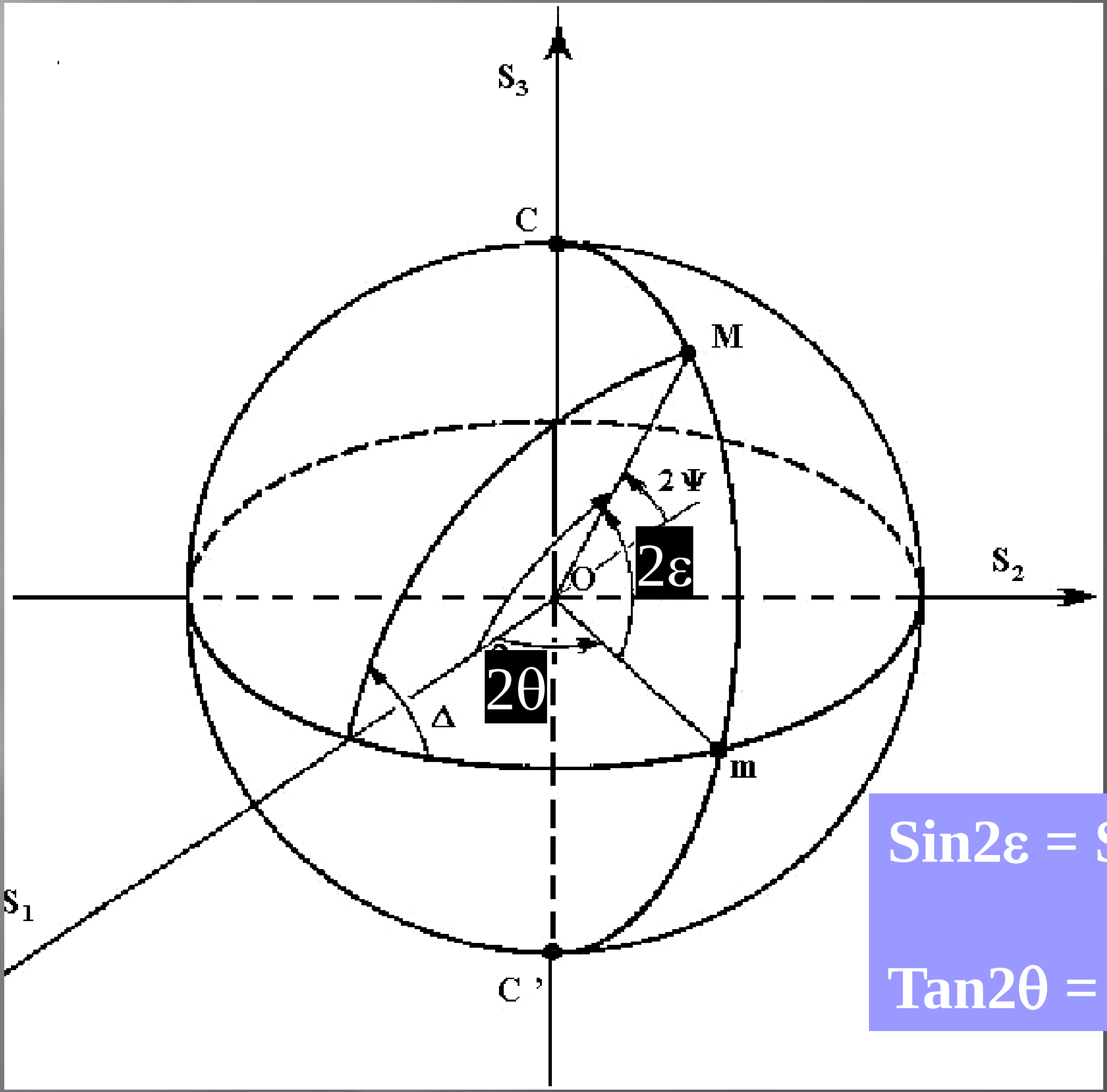






Source: Newport

Poincaré Sphere

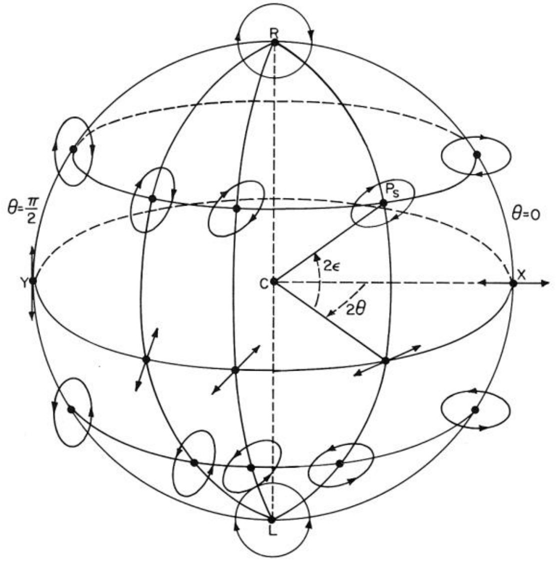


$\mathrm{Sin}2\varepsilon = \mathrm{Sin}2\psi\mathrm{Sin}\Delta$

$\mathrm{Tan}2\theta = \mathrm{Tan}2\psi\mathrm{Cos}\Delta$

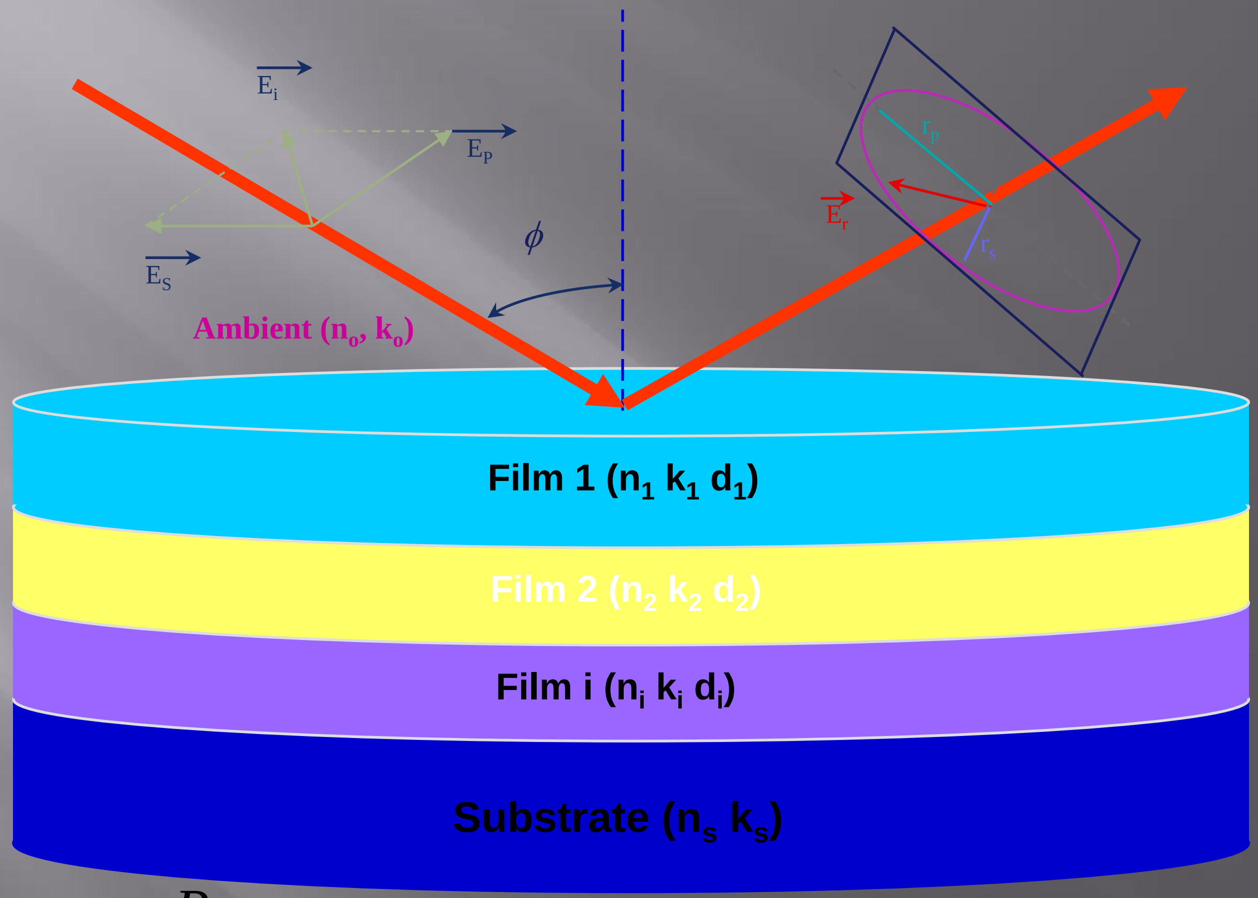
Poincaré Sphere

R.M.A Azzam & N.M. Bashara: Ellipsometry and Polarized Light, Elsevier Sci., New York, 1999



The Poincaré-sphere representation of polarization. The longitude 2θ and latitude 2ϵ determine a point P_s that represents an ellipse of polarization with azimuth θ and ellipticity angle ϵ. The lines of longitude and latitude represent the equi-azimuth and equi-ellipticity contours, respectively. The correspondence between polarization states and points on the sphere is indicated.

Reflection of Light



Ambient (n_o, k_o)

Film 1 (n_1 k_1 d_1)

Film 2 (n_2 k_2 d_2)

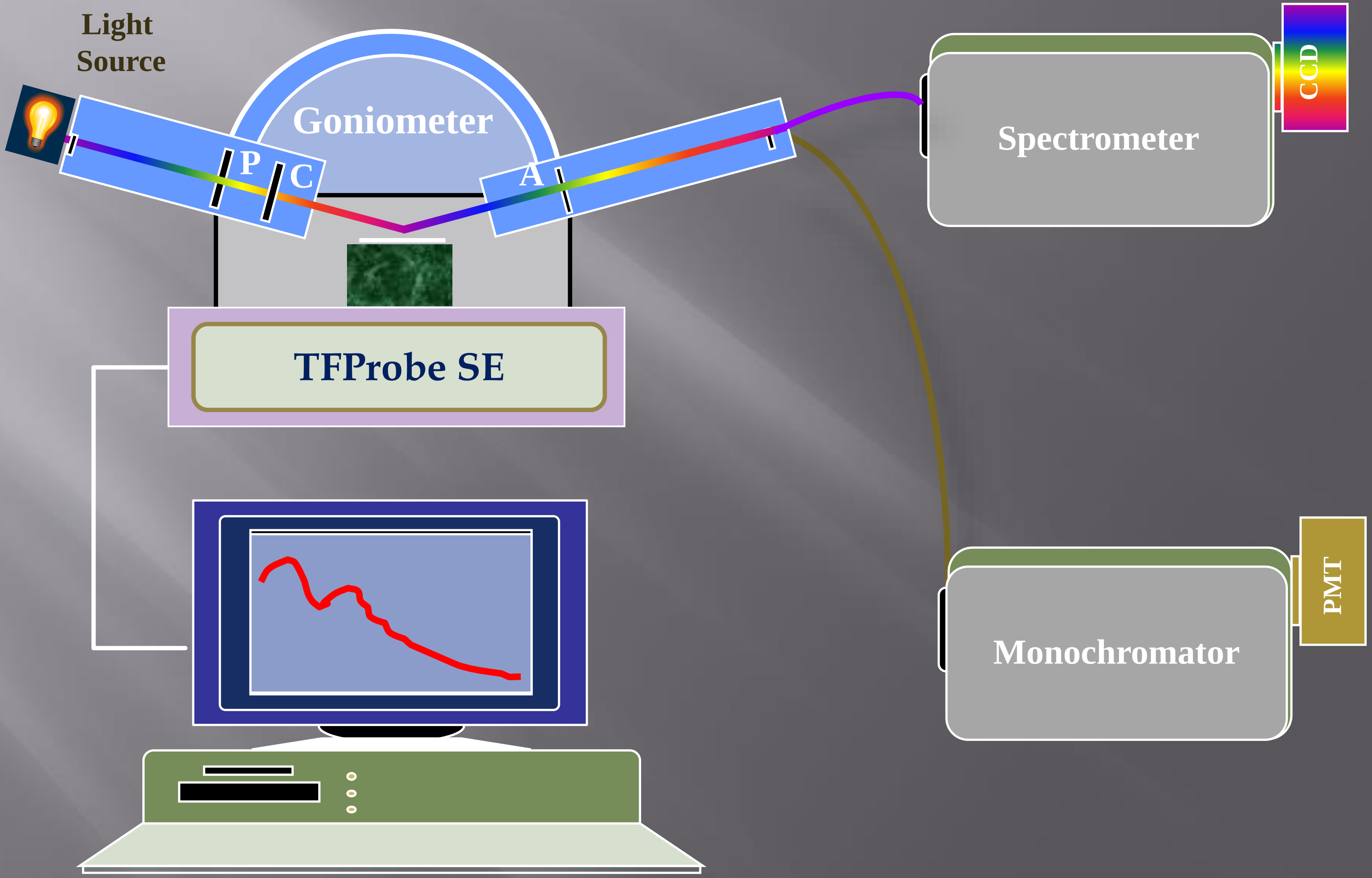
Film i (n_i k_i d_i)

Substrate (n_s k_s)

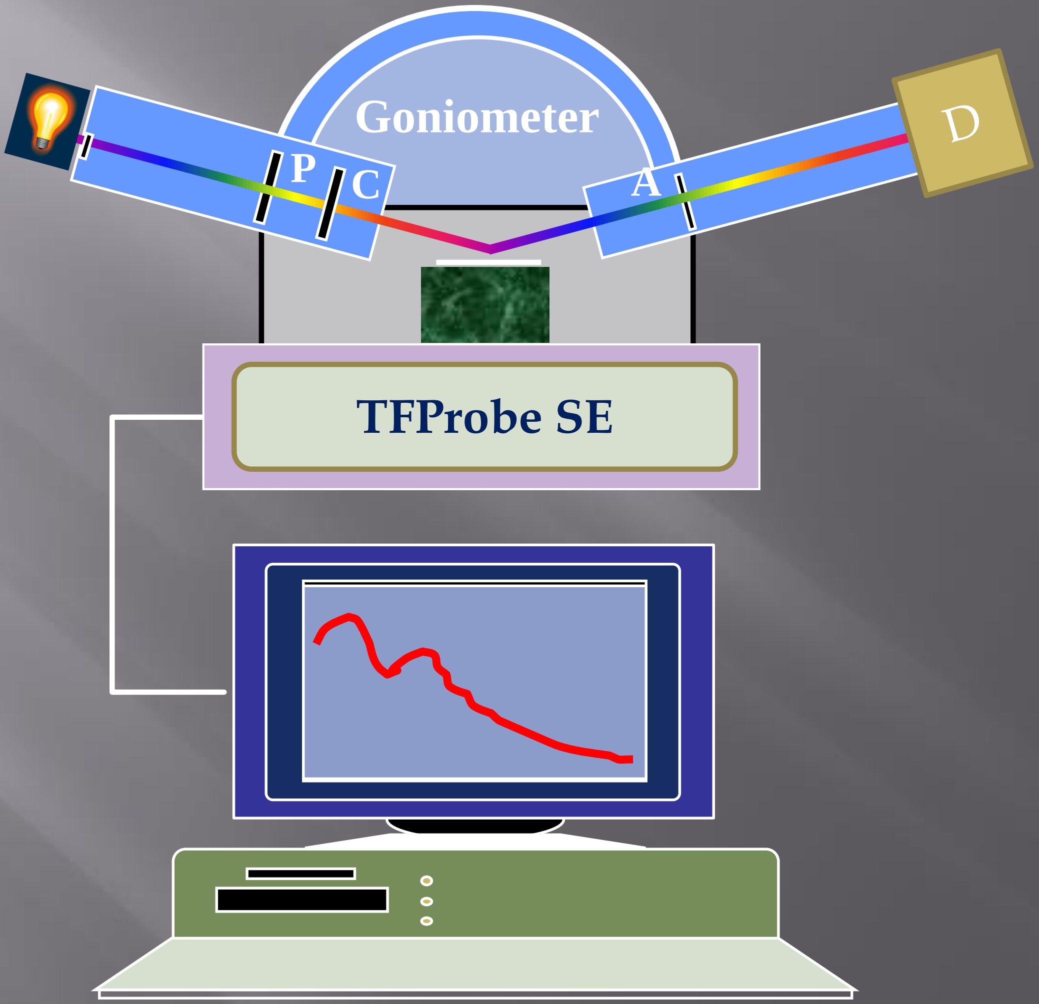
$$\rho = \frac{R^P}{R^S} = Tan\psi \cdot e^{j\Delta} = f(n_i, k_i, d_i \cdots)$$

Instrumentation

Typical SE Layout

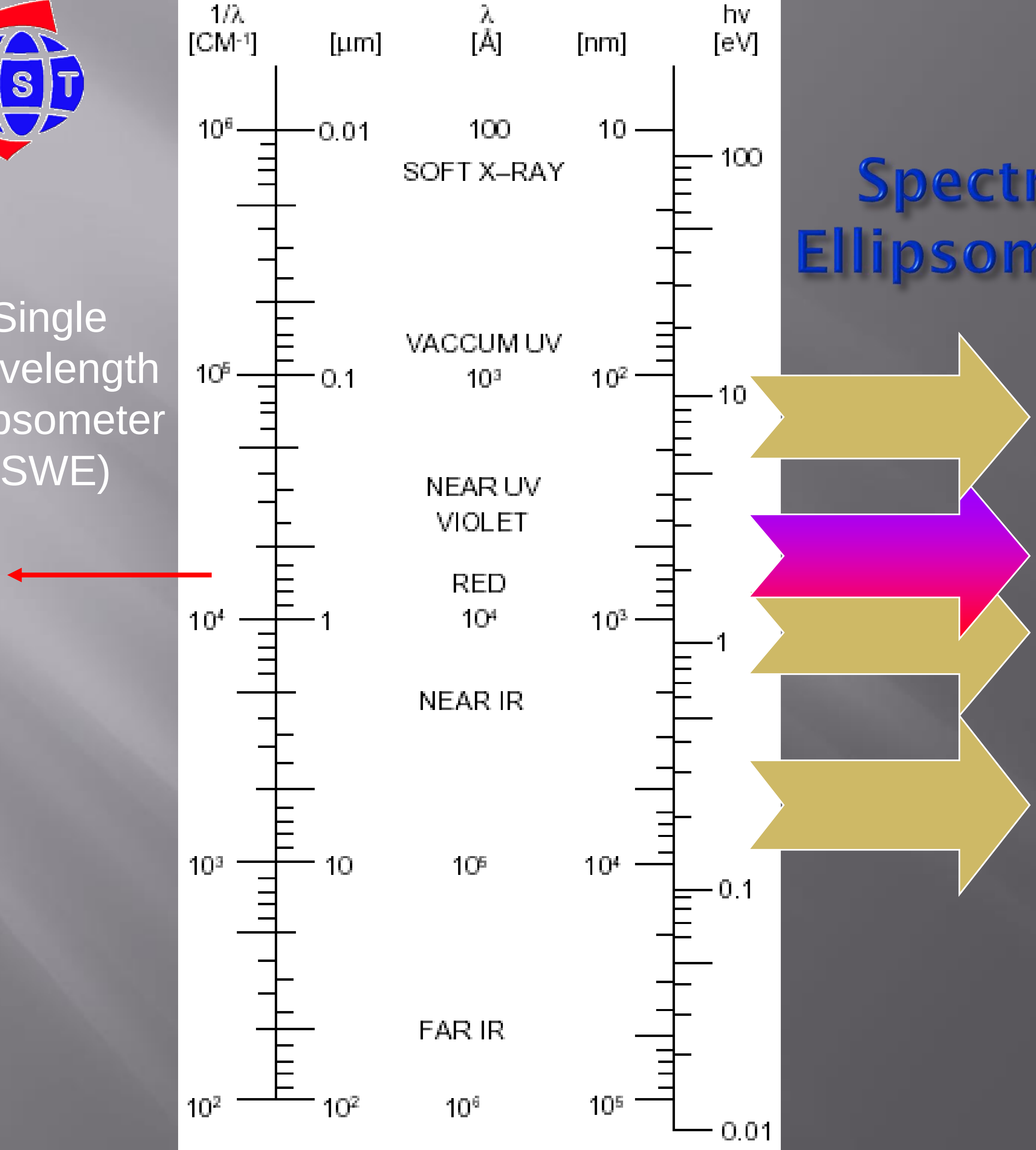


Typical SE Layout



Spectroscopic Ellipsometers (SE)

Single Wavelength Ellipsometer (SWE)



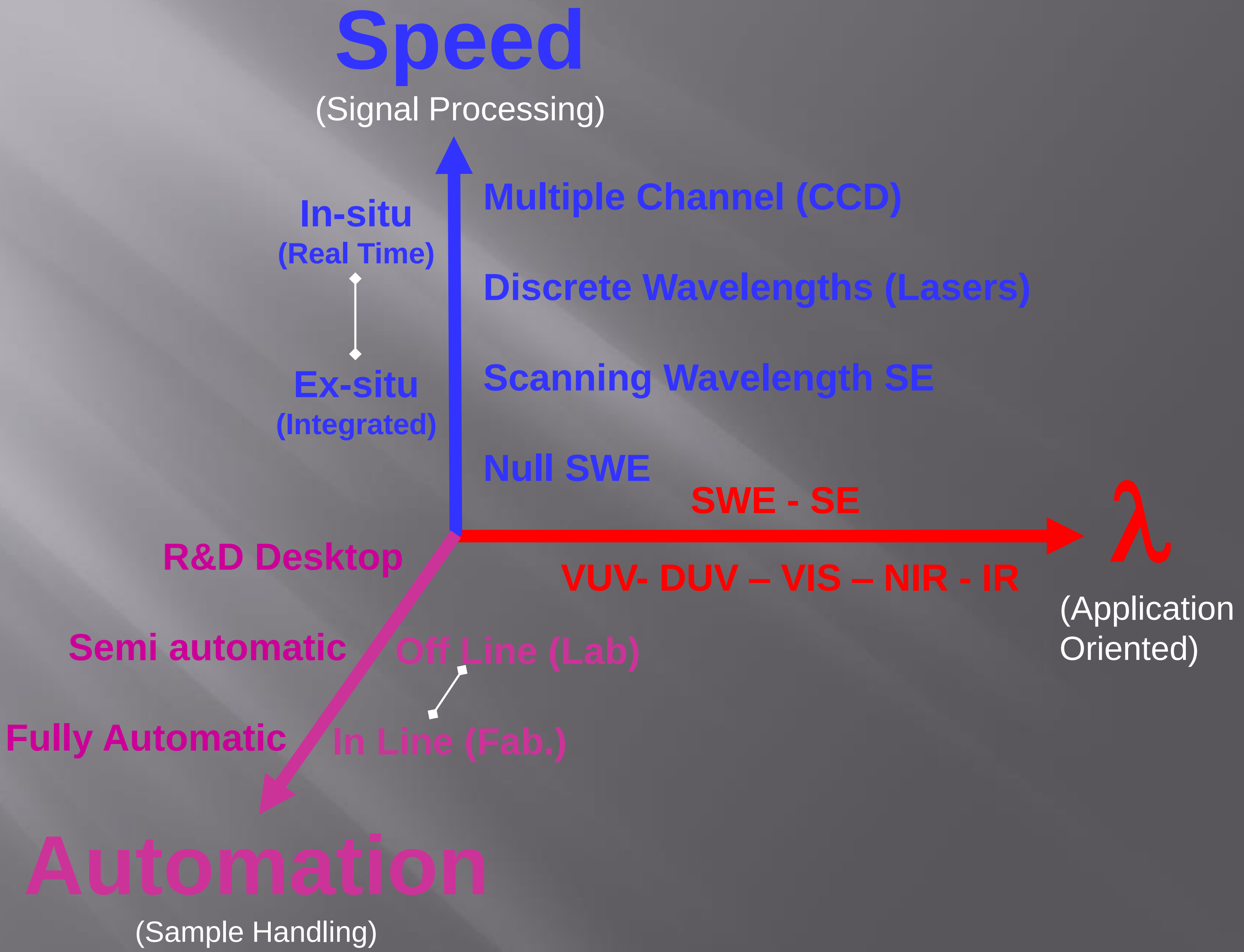
VUV / PUV

Vis

Vis + NIR

IR-SE

Ellipsometer Classification



Speed

(Signal Processing)

In-situ

(Real Time)

Ex-situ

(Integrated)

Multiple Channel (CCD)

Discrete Wavelengths (Lasers)

Scanning Wavelength SE

Null SWE

SWE - SE

λ

VUV- DUV – VIS – NIR - IR

(Application Oriented)

R&D Desktop

Semi automatic

Fully Automatic

Off Line (Lab)

In Line (Fab.)

Automation

(Sample Handling)

PRINCIPLE, INSTRUMENTATION AND MODELING

On Spectroscopic Ellipsometry

Modeling

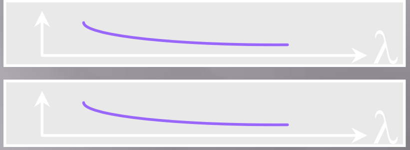
Model and Its Analyses

$$\rho = \frac{R^P}{R^S} = Tan\psi \cdot e^{j\Delta} = f(n_i, k_i, d_i \cdots)$$

Measured Data

TanΨ

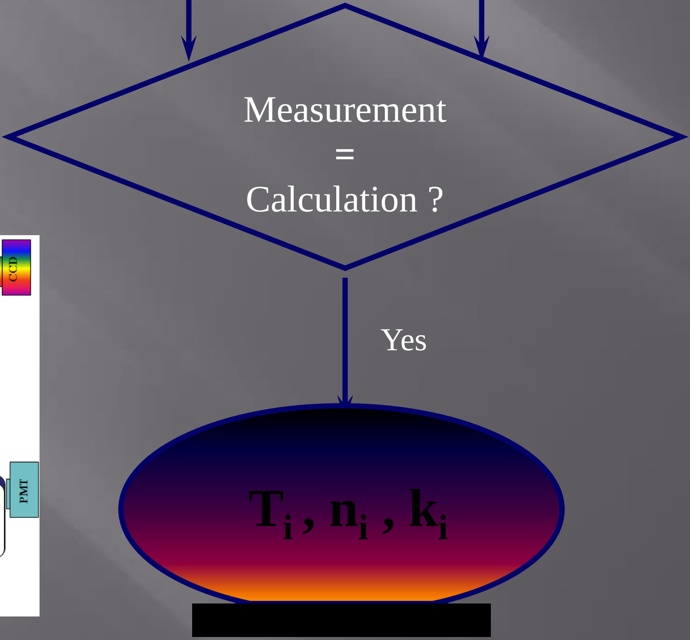
CosΔ



Physical Model

Estimated sample structure

- Film Stack and structure
- Material n, k, dispersion
- Composition Fraction of Mixture

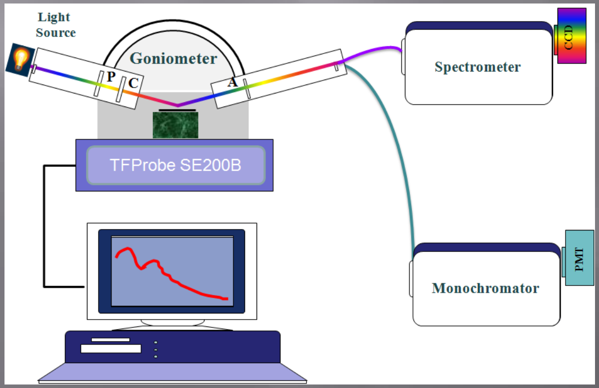


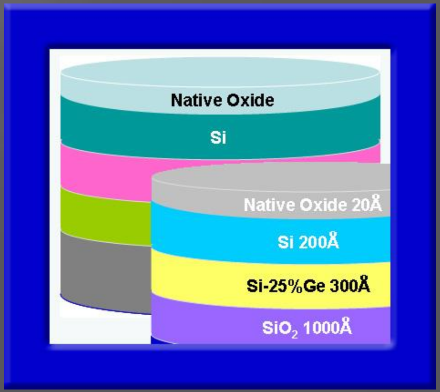
Measurement = Calculation ?

No

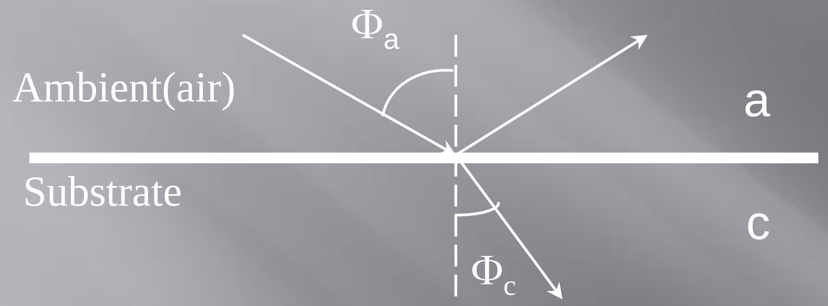
Yes

T_i, n_i, k_i





Constants for BULK



1. Fresnel Reflection Coefficients:

$$r_{ac}^{P} = \frac{\tilde{N}_c Cos\Phi_a - \tilde{N}_a Cos\Phi_c}{\tilde{N}_c Cos\Phi_a + \tilde{N}_a Cos\Phi_c}$$

$$r_{ac}^{S} = \frac{\tilde{N}_a Cos\Phi_a - \tilde{N}_c Cos\Phi_c}{\tilde{N}_a Cos\Phi_a + \tilde{N}_c Cos\Phi_c}$$

2. Snell's Law:

$$\tilde{N}_a Sin\Phi_a = \tilde{N}_c Sin\Phi_c$$

3. Ellipsometry Equation

$$\rho = \frac{r_{ac}^{P}}{r_{ac}^{S}}$$

4. Optical Constants

$$\tilde{N} = Sin\Phi_a \sqrt{1 + \left(\frac{1-\rho}{1+\rho}\right)^2 Tan^2\Phi_a}$$

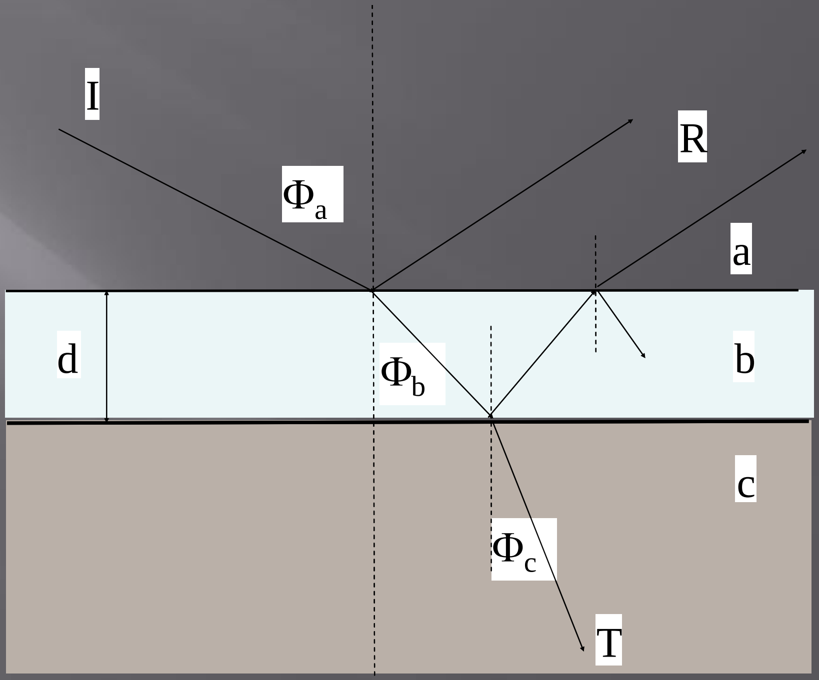
Air/Film/Substrate

- Multi reflections between interface a/b and interface b/c
- From the Fresnel coefficients at the interface a/b and b/c, the total reflection coefficients can be calculated as:

$$R^P = \frac{r_{ab}^P + r_{bc}^P e^{-j2\beta}}{1 + r_{ab}^P r_{bc}^P e^{-j2\beta}}$$

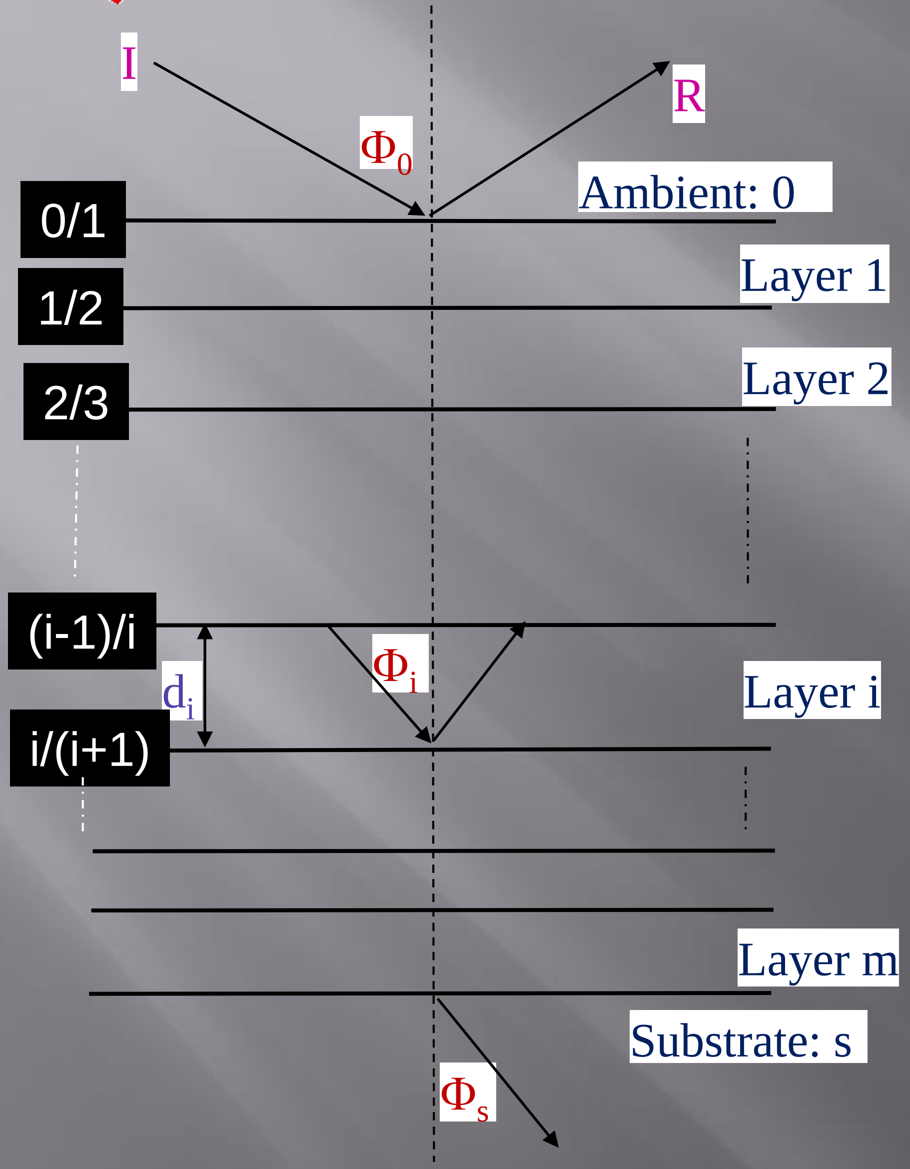
$$R^S = \frac{r_{ab}^S + r_{bc}^S e^{-j2\beta}}{1 + r_{ab}^S r_{bc}^S e^{-j2\beta}}$$

$$\beta = 2\pi(\frac{d}{\lambda})(n_b - jk_b)Cos\Phi_b$$



$$\rho = \frac{R^P}{R^S} = Tan\psi \cdot e^{j\Delta}$$

Analysis for Multilayer



- ▣ M films in structure
- ▣ Planar assumed
- ▣ Isotropic and homogenous
- ▣ Incident angle known

- **Facts:**
  - **M layers + one substrate**
  - **M+1 interfaces**
- **Unknowns:**
  - **Each layer thickness (m)**
  - **Optical constants (n & k, 2m)**
- **Ellipsometer Data:**
  - **One set of Ψ & Δ at each wavelength**

Reflection and Transmission at Interface

1. Fresnel Reflection Coefficients:

$$r^{P}_{(i-1)/i} = \frac{\tilde{N}_i Cos\Phi_{i-1} - \tilde{N}_{i-1} Cos\Phi_i}{\tilde{N}_i Cos\Phi_{i-1} + \tilde{N}_{i-1} Cos\Phi_i}$$

$$r^{S}_{(i-1)/i} = \frac{\tilde{N}_{i-1} Cos\Phi_{i-1} - \tilde{N}_i Cos\Phi_i}{\tilde{N}_{i-1} Cos\Phi_{i-1} + \tilde{N}_i Cos\Phi_i}$$

2. Fresnel Transmission Coefficients:

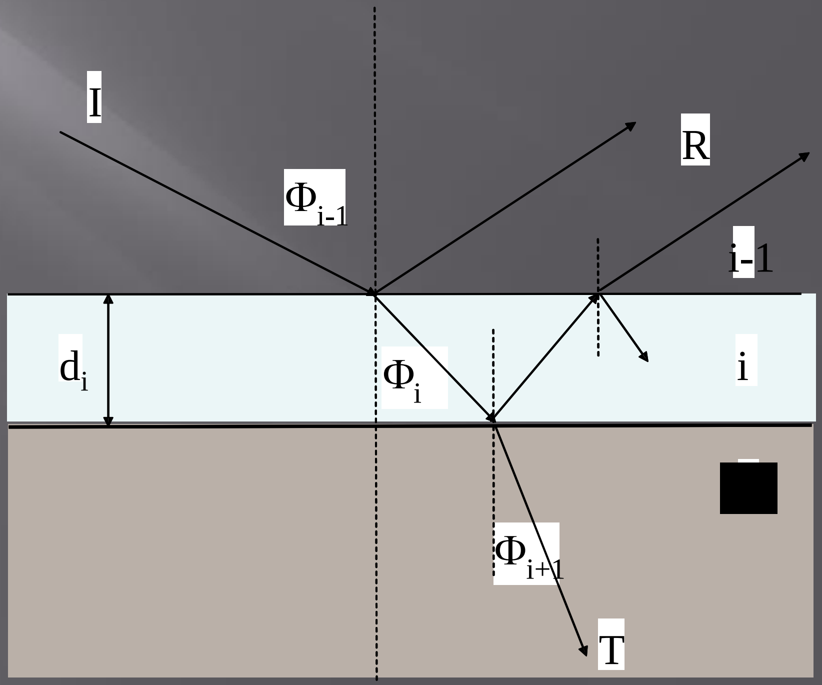
$$t^{P}_{(i-1)/i} = \frac{2\tilde{N}_{i-1} Cos\Phi_{i-1}}{\tilde{N}_i Cos\Phi_{i-1} + \tilde{N}_{i-1} Cos\Phi_i}$$

$$t^{S}_{(i-1)/i} = \frac{2\tilde{N}_i Cos\Phi_i}{\tilde{N}_{i-1} Cos\Phi_{i-1} + \tilde{N}_i Cos\Phi_i}$$

3. Snell's Law $\tilde{N}_i Sin\Phi_i = \tilde{N}_{i+1} Sin\Phi_{i+1}$

4. Phase Factor

$$\beta_i = 2\pi(\frac{d_i}{\lambda})\tilde{N}_i Cos\Phi_i$$



Ellipsometry Equations

Interface Matrix I (a &b)

$$I_{ab} = \begin{bmatrix} 1/t_{ab} & r_{ab}/t_{ab} \\ r_{ab}/t_{ab} & 1/t_{ab} \end{bmatrix} = (1/t_{ab}) \begin{bmatrix} 1 & r_{ab} \\ r_{ab} & 1 \end{bmatrix}$$

Layer Matrix

$$L = \begin{bmatrix} e^{j\beta} & 0 \\ 0 & e^{j\beta} \end{bmatrix}$$

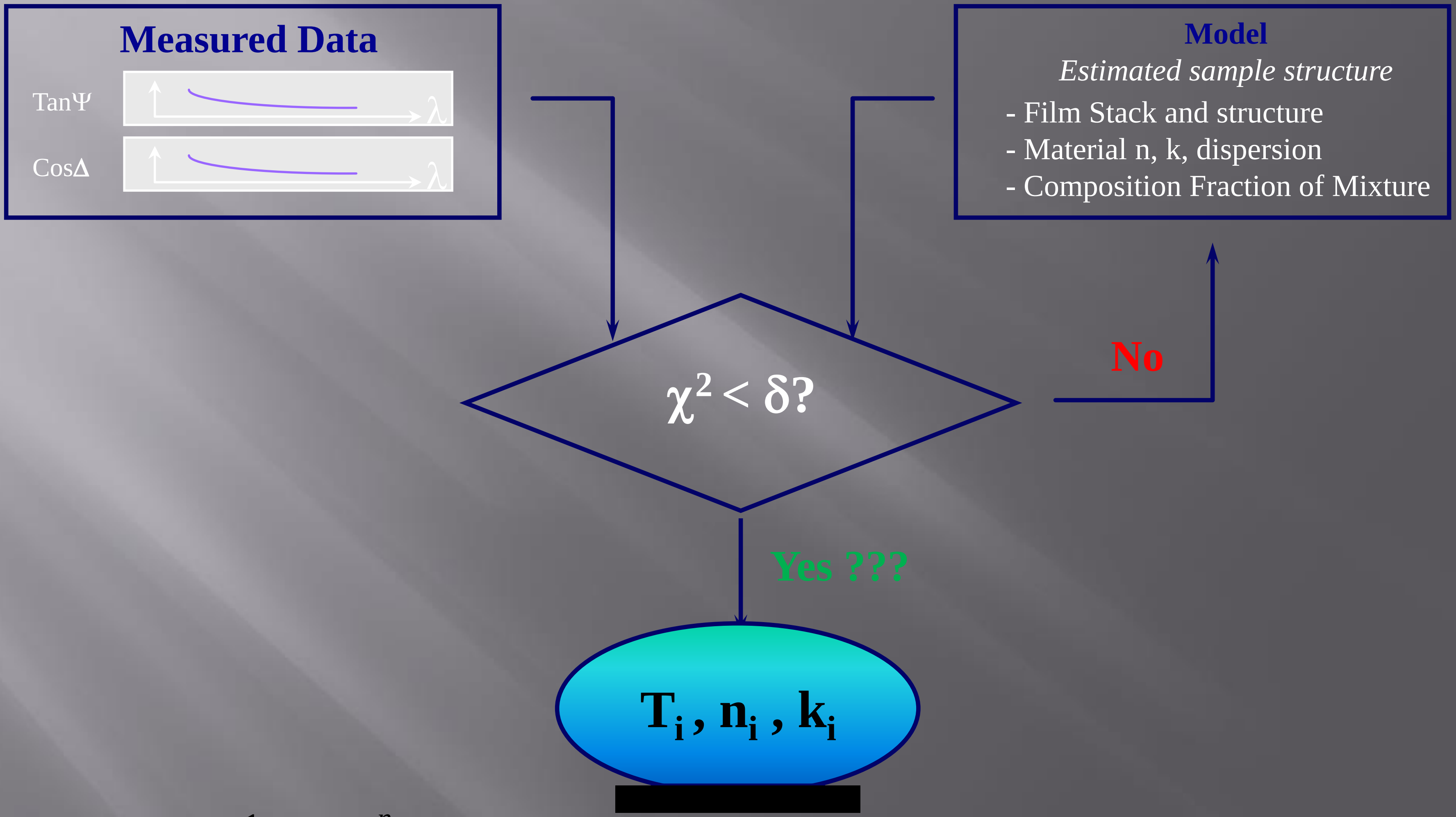
$$S = I_{01} L_1 I_{12} L_2 I_{23} L_3 I_{34} L_4 \ldots I_{(m-1)m} L_m I_{ms} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix}$$

$$R = \frac{S_{21}}{S_{11}} \qquad T = \frac{1}{S_{11}}$$

⟺

$$\rho = \frac{R^P}{R^S} = Tan\psi \cdot e^{j\Delta} = f(n_i, k_i, d_i \cdots)$$

Model and Its Analyses



Measured Data

Model

Estimated sample structure

- Film Stack and structure
- Material n, k, dispersion
- Composition Fraction of Mixture

$\chi^2 < \delta?$

No

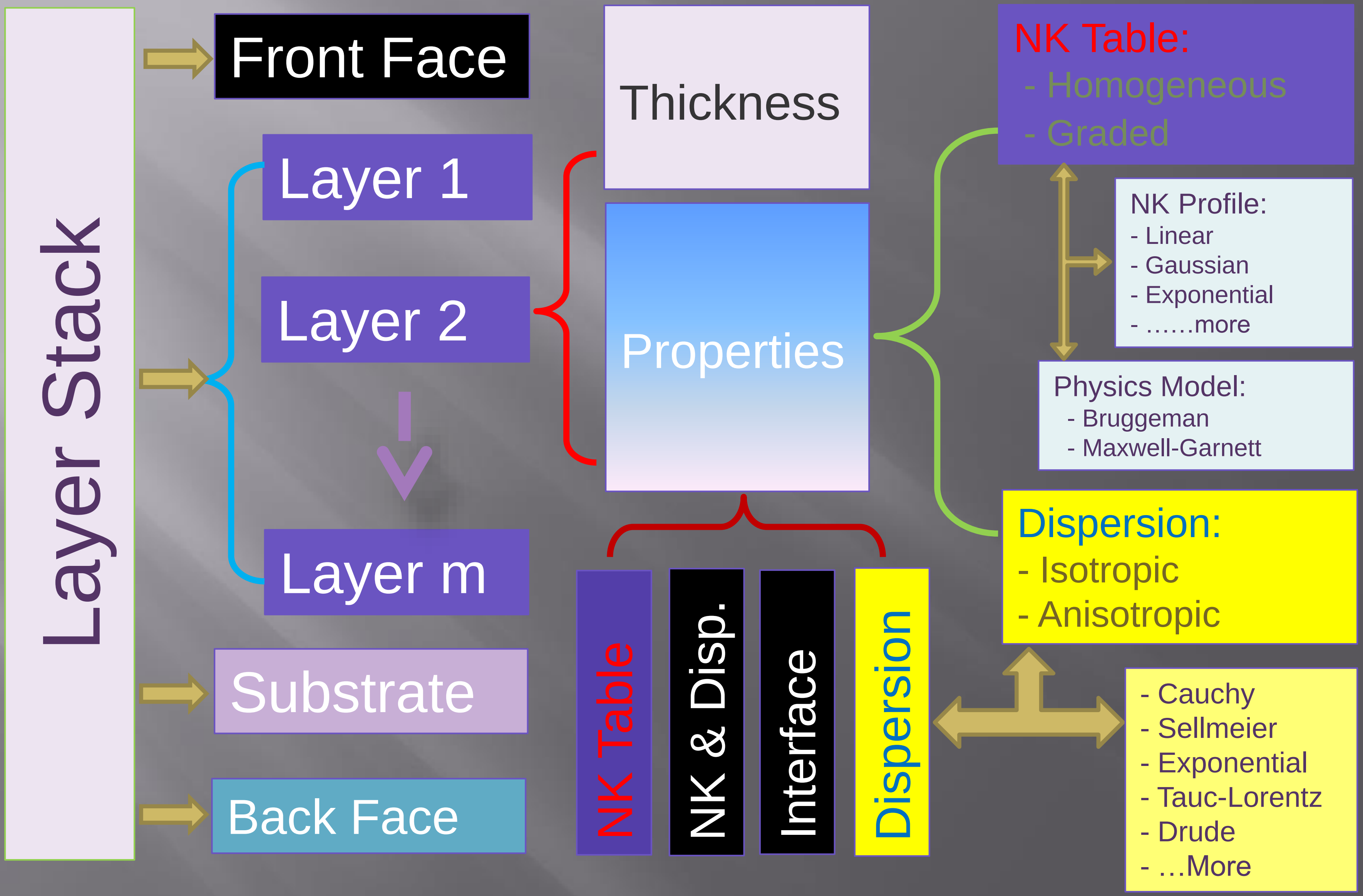
Yes ???

$\mathbf{T_i , n_i , k_i}$

$$\chi^2 = \frac{1}{2n-m-1}\sum_{i=1}^{n}[(Tan\Psi^i_{Theory} - Tan\Psi^i_{Exp})^2 + (Cos\Delta^i_{Theory} - Cos\Delta^i_{Exp})^2]$$

How to Set up MODEL?

Layer Stack in SE Analysis



Layer Stack

Front Face

Layer 1

Layer 2

Layer m

Substrate

Back Face

Thickness

Properties

NK Table

NK & Disp.

Interface

Dispersion

NK Table:
- Homogeneous
- Graded

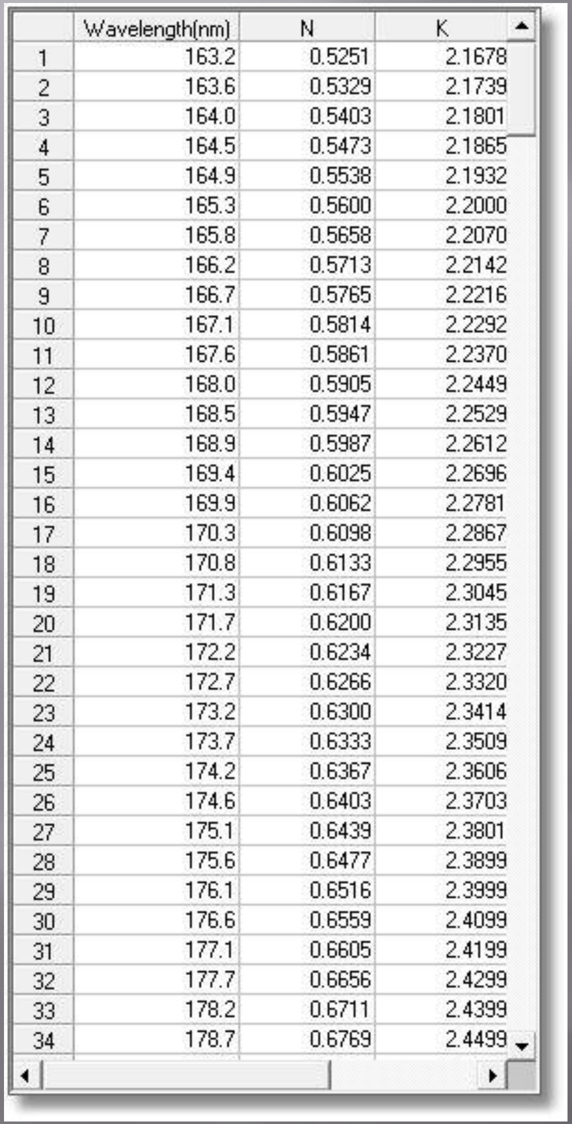
NK Profile:
- Linear
- Gaussian
- Exponential
- ……more

Physics Model:
- Bruggeman
- Maxwell-Garnett

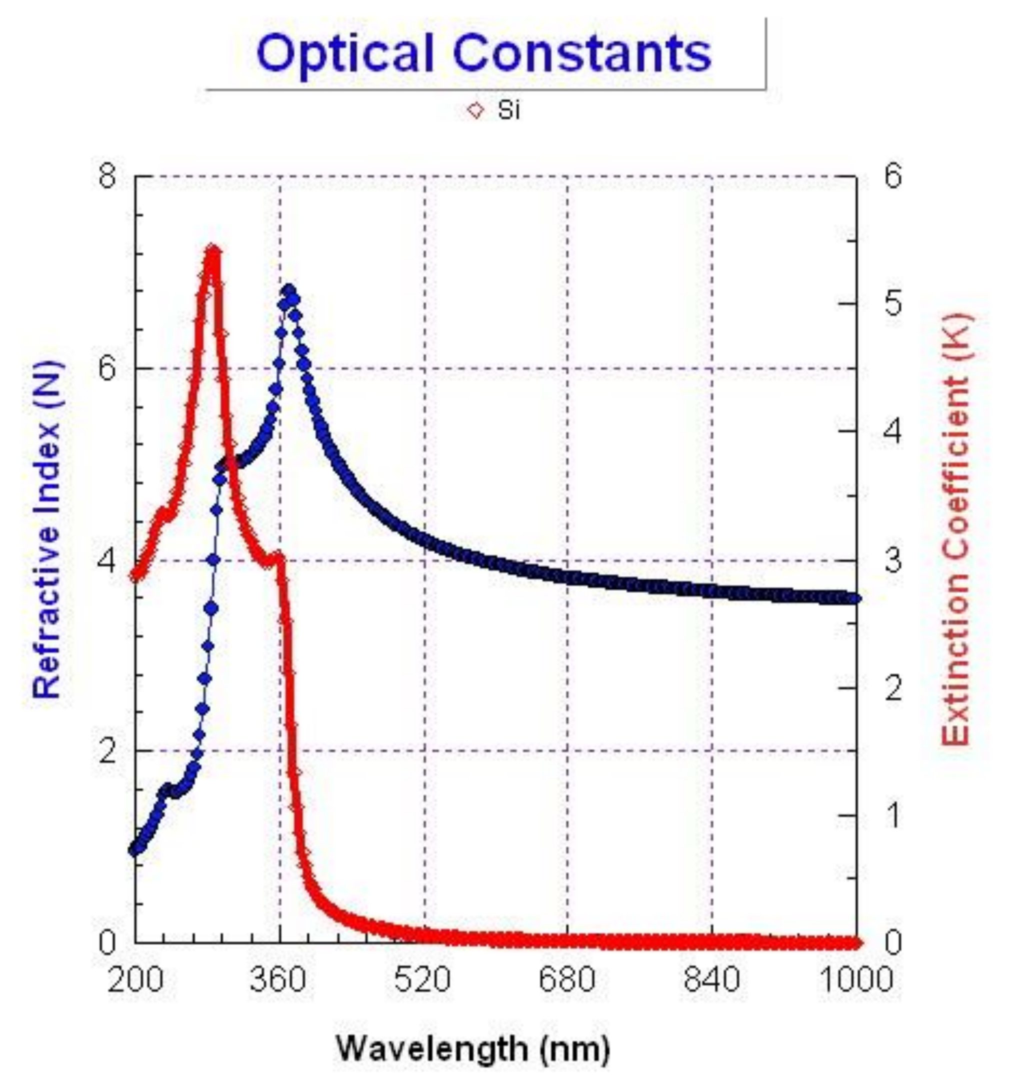
Dispersion:
- Isotropic
- Anisotropic

- Cauchy
- Sellmeier
- Exponential
- Tauc-Lorentz
- Drude
- …More

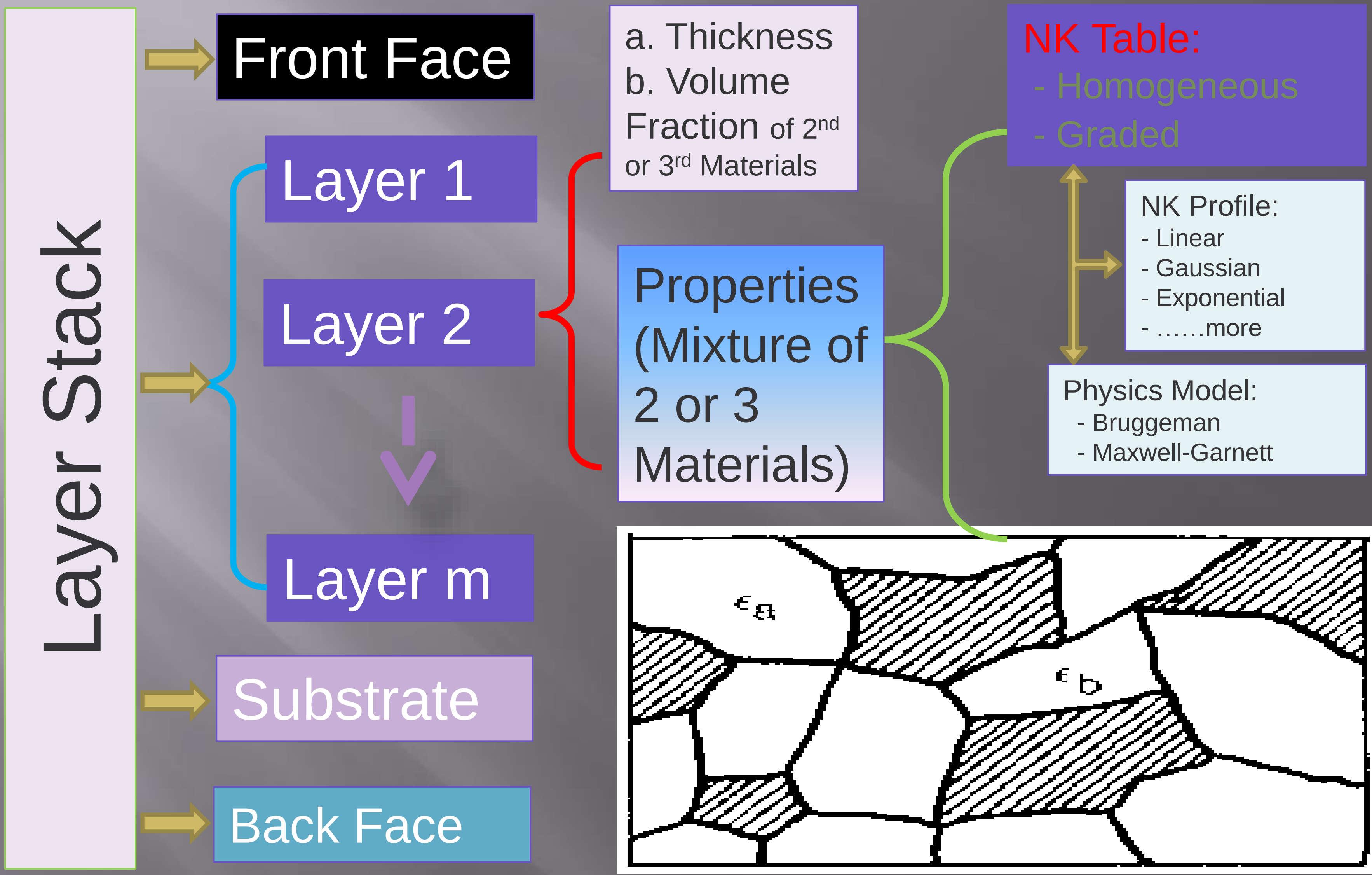
NK Table



	Wavelength(nm)	N	K
1	163.2	0.5251	2.1678
2	163.6	0.5329	2.1739
3	164.0	0.5403	2.1801
4	164.5	0.5473	2.1865
5	164.9	0.5538	2.1932
6	165.3	0.5600	2.2000
7	165.8	0.5658	2.2070
8	166.2	0.5713	2.2142
9	166.7	0.5765	2.2216
10	167.1	0.5814	2.2292
11	167.6	0.5861	2.2370
12	168.0	0.5905	2.2449
13	168.5	0.5947	2.2529
14	168.9	0.5987	2.2612
15	169.4	0.6025	2.2696
16	169.9	0.6062	2.2781
17	170.3	0.6098	2.2867
18	170.8	0.6133	2.2955
19	171.3	0.6167	2.3045
20	171.7	0.6200	2.3135
21	172.2	0.6234	2.3227
22	172.7	0.6266	2.3320
23	173.2	0.6300	2.3414
24	173.7	0.6333	2.3509
25	174.2	0.6367	2.3606
26	174.6	0.6403	2.3703
27	175.1	0.6439	2.3801
28	175.6	0.6477	2.3899
29	176.1	0.6516	2.3999
30	176.6	0.6559	2.4099
31	177.1	0.6605	2.4199
32	177.7	0.6656	2.4299
33	178.2	0.6711	2.4399
34	178.7	0.6769	2.4499



Mixture of Materials



Layer Stack

Front Face

Layer 1

Layer 2

Layer m

Substrate

Back Face

a. Thickness
b. Volume Fraction of 2nd or 3rd Materials

Properties (Mixture of 2 or 3 Materials)

NK Table:
- Homogeneous
- Graded

NK Profile:
- Linear
- Gaussian
- Exponential
- ……more

Physics Model:
- Bruggeman
- Maxwell-Garnett

Mixture of Materials

Layer Stack

Front Face

Layer 1

Layer 2

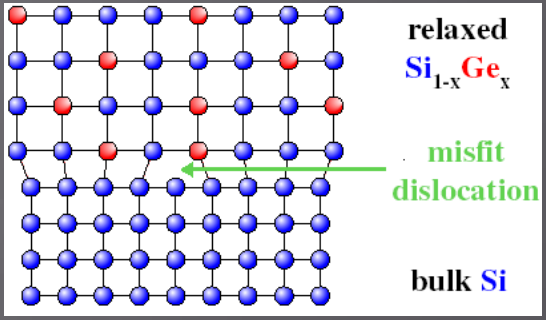
Layer m

Substrate

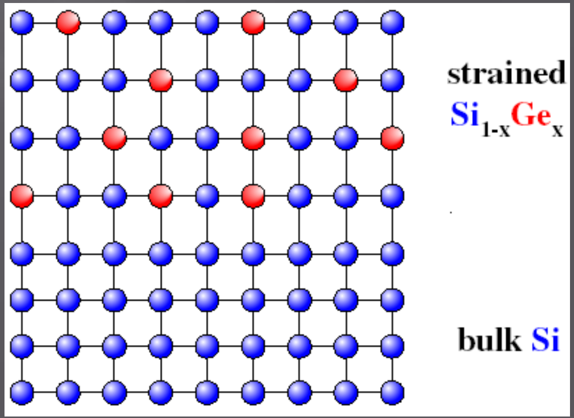
Back Face

a. Thickness
b. Concentration of 2nd Element

Properties (Alloy)



NK Table:
- Relaxed
- Strained



Mixture of Materials
(Interface)

Layer Stack

Front Face

Layer 1

Layer 2

Layer m

Substrate

Back Face

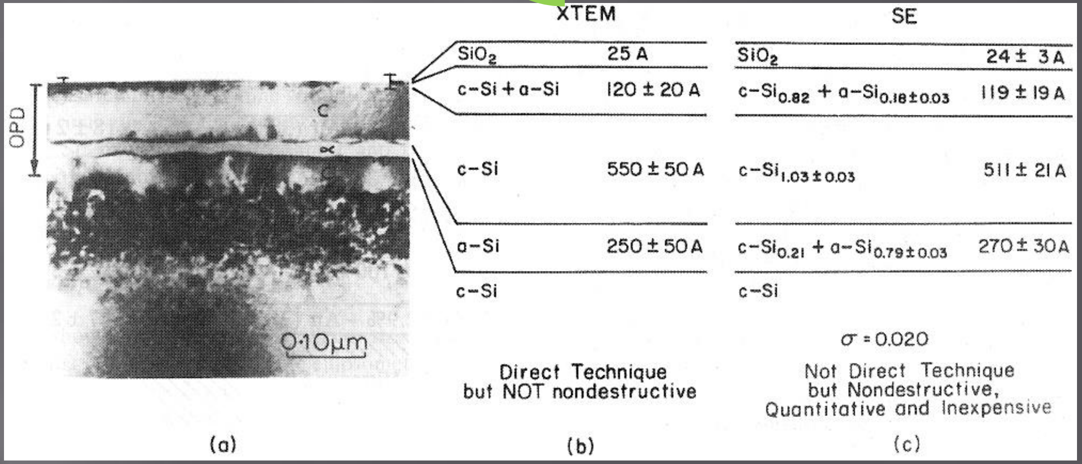
a. Thickness
b. Volume Fraction of Lower Material

Properties (Mixture of Above and Beneath Material)

NK Table:
- Homogeneous
- Graded

NK Profile:
- Linear
- Gaussian
- Exponential
- ……more

Physics Model:
- Bruggeman
- Maxwell-Garnett



Mixture of Materials
(Surface Roughness)

Layer Stack

- Front Face
- Layer 1
- Layer 2
- Layer m
- Substrate
- Back Face

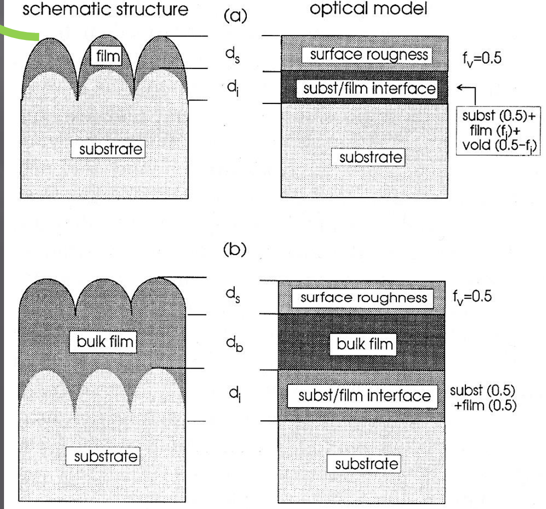
a. Thickness
b. Volume Fraction of Lower Material

Properties (Mixture of Air and Top Material)

NK Table:
- Homogeneous
- Graded

NK Profile:
- Linear
- Gaussian
- Exponential
- ……more

Physics Model:
- Bruggeman
- Maxwell-Garnett



Physics for Mixture of Materials

Microscopic Property

Polarizability: α

$$\frac{4\pi}{3} N\alpha = \frac{\varepsilon - 1}{\varepsilon + 2}$$

Macroscopic Property

Dielectric Response: ε

Clausius-Massotti Equation

(N is the density of polarizable units)

$$\frac{\varepsilon - 1}{\varepsilon + 2} = f_a \frac{\varepsilon_a - 1}{\varepsilon_a + 2} + f_b \frac{\varepsilon_b - 1}{\varepsilon_b + 2}$$

Lorentz-Lorentz Equation

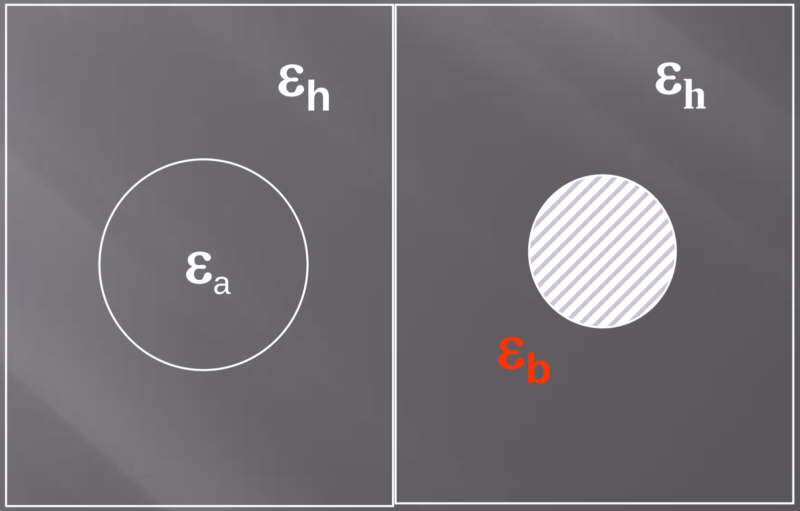
(f’s are volume fractions for each polarizable components a & b)

Maxwell-Garnett Equation

$$\frac{\varepsilon-\varepsilon_h}{\varepsilon+2\varepsilon_h}=f_a\,\frac{\varepsilon_a-\varepsilon_h}{\varepsilon_a+2\varepsilon_h}+f_b\,\frac{\varepsilon_b-\varepsilon_h}{\varepsilon_b+2\varepsilon_h}$$

a and b are in a host with dielectric constant of ε_h

(Philos. Trans. R. Soc., London, 205,1906, 237)

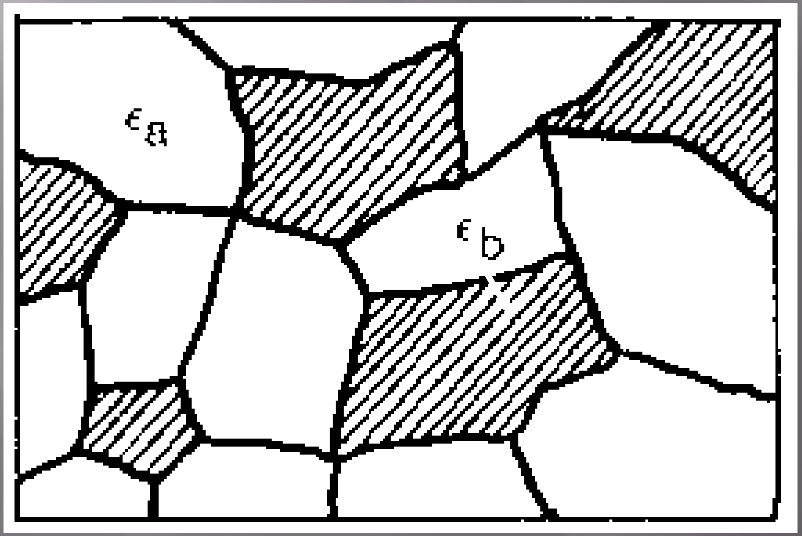


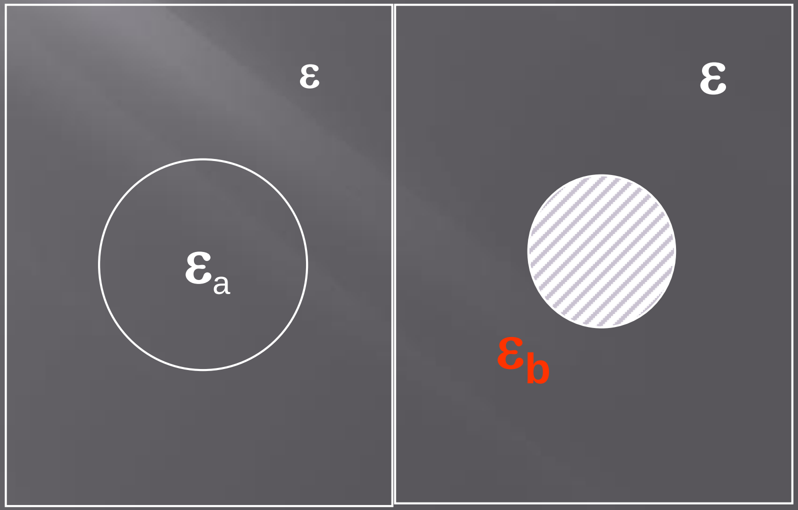
Effective Medium Approximation (EMA)

A.G. Bruggeman, Ann. Phys. (Liepzig) 24, 636 (1935)

The Bruggeman model is also called Effective Medium Approximation (EMA). In this model, the two media play exactly the same role. The effective dielectric function of the mixture is given by the second order equation :

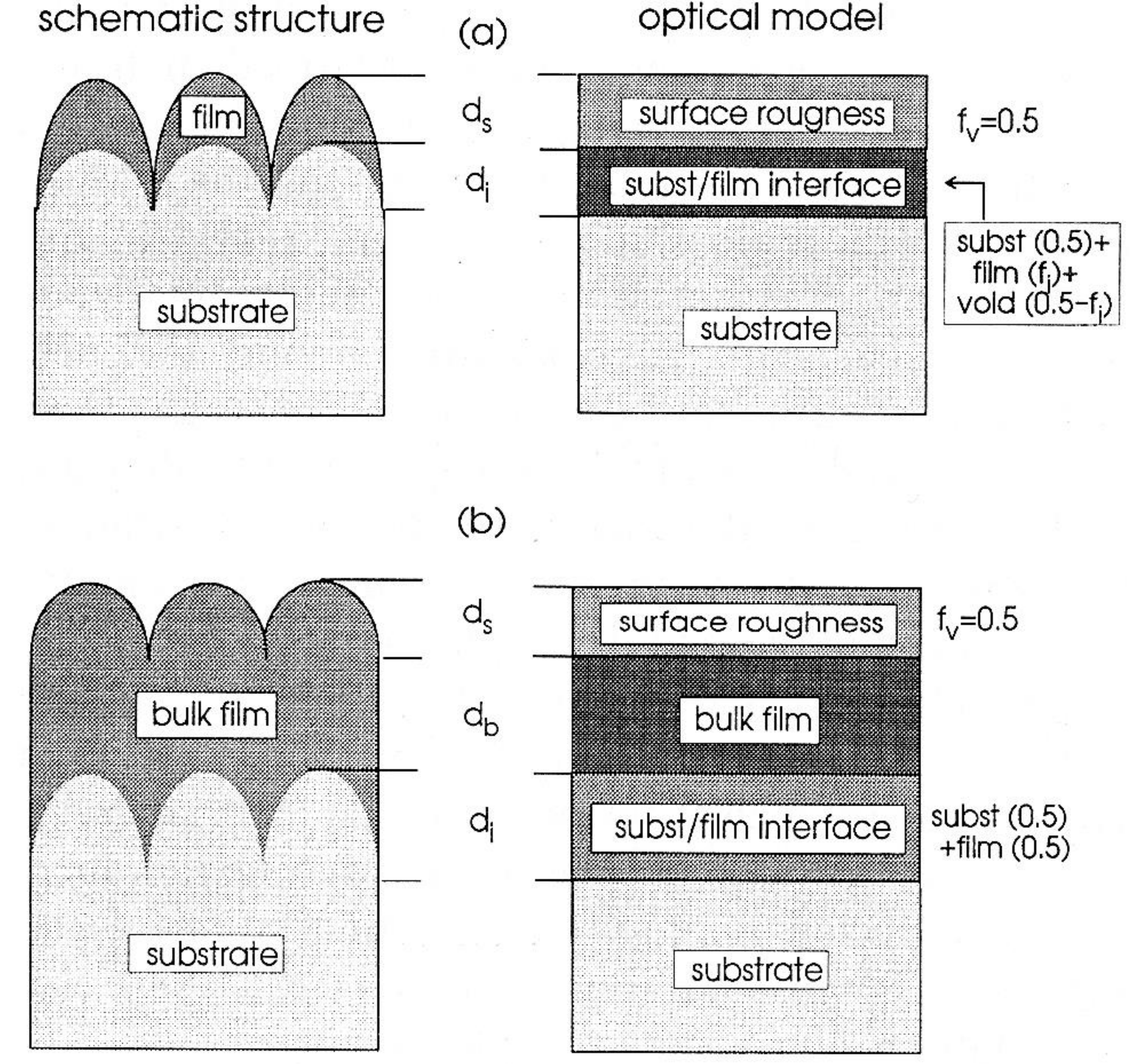
$$\varepsilon = \varepsilon_h \quad \Rightarrow \quad 0 = f_a \frac{\varepsilon_a - \varepsilon}{\varepsilon_a + 2\varepsilon} + f_b \frac{\varepsilon_b - \varepsilon}{\varepsilon_b + 2\varepsilon}$$





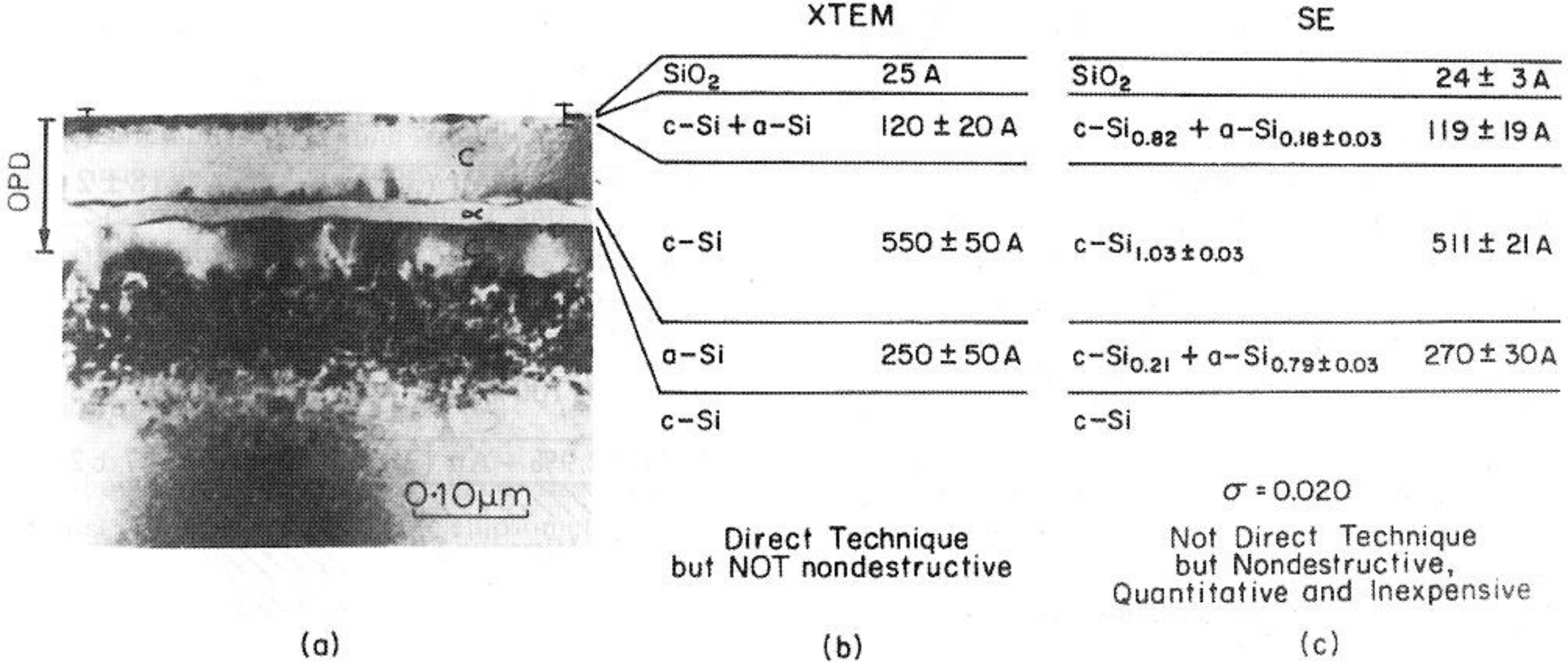
The two materials plays the same role but they are in interaction. Each type of inclusion is in interaction with the medium (it is supposed nevertheless spherical, depolarization coefficient equal to 1/3).

Surface and Interface



R.W.Collins, et al., Thin Solid Films,313-314,1998, pp18-32

Direct and Non-Direct Technique



XTEM		SE	
SiO_2	25 A	SiO_2	24 ± 3 A
c−Si + a−Si	120 ± 20 A	$c\text{−}Si_{0.82} + a\text{−}Si_{0.18 \pm 0.03}$	119 ± 19 A
c−Si	550 ± 50 A	$c\text{−}Si_{1.03 \pm 0.03}$	511 ± 21 A
a−Si	250 ± 50 A	$c\text{−}Si_{0.21} + a\text{−}Si_{0.79 \pm 0.03}$	270 ± 30 A
c−Si		c−Si	

$\sigma = 0.020$

Direct Technique
but NOT nondestructive

(b)

Not Direct Technique
but Nondestructive,
Quantitative and Inexpensive

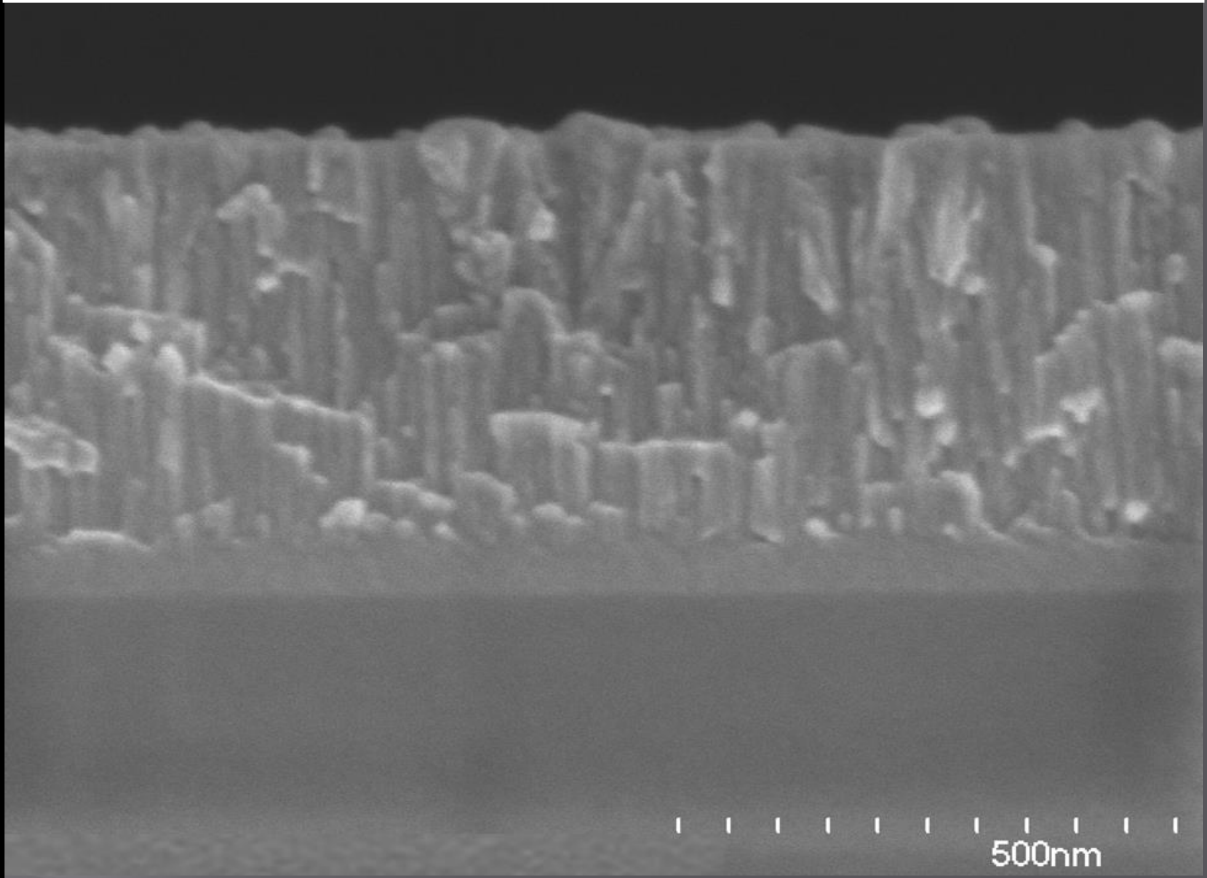
(c)

Source: K. Vedam, Thin Solid Film14 (1998) pp. 1-9

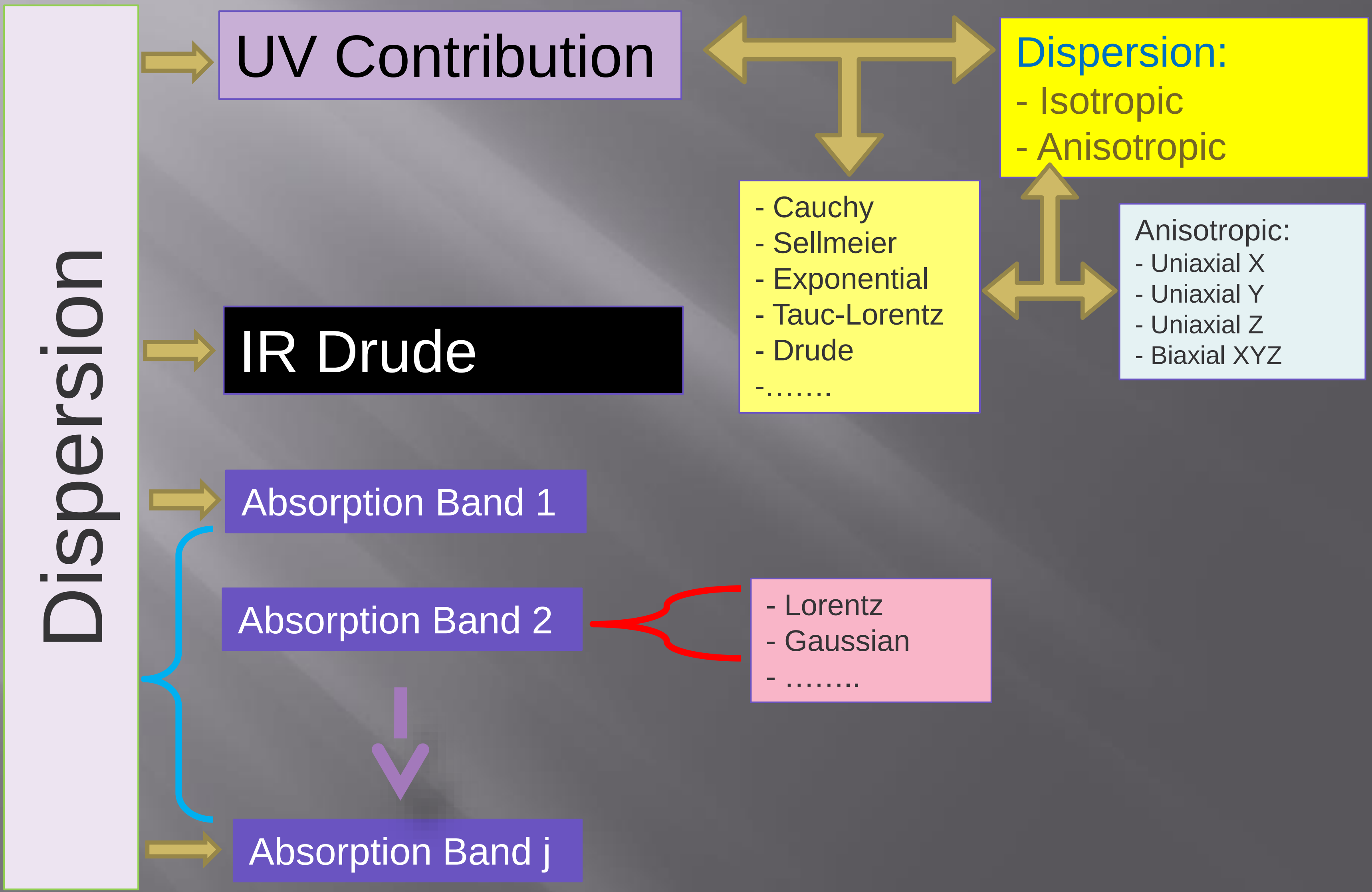
SE vs SEM for Inhomogeneous Film TiO_2

SE Model	
Thickness (nm)	n@1550nm
13.5	1.7211
424.42	2.2363
66.71	2.2825
Si Substrate	

SEM Photo



Dispersion



Dispersion

UV Contribution

IR Drude

Absorption Band 1

Absorption Band 2

Absorption Band j

- Cauchy
- Sellmeier
- Exponential
- Tauc-Lorentz
- Drude
-…….

Dispersion:
- Isotropic
- Anisotropic

Anisotropic:
- Uniaxial X
- Uniaxial Y
- Uniaxial Z
- Biaxial XYZ

- Lorentz
- Gaussian
- ……..

Dispersion (UV Contribution)

Dispersion

UV Contribution

- Cauchy NK

$$n = A + B/\lambda^2 + C/\lambda^4$$

$$k = D + E/\lambda^2 + F/\lambda^4$$

- Cauchy $\varepsilon_r/\varepsilon_i$

$$\varepsilon_r = A + B/\lambda^2 + C/\lambda^4$$

$$\varepsilon_i = D/\lambda + E/\lambda^3 + F/\lambda^5$$

- Sellmeier

$$\varepsilon_r = 1 + (A^2 - 1)\lambda^2/(\lambda^2 - B)$$

$$\varepsilon_i = C/\lambda + D/\lambda^2 + E/\lambda^3$$

- Exponential

$$\varepsilon_r = A + B\lambda^2 + C(D + (E + F/\lambda^2)/\lambda^2)/\lambda^2)\lambda^2$$

$$\varepsilon_i = 0$$

-Tauc-Lorentz

$$\varepsilon_i(E) = \frac{AE_0C(E - E_g)^2}{((E^2 - E_0)^2 + C^2E^2)E}$$ for E > Eg

$$\varepsilon_i(E) = 0$$ for E < Eg

- more

Dispersion (IR Contribution)

Dispersion

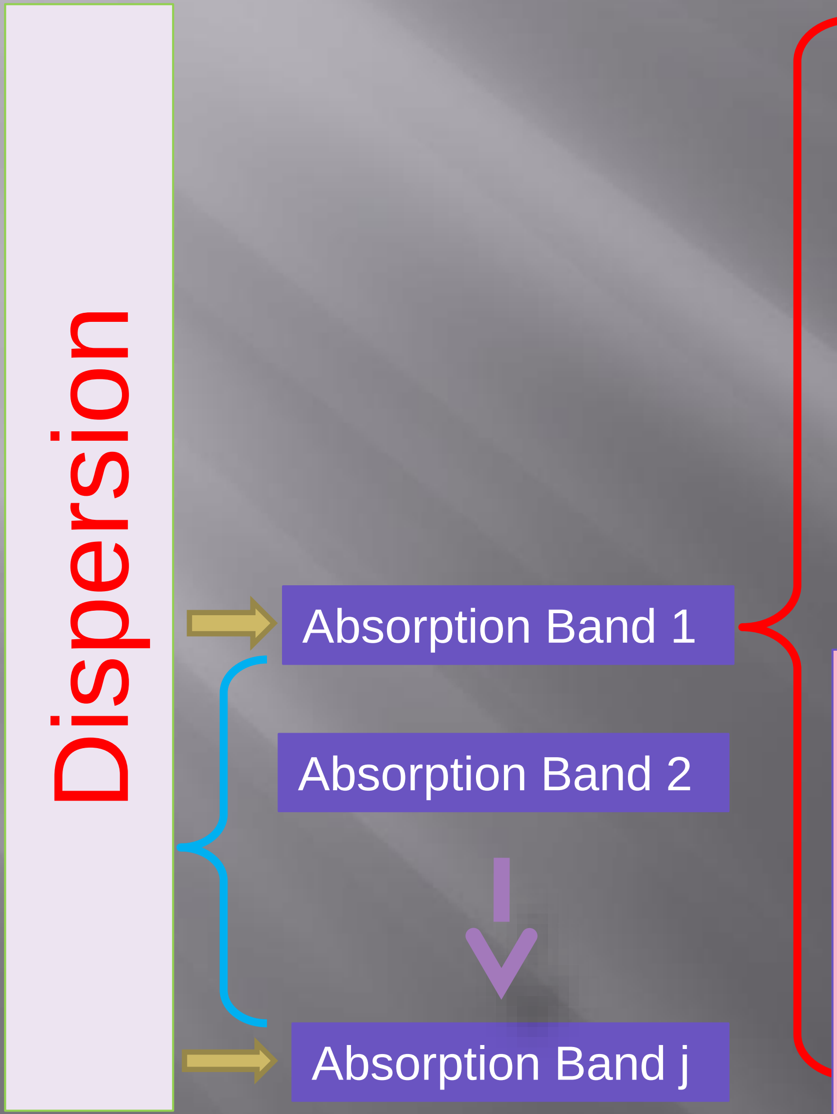
$$\varepsilon_r = P - (1/L_o)^2\lambda^2/(1+((1/\tau)\lambda)^2)$$

$$\varepsilon_i = (1/\tau)(1/L_o)^2\lambda^3/(1+((1/\tau)\lambda)^2)$$

IR Drude

Note: P is the polarization, 1/τ the mean free pass and 1/Lo the inverse of the plasma wavelength.

Dispersion (Absorption Bands)



- Lorentz

$$\varepsilon_r = A\lambda^2(\lambda^2 - L_0{}^2)/\left[(\lambda^2 - L_0{}^2)^2 + \gamma^2\lambda^2\right]$$

$$\varepsilon_i = A\lambda^3\gamma/\left[(\lambda^2 - L_0{}^2)^2 + \gamma^2\lambda^2\right]$$

Note: *A is the amplitude , Lo is the central wavelength and γ is the width of the band or peak.*

$$\varepsilon_r = A\cdot imag(DoubleW(z))$$

$$\varepsilon_i = A\cdot real(DoubleW(z))$$

$$DoubleW(z) = (\exp(-z^2)\cdot erfc(-iz)$$

$$z = (1/L_0 - 1/\lambda)/\gamma$$

- Gaussian

APPLICATIONS

with Spectroscopic Ellipsometry

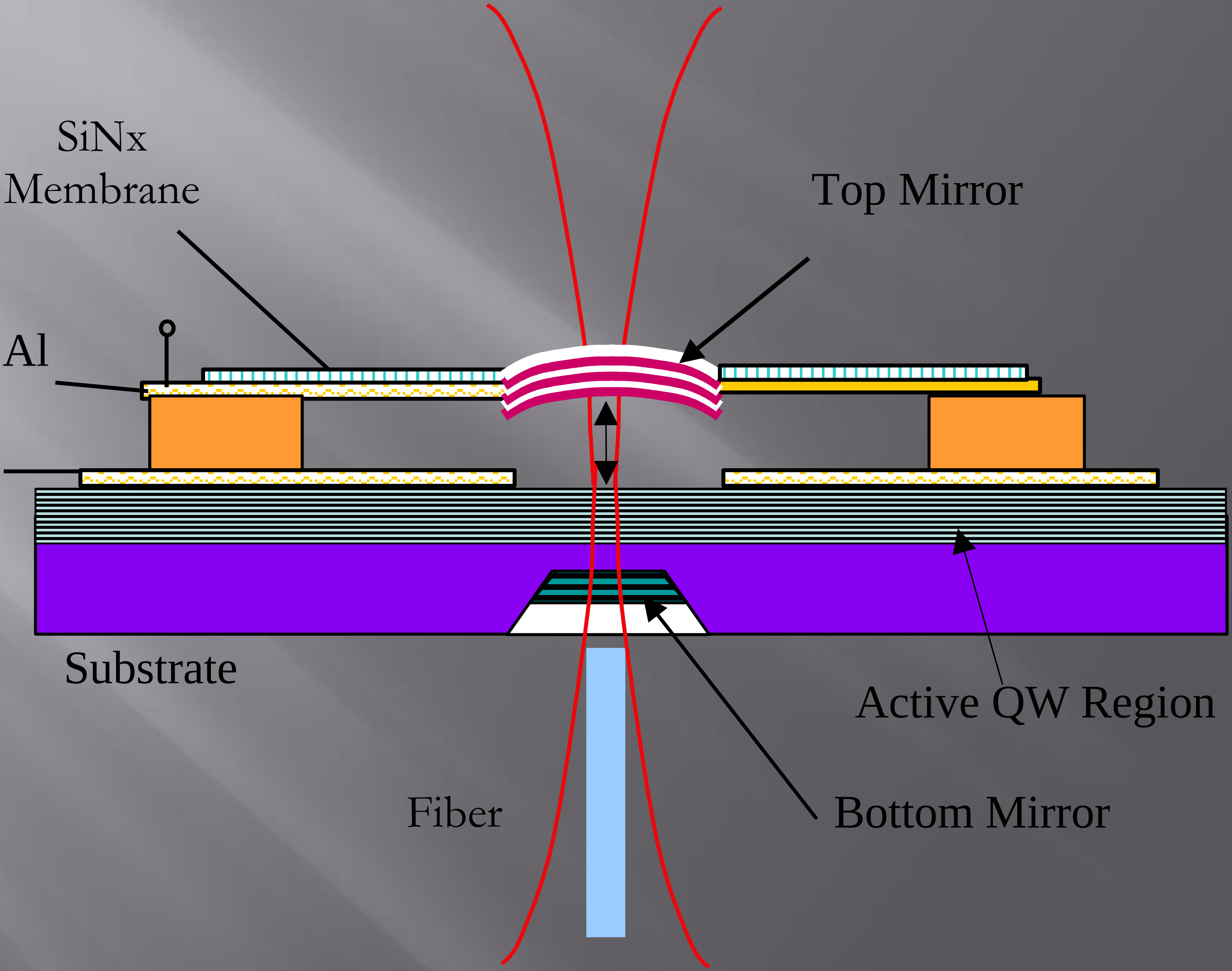
Applications

- Optical constants or dielectric constants for bulk materials
- Optical constants and thickness for films
- Surface, Interface and Composites
- Alloy concentration determination
- Real time monitoring for growth or etching kinetics study
- Band gaps
- Porosity
- Other properties derived from optical /dielectric constants

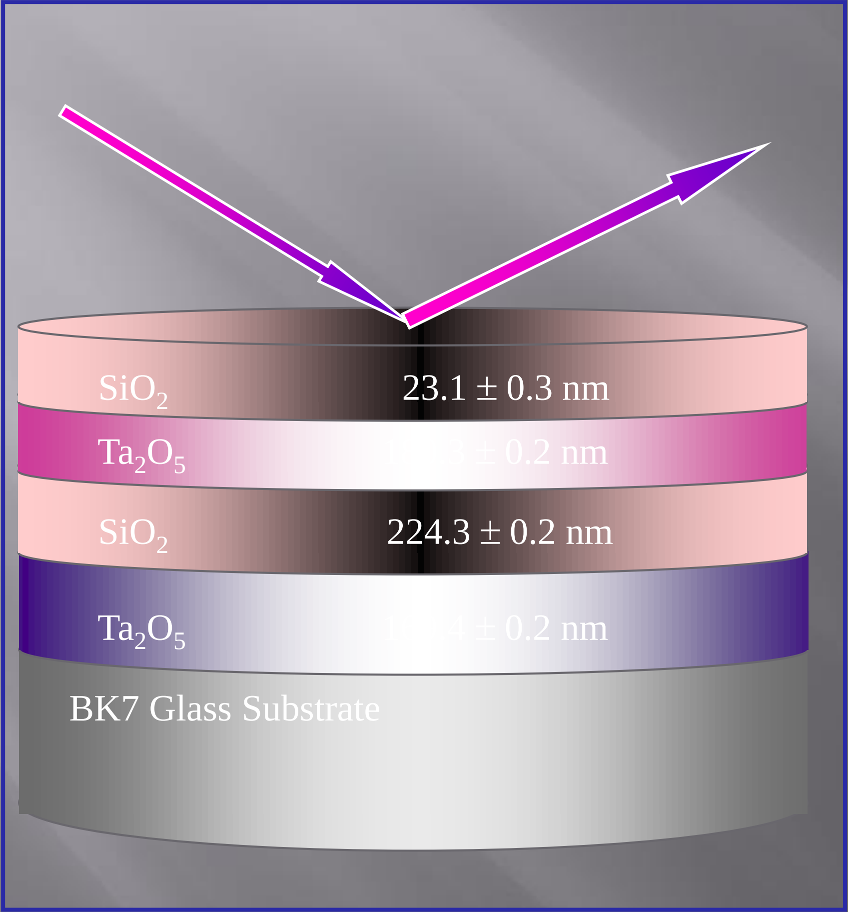
General Applications

- Materials:
    - Metals
    - Polymers
    - Ceramics and Glasses
    - Semiconductors and its Compounds
    - Composites
- Application Fields
    - **Semiconductor Industry**: Photoresist, Gate dielectrics, Semiconductors and their alloys or compounds such as, SiGe, InGaAs, AlInGaAs
    - **Photonics**
        - Optical coatings
        - Semiconductor compounds
        - Functional films in Optical MEMS
    - **Data Storage**
        - Diamond-like carbon (DLC)
        - Magnetic films
    - **Flat Panel Display** (FPD)
        - Thin film transistors (TFT) stack
        - Conductive oxide: Indium Tin Oxide (ITO)
    - **Solar Cell Industry**

Applications



Multilayer Dielectric Stack



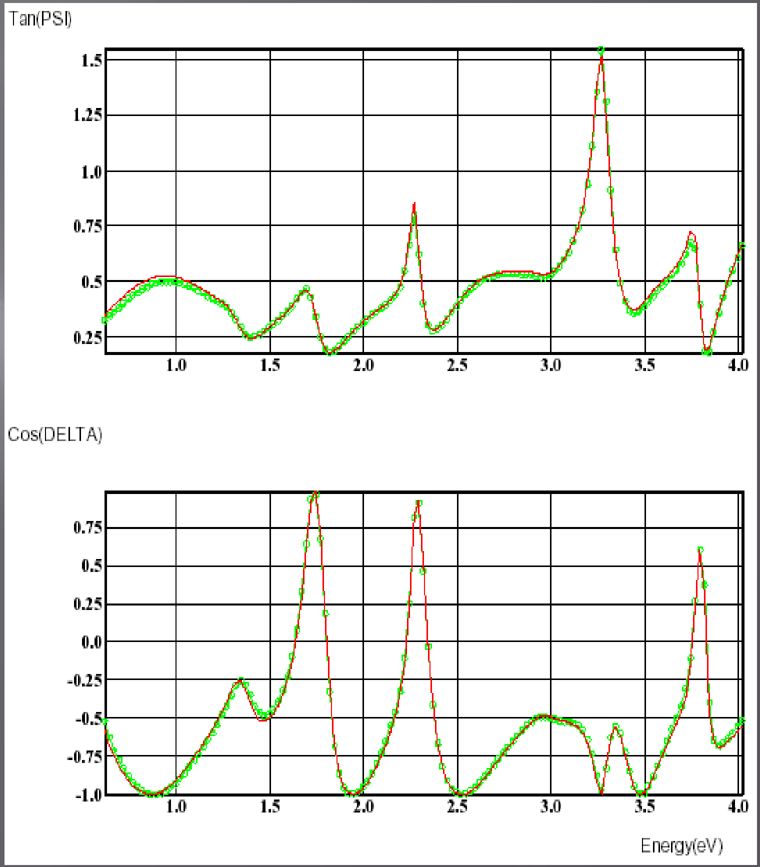
SiO_2 23.1 ± 0.3 nm

Ta_2O_5 18[illegible].3 ± 0.2 nm

SiO_2 224.3 ± 0.2 nm

Ta_2O_5 10[illegible].4 ± 0.2 nm

BK7 Glass Substrate



Summary

- Ellipsometry is a technique through monitoring the polarization state changes.
  - It offers nondestructive way to accurately determine film thickness and optical constants
- Many types of ellipsometers are available in the market. The selection and use of ellipsometer are highly application-oriented.
- SE has advantages over many other techniques.
- The ellipsometry is the *MODEL* based technique. It is not direct readout type instrument. Therefore:
  - **It is critical to use the right model to get right results**

Ellipsometry Advantages

Ellipsometry has many advantages over other techniques:

1. More ***comprehensive*** than any other tools: Optical, electrical, physical (or structural) and chemical (composition, bonding). All these information may be obtained from only one measurement.

2. ***Nondestructive*** compared with SIMS for composition

3. ***Non-contact*** compared with four-point probe for conductivity

4. ***Non-contact*** and no pattern needed compared with stylus profilometer for thickness

5. ***No vacuum*** requirement compared with all e-beam or ion-beam based instrument

Advantages – cont.

6. Ellipsometry is an ***absolute*** technique (no need of reference or standards)

7. Ellipsometry gives ***twice*** more information (both phase and amplitude ratio) than reflectometry (only intensity). In addition, as ellipsometer measures the polarisation state and not the intensity, it is less sensitive to light intensity fluctuations.

8. The phase information from ellipsometry is very ***sensitive to surface*** layers. Therefore, it is the best non-destructive technique for thin film characterisation.

Further Information Available

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