Study of Optical Properties of Isotropic Materials by Reflection Spectroscopic Ellipsometry

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Abstract

Ellipsometry is a versatile and invasive optical technique to study the optical properties of wide range of materials. The optical properties involves complex and real coefficients of refractive index in to $n - \iota\kappa$, absorption coefficient for lossy materials, dielectric constant and optical band gap. The principle of this technique is based on how s- and $p-$components of incident light change upon reflection, refraction or transmission from the sample material. The output polarization collected at detector helps to find ellipsometric parameters Ψ and Δ, which further helps to find optical properties of the sample material. This technique is also useful for characterization of thickness, roughness, composition, electrical conductivity etc. for isotropic materials. The study can further be expanded for anisotropic materials using Mueller-matrix formalism. In this experiment, we are studying isotropic thin films and are willing to find ellipsometric parameters Ψ and Δ, find n, k and d by using Ψ and Δ with the help of J.A. Woollam's Alpha-SE Ellipsometer and verify complex reflection coefficient ρ by using MATLAB.

KEYWORDS: Ellipsometry · Spectroscopic ellipsometry · Fresnel equations · Polarization · Tauc plot · Band gap · Mueller matrices · MATLAB for ellipsometry

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List of Symbols

A, B, C	Cauchy constants
I	Intensity
M	Mueller matrix
N, C, S	Mueller constants
R	Total reflected amplitude
S_i	Stokes vector for incident beam
S_r	Stokes vector for reflected beam
Δx	Path difference
Δ	Phase difference
$\vec{B}$	Magnetic field
$\vec{E}$	Electric field
$\vec{H}$	Magnetic field intensity
$\vec{k}$	Propagation vector
α	Absorption coefficient
δ	Phase-film thickness
κ	Extinction coefficient
λ	Wavelength
$\langle n \rangle$	Pesudo refractive index
ωt	Phase angle
ρ	Complex reflection coefficient (amplitude diminutions ratio)
$\tan \Psi$	Magnitude of reflectivity ratio
θ_B	Brewster angle
θ_c	Critical angle
θ_i	Angle of incidence
θ_r	Angle of reflection
θ_t	Angle of transmission
ε_r	Permittivity of medium
$\widetilde{n}$	Complex refractive index
d	Thickness of film
m_{ij}	Mueller matrix elements
n	Refractive index
r^p	Reflectance for p-polarization
r^s	Reflectance for s-polarization
t^p	Transmittance for p-polarization
t^s	Transmittance for s-polarization

Chapter 1

Introduction

This section provides a brief review of fundamental optics and light-matter interaction which is necessary for our study of spectroscopic ellipsometry. We will also discuss fundamental equations of polarization and use MATLAB to visualize propagation of wave.
For optical measurement[4], there are numerous techniques which are used to study different optical properties of electromagnetic radiations on the basis of reflection and transmission of light from a surface. Some of these are:

1. interferometry
2. reflectometry
3. ellipsometry

Interferometry It is a technique which uses the phenomenon of interference of waves to study different optical properties.

Reflectometry It uses the reflection of light at different surfaces for different mediums and interfaces. Usually, it is used for the characterization of thin films.

Ellipsometry It relies upon elliptical polarization and measures the change in polarization to study index of refraction and other optical characteristics of objects. It is classified into three categories:

1. scattering ellipsometry
2. transmission ellipsometry
3. reflection ellipsometry

All three techniques were developed in last decade for characterization of materials. A particular school of science owe their all progress to the revolution in this type of measurement techniques. Ellipsometry is one of those techniques which has revolutionized our research ideas. It is quite popular optical characterization technique and it is applied to wide research areas from semiconductors to organic materials.
The aim of this experiment is to provide deep and fundamental understanding for spectroscopic ellipsometry and how it helps to measure the optical parameters. This manual will comprehend the

data analysis techniques and measurement methods to be implemented practically in PhysLab. The prerequisite knowledge of optics is mandatory for better understanding of what is going behind the scene while working with alpha-SE Ellipsometer.
First, we will discuss 'optics' and 'polarization of light' and then we will study principle of ellipsometry. This will help to have a certain order and uniformity in our approach to ellipsometry and would be easy for reader to grasp the theoretical concepts.

1.1 Polarization of Light

Maxwell Rainbow constitutes the electromagnetic spectrum and in almost middle of that, we have an important type of radiation: visible light. Its wavelength ranges from $390\ \mathrm{nm}$ to $700\ \mathrm{nm}$ and they can easily be explained as sinusoidal waves in free space. But when light has its interaction with material at different angles, the behavior becomes complicated to understand and illustrate since light can be reflected, transmitted or it can be absorbed when it has some sort of interaction with matter.

Q 1. Derive wave equation using Maxwell equations.

1.1.1 What is Polarization of Light?

Light is an electromagnetic wave i.e. it has both electric and magnetic components. For the purpose of ellipsometric study, we are be more interested in behavior of electric field component in time and space, known as polarization. It is to clarify here that direction of propagation of light is always perpendicular to and direction. A propagating light in space or medium has three orthogonal directions associated with it:

1. direction of propagation $\vec{k}$
2. electric field $\vec{E}$
3. magnetic field $\vec{B}$

For example, if light is propagating along z-axis (z-polarized light), then $\vec{E}$ could be along y-axis and $\vec{B}$ along x-axis or vice versa. Mathematically,

$$\vec{E} = \hat{y}E_o\cos(kz - \omega t) \quad ; \quad \vec{B} = \hat{x}B_o\cos(kz - \omega t)$$

or

$$\vec{E} = \hat{x}E_o\cos(kz - \omega t) \quad ; \quad \vec{B} = \hat{y}B_o\cos(kz - \omega t)$$

These are the two possible set of equations for z-polarized light. Here ω the is angular frequency and k is the wave number. Temporal phase is represented by ωt while kz represents the spatial phase.

1.1.2 Visualization of Propagation of Light by using MATLAB

This is a sample code in MATLAB command window to visualize the propagation of light.

```
[x,y]=meshgrid(5:0.05:15,−5:0.05:5);
lambda=1;
k=2*pi/lambda;
f=3e8/lambda;
w=2*pi*f;
t=linspace(0,60e−9,200);
%z=exp(i*k*abs(x+i*y));
z=exp(i*k*x);
for n=1:length(t)
surf(x,y,real(z*exp(−i*w*t(n))));
%view(ceil(90*n*1/length(t)),ceil(90*n*2/length(t)));
view(3)
zlim([−1.5 1.5])
xlim([min(min(x)) max(max(x))])
ylim([min(min(y)) max(max(y))])
shading interp
getframe();
end
```

Q 2. Using MATLAB code given in section 2.2.2, visualize the electromagnetic wave propagation, write your observations and paste graph in your lab report.

1.1.3 Types of Polarization

When two orthogonal light waves are in-phase, the resulting light will be *linearly* polarized. The relative amplitudes determine the resulting orientation. If the orthogonal waves are $90°$ out-of-phase and equal in amplitude, the resultant light is *circularly* polarized. The most common polarization is *elliptical*, one that combines orthogonal waves of arbitrary amplitude and phase. This is where ellipsometry gets its name. Plane wave solution of electric field by Maxwell's equations is:

$$\vec{E} = \vec{E_o} \exp i(kz - \omega t) \tag{2.1}$$

Here, $\vec{E_o}$ is the polarization vector for electric field and it moves in the z direction. Since $\vec{E_o}$ is orthogonal to $\vec{k}$, so

$$\vec{E_o} = (E_x, E_y, 0)$$

where E_x and E_y are complex in nature.
Now, Eq. 2.1 can also be written as:

$$\vec{E} = E_x\hat{x}\cos(kz - \omega t + \phi_x) + E_y\hat{y}\cos(kz - \omega t + \phi_y) \tag{2.2}$$

For linear polarization, there is no phase difference i.e. if $E_y = 0$ then $E_x \neq 0$, so Eq. 2.2 becomes now

$$\vec{E} = E_o\hat{x} \exp i(kz - \omega t)$$

$$\boxed{\vec{E} = E_o\hat{x}\cos(kz - \omega t)}$$

This is *linearly polarized light in x-direction*.
Similarly,

$$\vec{E} = E_o \hat{y} \exp i(kz - \omega t)$$

$$\boxed{\vec{E} = E_o \hat{y} \cos(kz - \omega t)}$$

This is *linearly polarized light in y-direction*.

Q 3. On the same basis, solve Maxwell equation for circularly polarized light. Also show that linearly polarized light can be written as a sum of left and right circular light.

Q 4. Find and describe the electromagnetic field produced by a superposition of two equal-amplitude, monochromatic, plane waves that propagate in opposite directions. Let the wave propagating along $+z$ have left circular polarization and the wave propagating along $-z$ have right circular polarization.

1.2 Light-Matter Interaction

When light interacts with matter, its behavior is studied with the help of two coefficients:

1. refractive index (n)
2. extinction coefficient (κ)

Here, refractive index which is the ratio of speed of light in vacuum to speed of light in medium.

$$n = \frac{c}{v}$$

The refractive index for air is 1.0003, which shows speed of light in air is $2.99 \times 10^8\ \mathrm{m\,s^{-1}}$, a bit less than speed of light in vacuum (n = 1 for vacuum). And κ is attenuation coefficient or extinction coefficient.

Q 5. Show that for different wavelength of light, value of refractive index is also different?

Q 6. What is the difference in propagation of EM waves, when it travels through a transparent medium and an absorbing medium.

For transparent medium, electromagnetic wave propagation can be described completely by studying refractive index, but for absorbing media, it is merely not possible to describe wave propagation completely. This is where we require κ. Generally, wave propagation is a combination of both refractive index and extinction coefficient i.e.

$$\sqrt{\varepsilon_r} = n - i\kappa$$

Here, ε_r is the permittivity of the medium.

Q 7. If ε_r = 8.5 - 13.5i, then find the values of n and κ.

1.3 Absorption Coefficient

When light enters a material (having higher index), it slows down. Since the frequency of waves remains unchanged, this shortens the wavelength. The attenuation coefficient κ terms the loss of energy of the wave in lossy material. It can be related to the absorption coefficient as:

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

Beer's law explains how light loses intensity in the lossy material. Thus, the complex refractive index coefficient (extinction coefficient) describes that how rapidly light vanishes in an absorbing material. Mathematically,

$$I(x) = I_o e^{-i\alpha x}$$

Chapter 2

Reflection and Transmission by Planar Interfaces

When light interact with planar boundaries, a part of it is reflected and a part is transmitted. It is quite easy to understand the behaviour of incident light by splitting its plane of polarization into following components:

TE Polarization If magnetic field $\vec{B}$ is parallel to the plane of incidence and electric field $\vec{E}$ is perpendicular to the plane of incidence, then this is called *s-polarization*[1]*, TE polarization,* σ*-polarization* or *sagittal plane polarization*.

TM Polarization If electric field $\vec{E}$ is parallel to the plane of incidence then magnetic field $\vec{B}$ will surely be perpendicular to the plane of incidence, this is called *p-polarization, TM polarization,* π*-polarization* or *tangential plane polarization*.

It has been observed that reflection and transmission coefficients, for TE and TM waves, played a key role in development of optics. In 1823, Fresnel[6] was the first one who attempted to derive these coefficients theoretically.

2.1 TE Polarization

Consider an x polarized electric field $\vec{E}$ parallel to the plane of incidence. So

$$\vec{E_i} = \hat{x} E_i e^{-i\vec{k_i}.\vec{r}}$$
$$\vec{k_i} = k_1 \left(\hat{z}\cos\theta_i + \hat{y}\sin\theta_i\right)$$

[1]Label *'s'* stands for a German word *senkrecht* means *perpendicular*.

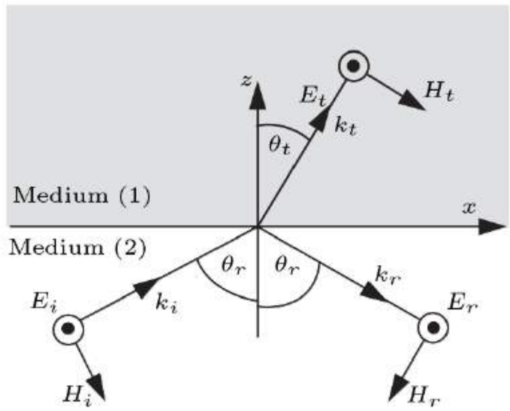


Figure 2.1: s-polarized wave perpendicular to the plane of incidence

It gives

$$\nabla \times \vec{E_i} = -\frac{\partial \vec{B}}{\partial t}$$
$$-i\vec{k_i} \times \vec{E_i} = -i\omega \vec{B}$$
$$\vec{B_i} = \frac{1}{\omega}\vec{k_i} \times \vec{E_i}$$
$$\vec{B_i} = \frac{E_i k_1}{\omega}\left(\hat{y}\cos\theta_i - \hat{z}\sin\theta_i\right) e^{-i\vec{k_i}.\vec{r}}$$

Similarly, for reflected and transmitted waves, we have

$$\vec{E_r} = \hat{x}E_r e^{-i\vec{k_r}.\vec{r}}$$
$$\vec{B_r} = \frac{E_r k_1}{\omega}\left(-\hat{z}\sin\theta_r - \hat{y}\cos\theta_r\right) e^{-i\vec{k_r}.\vec{r}}$$

And

$$\vec{E_t} = \hat{x}E_t e^{-i\vec{k_t}.\vec{r}}$$
$$\vec{B_t} = \frac{E_t k_2}{\omega}\left(\hat{y}\cos\theta_t - \hat{z}\sin\theta_t\right) e^{-i\vec{k_t}.\vec{r}}$$

By applying boundary conditions for tangential and normal components, it is revealed that

$$E_r = E_i\left(\frac{z_2\cos\theta_i - z_1\cos\theta_t}{z_2\cos\theta_i + z_1\cos\theta_t}\right)$$
$$r^s = \frac{E_r}{E_i} = \frac{z_2\cos\theta_i - z_1\cos\theta_t}{z_2\cos\theta_i + z_1\cos\theta_t} \tag{2.1}$$

And

$$E_t = E_i\left(\frac{2z_2\cos\theta_i}{z_2\cos\theta_i + z_1\cos\theta_t}\right)$$
$$t^s = \frac{E_t}{E_i} = \frac{2z_2\cos\theta_i}{z_2\cos\theta_i + z_1\cos\theta_t} \tag{2.2}$$

For two non-magnetic dielectric mediums (i.e., $\mu_1 = \mu_2 = 1$ but $\epsilon_1 \neq \epsilon_2 \neq 1$), we can rewrite Eqs. (2.1) and (2.2) in terms of refractive index by using the fact that

$$\frac{z_1}{z_2} = \frac{\mu_1 n_2}{\mu_2 n_1} = \frac{n_2}{n_1}$$

i.e.

$$r^s = \frac{n_1 \cos\theta_i - n_2 \cos\theta_t}{n_1 \cos\theta_i + n_2 \cos\theta_t} \tag{2.3}$$

And

$$t^s = \frac{2n_1 \cos\theta_i}{n_1 \cos\theta_i + n_2 \cos\theta_t} \tag{2.4}$$

Eqs. (2.3) and and (2.4) are the famous Fresnel equations.

Q 8. Derive the reflection and transmission amplitude of the magnetic field for the TM polarized incident plane wave from a planar interface located at $z = 0$. Now, compute the reflectance as the ratio of the z components of the time-averaged Poynting vector of the reflected and incident plane wave. Similarly, compute the transmittance.
Answer

Reflectance for p-polarized case is:

$$r^p = \frac{n_2 \cos\theta_i - n_1 \cos\theta_t}{n_2 \cos\theta_i + n_1 \cos\theta_t}$$

And transmittance is

$$t^p = \frac{2n_1 \cos\theta_i}{n_2 \cos\theta_i + n_1 \cos\theta_t}$$

2.2 Special Cases

Now, we will discuss some special cases for Fresnel equations.

2.2.1 Normal Incidence

For normal incidence, $\cos\theta_i = \cos\theta_t = 1$ because $\theta_i = \theta_t = 0$, so Eqs. (2.1) and (2.2) reduces to

$$r^s = \frac{z_2 - z_1}{z_2 + z_1} = \frac{n_1 - n_2}{n_1 + n_2}$$

And

$$t^s = \frac{2z_2}{z_2 + z_1} = \frac{2n_1}{n_1 + n_2}$$

Q 9. For normal incidence,find the transmittance and reflectance relations for TM polarization.

2.2.2 Total Internal Reflection

For total internal reflection, when If light is incident on a planar boundary in such a way that $\theta_i > \theta_c$, then light is totally reflected back and there is no transmission to other medium (as an ideal case). That special angle θ_c is known as 'critical angle'.

2.2.3 Brewster Angle

At Brewster angle θ_B, no light is reflected but all is transmitted to the second medium. It is given as

$$\theta_B = \tan^{-1}\left(\frac{n_2}{n_1}\right)$$

Note: In Ellipsometry technique, waves of s- and p- polarized light are irradiated onto the sample at a certain angle, known as Brewster angle. In the principle behind the ellipsometry technique, we are interested in measuring the ratio of the amplitude reflection coefficients for p- and s- polarized light waves r^p/r^s. At θ_B the difference between r^p and r^s is maximized and so the sensitivity of measurement, for this reason ellipsometry measurements are usually performed at θ_B.

Q 10. Using $r^s = 0$ in reflectance relation, Prove the relation for Brewster angle given above.

Q 11. For the air/glass interface, Find the value of θ_B.

Chapter 3

Spectroscopic Ellipsometry

As we have discussed about different types of ellipsometry: *scattering, transmission, reflection*. However, we are interested in reflection ellipsometry only. Since its name comes from phenomenon of elliptical polarization of light and it is based upon the change in polarization of light. It makes it a very versatile, non-invasive and non-destructive technique. It has been acknowledged that Paul Drude was the first one who established the fundamental principles of ellipsometry in 1888 [11] and its first documented use was done by A. Rothen [7] in 1945 to measure the thickness of thin surface films.
Ellipsometry is sometimes termed as spectroscopic ellipsometry. The reason is that all work is done as a function of light's energy or wavelength. The rule for ellipsometry is that it measures change in state of polarization as it is transmitted or reflected from a material. The resulting change in polarization of light is represented by phase difference (Δ) and amplitude ratio (Ψ) i.e.

$$\rho = \tan(\Psi)e^{i\Delta}$$

Optical properties as well as thickness of materials are the reason for change in polarization state so these parameters can be extracted from the information collected at the detector.
Most of ellipsometry interest lies in how p- and s- polarized components of light change when they are reflected or transmitted. Initially known polarized beam is transmitted or reflected from the sample material and output polarization is recorded and measured.

3.1 Fundamental Equation of Ellipsometry

Now, we are going to derive classical fundamental equation of ellipsometry i.e. we aim to relate amplitude diminutions ratio ρ to phase difference Δ and magnitude of reflectivity ratio $\tan\Psi$.
Consider an incident monochromatic plane wave falling on medium 1 has components parallel E_i^p and perpendicular E_i^s to the plane of incidence as shown in figure 3.1. Here, E_r^p and E_r^s are the reflected components of the plane wave.

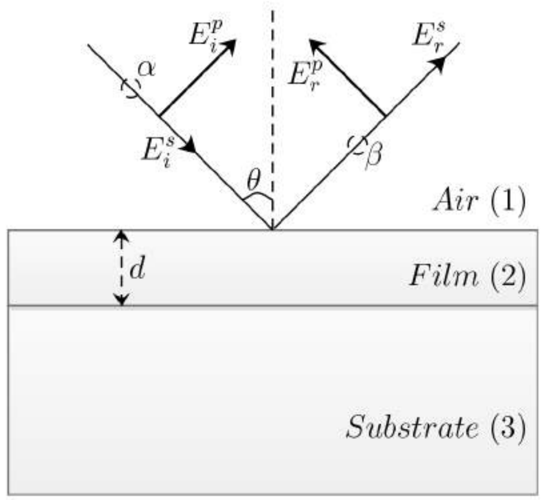


Figure 3.1: Reflection of an incident plane wave by an optical film of thickness d

Now, the incident wave is

$$E_i^p = E_{io}^p e^{\iota\alpha^p}$$
$$E_i^s = E_{io}^s e^{\iota\alpha^s}$$

Generally

$$E_i^j = E_{io}^j e^{\iota\alpha^j} \tag{3.1}$$

where $j = p, s$.
And, the reflected wave is

$$E_r^p = E_{ro}^p e^{\iota\beta^p}$$
$$E_r^s = E_{ro}^s e^{\iota\beta^s}$$

Generally

$$E_r^j = E_{ro}^j e^{\iota\beta^j} \tag{3.2}$$

where $j = p, s$.
Here, for brevity, we have suppressed the propagation phase factor $\omega t - k_i z$ to α and $\omega t - k_r z$ to β. For optically absorbing materials, the induced field will be attenuated and undergo a phase shift. It is expressed in terms of complex reflection coefficient (ρ) i.e.

$$\rho_r^j = \frac{E_r^j}{E_i^j} \tag{3.3}$$

By putting E_i^j and E_r^j from Eqs. (3.1) and (3.2) respectively, we get

$$\rho_r^j = \frac{E_{ro}^j e^{\iota\beta^j}}{E_{io}^j e^{\iota\alpha^j}}$$
$$\rho_r^j = \frac{E_{ro}^j}{E_{io}^j} e^{\iota\beta^j - \iota\alpha^j}$$
$$\rho_r^j = \frac{E_{ro}^j}{E_{io}^j} e^{\iota\left(\beta^j - \alpha^j\right)}$$

Let us define a complex relative amplitude attenuation as

$$\rho = \frac{\rho^p}{\rho^s}$$
$$\rho = \frac{\dfrac{E_{ro}^p}{E_{io}^p} e^{\iota(\beta^p - \alpha^p)}}{\dfrac{E_{ro}^s}{E_{io}^s} e^{\iota(\beta^s - \alpha^s)}}$$
$$\rho = \frac{E_{ro}^p / E_{io}^p}{E_{ro}^s / E_{io}^s} e^{\iota[(\beta^p - \beta^s) - (\alpha^p - \alpha^s)]}$$
$$\rho = \frac{E_{ro}^p / E_{io}^p}{E_{ro}^s / E_{io}^s} e^{\iota(\beta - \alpha)}$$

where $\beta = \beta^j - \beta^s$ and $\alpha = \alpha^j - \alpha^s$. Now by putting $\Delta = \beta - \alpha$, which is phase change, we get

$$\rho = \frac{E_{ro}^p / E_{io}^p}{E_{ro}^s / E_{io}^s} e^{\iota\Delta} \tag{3.4a}$$

And, we know that if the planes of polarization for the reflected and the transmitted light are rotated in opposite directions relative to the polarization plane of the incident light then the angle γ_i that the plane of polarization of the incident light form with the plane of incidence is:

$$\tan\gamma_i = \frac{E_{io}^p}{E_{io}^s}$$

And

$$\tan\gamma_r = \frac{E_r^p}{E_r^s}$$
$$\tan\gamma_r = \frac{\dfrac{E_{ro}^p}{E_{io}^p} E_{io}^p}{\dfrac{E_{ro}^s}{E_{io}^s} E_{io}^s}$$
$$\tan\gamma_r = \frac{E_{ro}^p / E_{io}^p}{E_{ro}^s / E_{io}^s} \tan\gamma_i$$
$$\frac{\tan\gamma_r}{\tan\gamma_i} = \frac{E_{ro}^p / E_{io}^p}{E_{ro}^s / E_{io}^s}$$

So, Eq. (3.4a) becomes now

$$\rho = \frac{\tan \gamma_r}{\tan \gamma_i} e^{\iota \Delta}$$

By putting $\frac{\tan \gamma_r}{\tan \gamma_i} = \tan \Psi$, we get

$$\rho = \tan \Psi e^{\iota \Delta} \tag{3.4b}$$

It is the classical fundamental equation of ellipsometry[2]. By measuring Ψ and Δ, optical constants n, k and d can also be found.

3.2 Three-Phase Optical System (Air-Film-Substrate System)

Let us consider a parallel-sided three-phase optical system, shown in figure 3.2 i.e. air-film-substrate system named as medium 1, medium 2 and medium 3 having refractive indices n_1, n_2 and n_3. We are aiming to find reflection coefficient for multiple reflections by using method of summation[3]. For simplicity, we are considering

- monochromatic plane wave is incident on medium 1,
- medium 1 is non-amplifying,
- system is parallel-sided,
- medium 2 is of very small thickness (up to few microns),
- media 1 and 3 are of infinite thickness,
- system is homogeneous and isotropic.

Remember: We are using notation, generally, r_{ab} which means that incident wave is coming from medium a and falling on medium b.

Normally, for single interface (two-phase), incident plane wave transmits to medium 2 and continues its motion. But for dual interface (three-phase system), a part of plane wave is transmitted to medium 3 and a part is reflected back to medium 2 which heads towards medium 1. This is termed as a partial wave. For example, we have regarded second partial wave R_2 as $t_{12}r_{23}$. Same process repeats, somehow many times, for all partial waves. Plane wave will also experience a phase change as it will traverse from interface to another. So, a phase factor $e^{-2\iota\delta}$ is included in complex reflection amplitude where δ is film-phase thickness and we will use the following recipe to deduce δ. Consider figure 3.3 Since

$$path\ difference = n_2 \left(\overline{AB} + \overline{BC}\right) - n_1 \left(\overline{AD}\right) \tag{3.5}$$

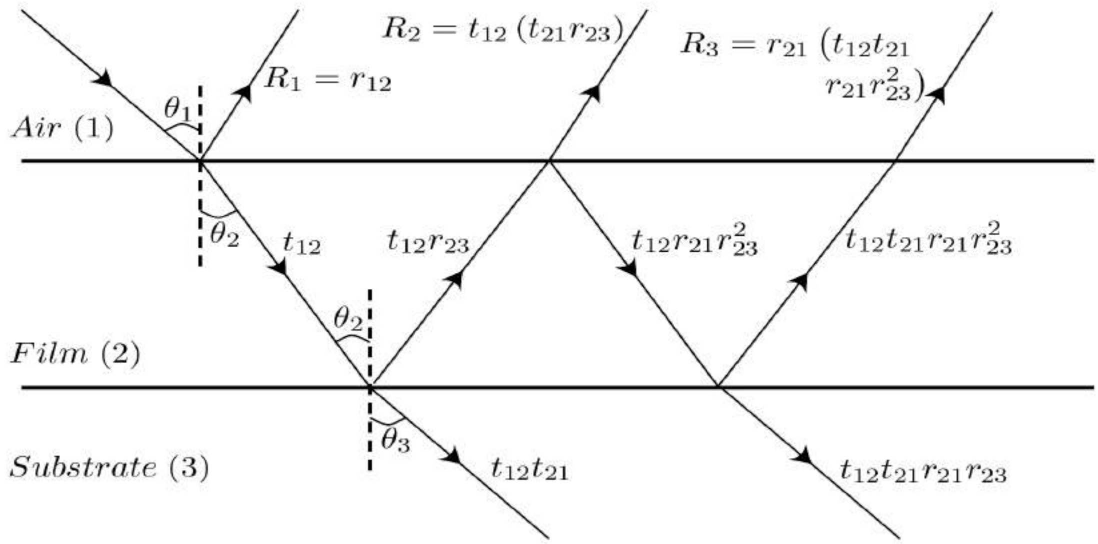


Figure 3.2: Propagation of plane wave through air-film-substrate system

Since

$$\cos\theta_2 = \frac{\overline{BO}}{\overline{AB}} \qquad ; \qquad \cos\theta_2 = \frac{\overline{BO}}{\overline{BC}}$$
$$\overline{AB} = \frac{d}{\cos\theta_2} \qquad ; \qquad \overline{BC} = \frac{d}{\cos\theta_2}$$

And

$$\frac{\overline{AD}}{\overline{AC}} = \sin\theta_1 \qquad \Rightarrow \qquad \overline{AD} = \overline{AC}\sin\theta_1 \tag{3.6}$$
$$\tan\theta_2 = \frac{\overline{AO}}{\overline{BO}} \qquad \Rightarrow \qquad \overline{AO} = d\tan\theta_2$$

It gives

$$\overline{AC} = 2\left(\overline{AO}\right) \qquad \Rightarrow \qquad \overline{AC} = 2d\tan\theta_2$$

Eq. (3.6) becomes now

$$\overline{AD} = 2d\sin\theta_1\tan\theta_2$$

By substituting these values to Eq. (3.5), we get

$$path\ difference = \frac{2n_2 d}{\cos\theta_2} - 2n_1 d\sin\theta_1\tan\theta_2$$

By Snell's law

$$n_1\sin\theta_1 = n_2\sin\theta_2$$

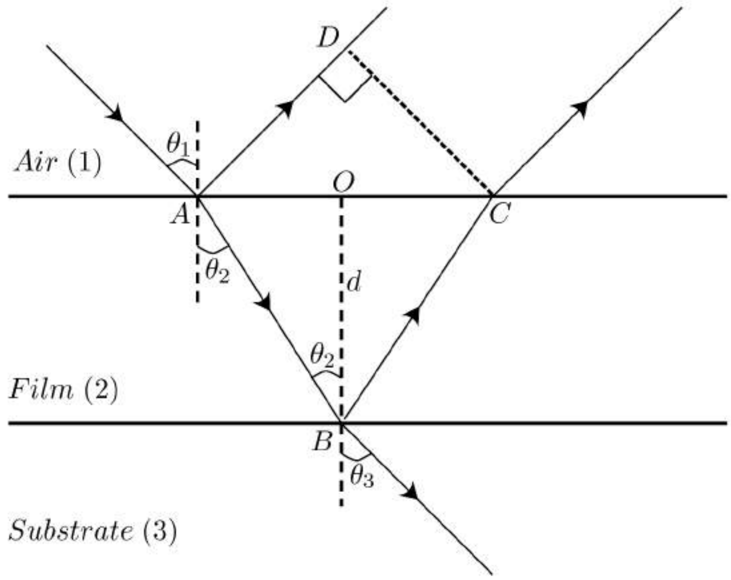


Figure 3.3: Phase film thickness

So

$$path\ difference = \frac{2n_2 d}{\cos\theta_2} - 2d\frac{\sin\theta_2}{\cos\theta_2} n_2 \sin\theta_2$$
$$\Delta x = 2n_2 d\cos\theta_2$$

Since

$$phase\ difference = \frac{2\pi}{\lambda}(\Delta x)$$
$$\delta' = \frac{2\pi}{\lambda}\left(2n_2 d\cos\theta_2\right)$$
$$\delta' = 2\left(\frac{2\pi}{\lambda} n_2 d\cos\theta_2\right)$$
$$\delta' = 2\delta$$

where

$$\delta = \frac{2\pi}{\lambda} n_2 d\cos\theta_2$$

So, the successive partial waves can now be written as:

$$R_1 = r_{12} e^{-0\iota\delta}$$
$$R_2 = t_{12} t_{21} r_{23} e^{-2\iota\delta}$$
$$R_3 = t_{12} t_{21} r_{21}^2 r_{23}^2 e^{-4\iota\delta}$$

and so on.

Now, the total reflected amplitude is

$$\begin{aligned}
R &= R_1 + R_2 + R_3 + \cdots \\
R &= r_{12}e^{-0\iota\delta} + t_{12}t_{21}r_{23}e^{-2\iota\delta} + t_{12}t_{21}r_{21}^2r_{23}^2e^{-4\iota\delta} + \cdots \\
R &= r_{12} + t_{12}t_{21}r_{23}\left[1 + \left(r_{21}r_{23}e^{-2\iota\delta}\right) + \cdots\right]
\end{aligned}$$

Using

$$\frac{1}{1-x} = 1 + x + x^2 + \cdots$$

So

$$R = r_{12} + \frac{t_{12}t_{21}r_{23}e^{-2\iota\delta}}{1 - r_{21}r_{23}e^{-2\iota\delta}} \tag{3.7}$$

From Fresnel coefficients, we know that

$$r_{21} = -r_{12} \qquad ; \qquad t_{21} = \frac{1-r_{12}^2}{t_{12}} \qquad \Rightarrow \qquad t_{12}t_{21} = 1 - r_{12}^2$$

Eq. (3.7) becomes now

$$R = \frac{r_{12} + r_{23}e^{-2\iota\delta}}{1 + r_{21}r_{23}e^{-2\iota\delta}}$$

For *s*-polarization

$$R^s = \frac{r_{12}^s + r_{23}^s e^{-2\iota\delta}}{1 + r_{21}^s r_{23}^s e^{-2\iota\delta}}$$

And for *p*-polarization

$$R^p = \frac{r_{12}^p + r_{23}^p e^{-2\iota\delta}}{1 + r_{21}^p r_{23}^p e^{-2\iota\delta}}$$

where

$$r_{12}^s = \frac{n_1\cos\theta_1 - n_2\cos\theta_2}{n_1\cos\theta_1 + n_2\cos\theta_2} \qquad ; \qquad r_{23}^s = \frac{n_2\cos\theta_2 - n_3\cos\theta_3}{n_2\cos\theta_2 + n_3\cos\theta_3}$$

and

$$r_{12}^p = \frac{n_1\cos\theta_2 - n_2\cos\theta_1}{n_1\cos\theta_2 + n_2\cos\theta_1} \qquad ; \qquad r_{23}^p = \frac{n_2\cos\theta_3 - n_3\cos\theta_2}{n_2\cos\theta_3 + n_3\cos\theta_2}$$

3.2.1 Solution of Fundamental Equation of Ellipsometry for n_3

Since we know that

$$r_{13}^p = \frac{n_3 \cos\theta_1 - n_1 \cos\theta_3}{n_3 \cos\theta_1 + n_1 \cos\theta_3} \qquad ; \qquad r_{13}^s = \frac{n_1 \cos\theta_1 - n_3 \cos\theta_3}{n_1 \cos\theta_1 + n_3 \cos\theta_3}$$

For $n_1 = 1$

$$r_{13}^p = \frac{n_3 \cos\theta_1 - \sqrt{1-\sin^2\theta_3}}{n_3 \cos\theta_1 + \sqrt{1-\sin^2\theta_3}} \qquad ; \qquad r_{13}^s = \frac{\cos\theta_1 - n_3\sqrt{1-\sin^2\theta_3}}{\cos\theta_1 + n_3\sqrt{1-\sin^2\theta_3}}$$

And by using Snell's law

$$n_1 \sin\theta_1 = n_3 \sin\theta_3 \qquad \Rightarrow \qquad \sin\theta_3 = \frac{\sin\theta_1}{n_3}$$

We get

$$r_{13}^p = \frac{n_3 \cos\theta_1 - \sqrt{1-\dfrac{\sin^2\theta_1}{n_3^2}}}{n_3 \cos\theta_1 + \sqrt{1-\dfrac{\sin^2\theta_1}{n_3^2}}} \qquad ; \qquad r_{13}^s = \frac{\cos\theta_1 - n_3\sqrt{1-\dfrac{\sin^2\theta_1}{n_3^2}}}{\cos\theta_1 + n_3\sqrt{1-\dfrac{\sin^2\theta_1}{n_3^2}}}$$

$$r_{13}^p = \frac{n_3^2 \cos\theta_1 - \sqrt{n_3^2-\sin^2\theta_1}}{n_3^2 \cos\theta_1 + \sqrt{n_3^2-\sin^2\theta_1}} \qquad ; \qquad r_{13}^s = \frac{\cos\theta_1 - \sqrt{n_3^2-\sin^2\theta_1}}{\cos\theta_1 + \sqrt{n_3^2-\sin^2\theta_1}}$$

So

$$\rho = \frac{r_{13}^p}{r_{13}^s}$$

$$\rho = \left[\frac{n_3^2 \cos\theta_1 - \sqrt{n_3^2-\sin^2\theta_1}}{n_3^2 \cos\theta_1 + \sqrt{n_3^2-\sin^2\theta_1}}\right] \left[\frac{\cos\theta_1 + \sqrt{n_3^2-\sin^2\theta_1}}{\cos\theta_1 - \sqrt{n_3^2-\sin^2\theta_1}}\right]$$

By putting $n_3^2 = x^2 \;\; ; \;\; \cos\theta_1 = a \;\; ; \;\; \sqrt{n_3^2-\sin^2\theta_1} = b$, we get

$$\rho = \left(\frac{ax^2-b}{ax^2+b}\right)\left(\frac{a+b}{a-b}\right)$$

$$\rho = \frac{a^2x^2 - b^2 - ab\left(1-x^2\right)}{a^2x^2 - b^2 + ab\left(1-x^2\right)}$$

Let $M = a^2x^2 - b^2$ and $N = ab\left(1-x^2\right)$, so

$$\rho = \frac{M-N}{M+N}$$

$$\rho = \frac{N\left(\dfrac{M}{N}-1\right)}{N\left(\dfrac{M}{N}+1\right)}$$

By putting $\dfrac{M}{N} = u$, we get

$$\begin{aligned}
\rho &= \frac{u-1}{u+1} \\
u &= \frac{1+\rho}{1-\rho}
\end{aligned}$$

As, we have

$$\begin{aligned}
N &= ab\left(1 - x^2\right) \\
N &= \cos\theta_1\sqrt{n_3^2 - \sin^2\theta_1}\left(1 - 1 + \frac{M}{\sin^2\theta_1}\right) \\
\frac{N}{M} &= \cos\theta_1\sqrt{n_3^2 - \sin^2\theta_1}\csc^2\theta_1 \\
\frac{1}{u} &= \cot\theta_1\csc\theta_1\sqrt{n_3^2 - \sin^2\theta_1} \\
\frac{1}{u^2} &= \cot^2\theta_1\csc^2\theta_1\left(n_3^2 - \sin^2\theta_1\right) \\
n_3^2 &= \sin^2\theta_1 + \frac{\tan^2\theta_1\sin^2\theta_1}{u^2} \\
n_3^2 &= \sin^2\theta_1 + \frac{\tan^2\theta_1\sin^2\theta_1}{\left(\frac{1+\rho}{1-\rho}\right)^2} \\
n_3 &= \sin\theta_1\sqrt{1 + \left(\frac{1-\rho}{1+\rho}\right)^2\tan^2\theta_1} \qquad (3.8)
\end{aligned}$$

This is our require solution. However, by further simplification

$$\begin{aligned}
n_3 &= \sin\theta_1\sqrt{\frac{(1+\rho)^2\cos^2\theta_1 - (1-\rho)^2\sin^2\theta_1}{(1+\rho)^2\cos^2\theta_1}} \\
n_3 &= \frac{\sin\theta_1}{\cos\theta_1}\sqrt{\frac{2\rho + \rho^2 + 1 - 4\rho\sin^2\theta_1}{(1+\rho)^2}} \\
n_3 &= \tan\theta_1\sqrt{1 - \frac{4\rho}{(1+\rho)^2}\sin^2\theta_1}
\end{aligned}$$

It is another simplified form of Eq. (3.8).[10]

Chapter 4

Experiment

To study optical properties of materials, we're using Alpha Spectroscopic Ellipsometer (α-SE) by J. A. Woollam, shown in figure 4.1. CompleteEASE is used with alpha-SE ellipsometer. Although it is the only available apparatus in PhysLab to study ellipsometry yet we are using it because:

- It is easy-to-use with a push button operative approach.
- It has less uncertainty in refractive index and thickness than other available machines.
- It can be used for wide range range of materials i.e. from dielectrics to organic materials, conductors to semiconductors, isotropic to anisotropic and many more.
- Its operation is very fast as it operates for hundreds of wavelength in just seconds.

Specifications of alpha-SE by J. A. Woollam are given in table 4.1

Angle of Incidence	60°, 70°, 75°	Normal measurement
	90°	S-T mode
Spectral Range	380 nm to 900 nm	180 wavelengths
Data Acquisition Rate	3 s	Fast mode
	10 s	Standard mode
	30 s	High-precision mode
Beam Diameter	~ 3 mm	Collimated
	~ 0.3 mm	Focused

Table 4.1: Specifications of Alpha-SE by J. A. Woollam

4.1 Procedure

To perform experiment with an increased and improved accuracy of results, follow the procedure:

1. Calibrate the ellipsometer by doing S-T baseline from 'Hardware' tab. If MSE > 1, then S-T baseline will be unsuccessful, so do it again and again till an MSE less than 1 is achieved (refer to figure 4.2).

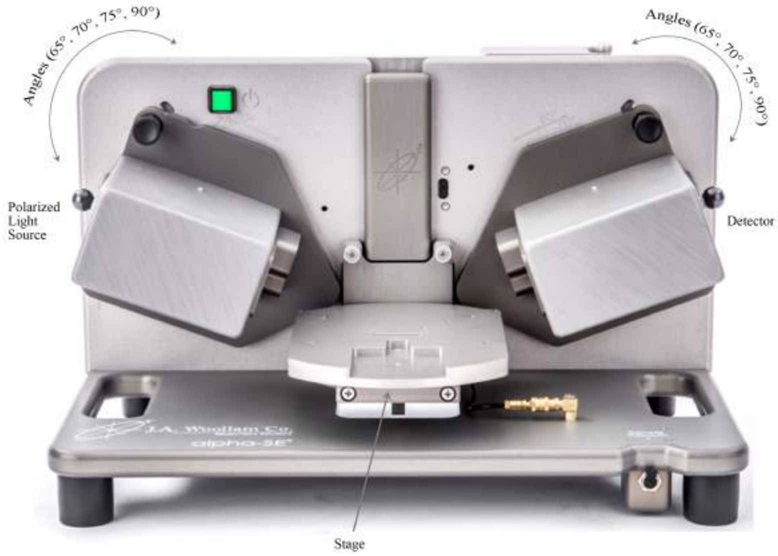


Figure 4.1: Woollam's Alpha-SE Ellipsometer (Source: J. A. Woollam)

2. Mount your sample on the wafer carrier or stage.

3. Move stage to your desired angle, as in our case it is 70°, by holding and pulling out the black knobs.

4. Set measurement mode to 'standard' (refer to figure 4.5).

5. Set sample alignment to 'standard' (refer to figure 4.5).

6. Press 'Measure'.

7. α-SE will automatically be aligned.

8. SE data will be measured on the sample.

9. Save your file (refer to figure 4.6).

10. Open the built in optical models and generate SE data. CompleteEASE will not automatically fit the data (refer to figure 4.7).

11. From the analysis done by α-SE, refractive index, thickness, attenuation, band gap, band energy and many other parameters can be found.

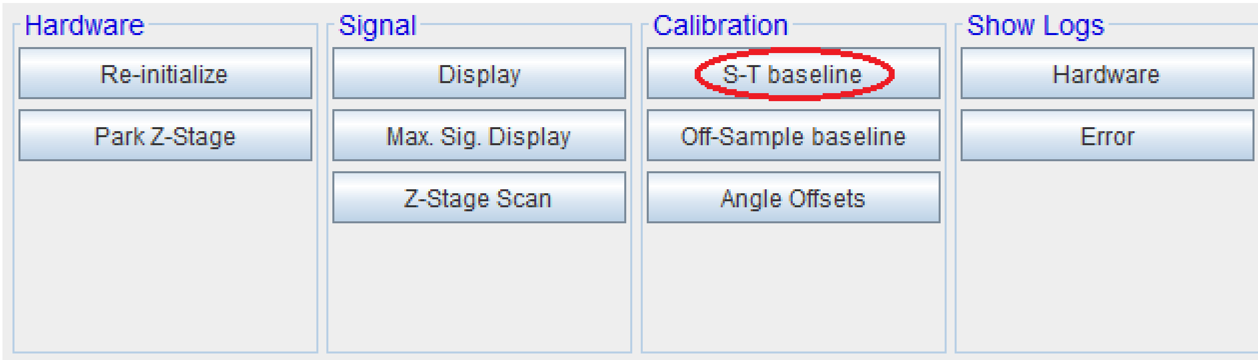


Figure 4.2: S-T baseline

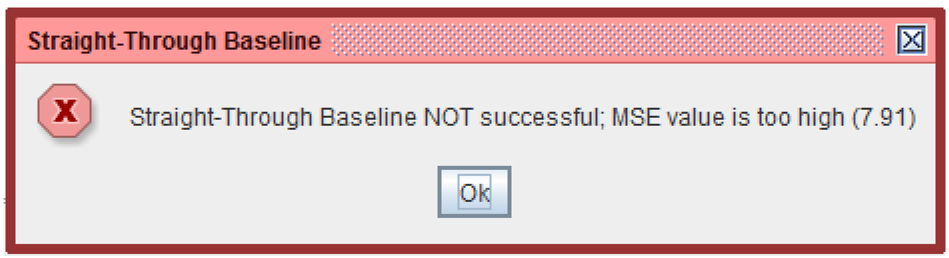


Figure 4.3: Unsuccessful S-T baseline

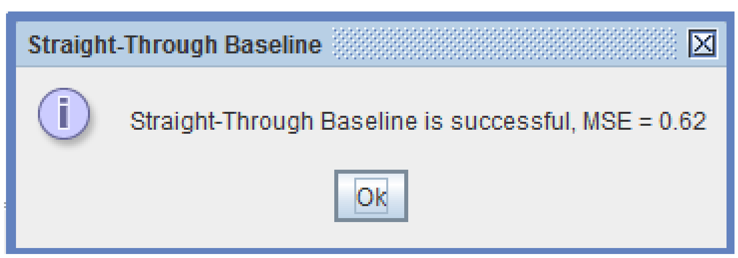


Figure 4.4: Successful S-T baseline

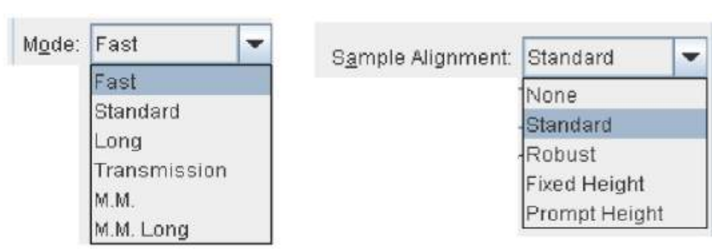


Figure 4.5: Measurement mode and sample mode dialog box

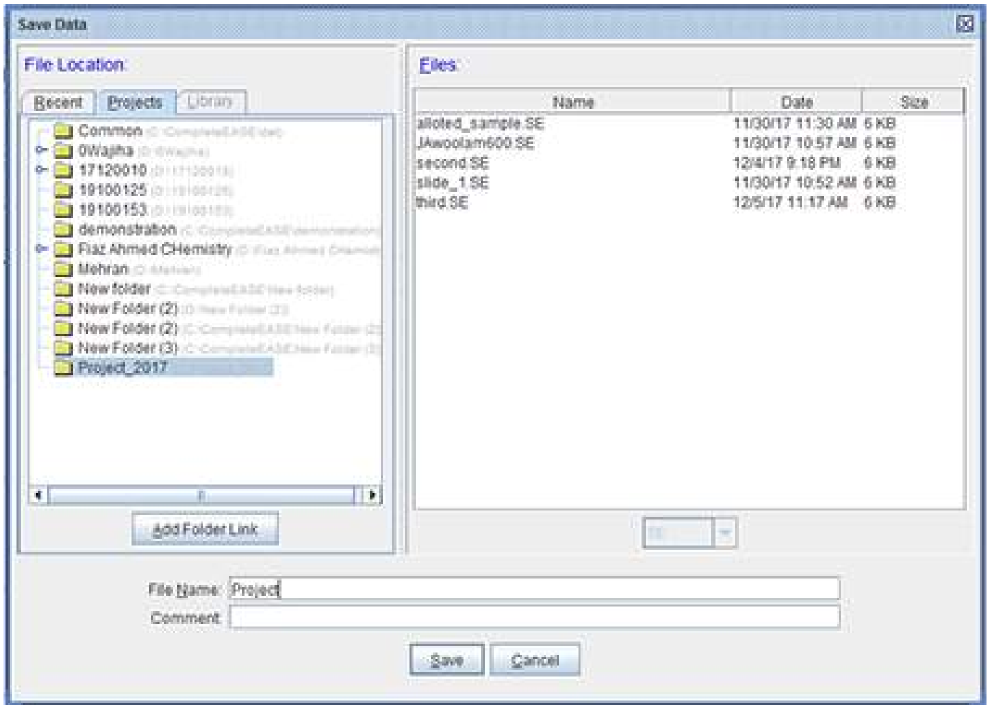


Figure 4.6: Save dialog box

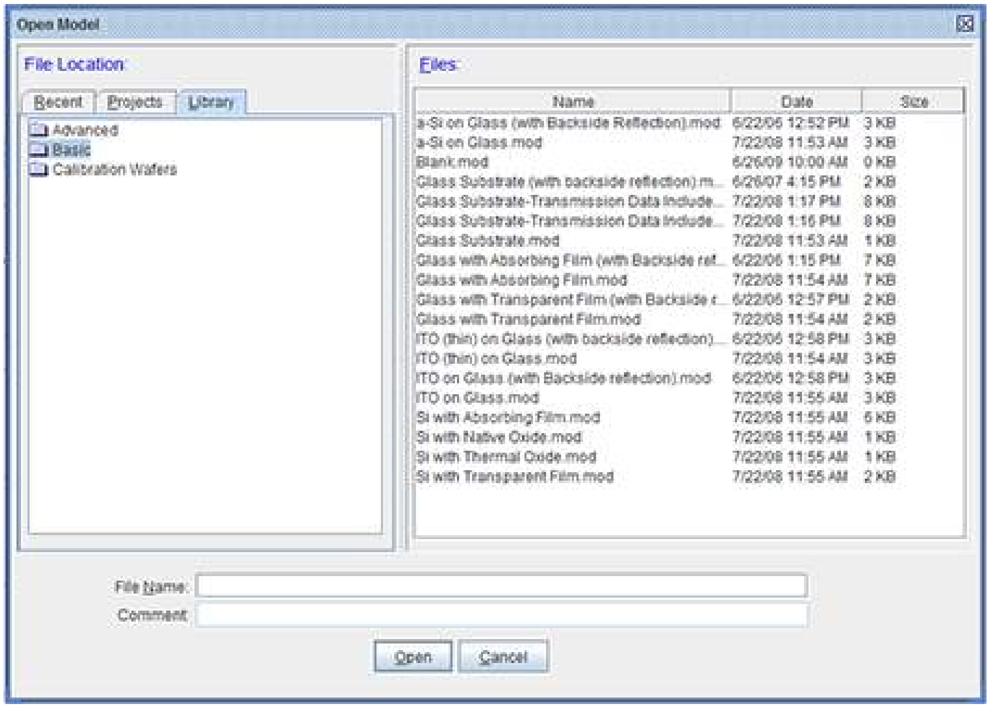


Figure 4.7: Open model dialog box

4.2 Results and Discussion

We will discuss and analyze two types of systems:

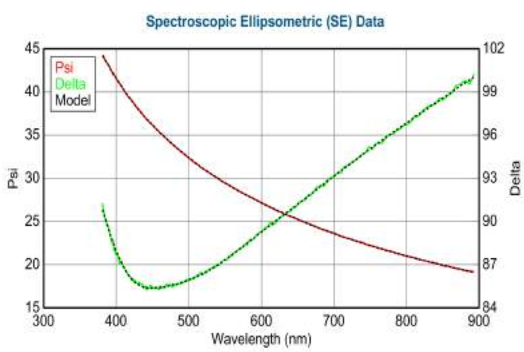
1. Air-film-substrate
2. Glass substrate

4.2.1 Air-Film-Substrate

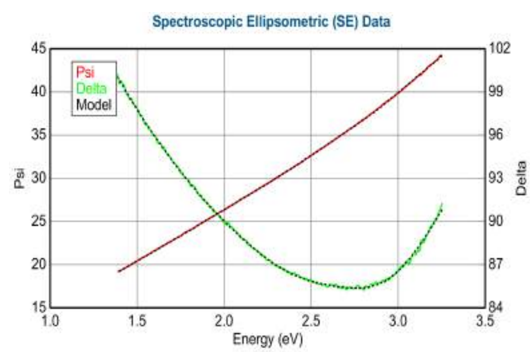
Following results are deduced from analysis.

4.2.1.1.0 Fit Model Set

Model fit is done by selecting 'glass substrate with absorbing film' as it gives the best fit model. It helps to achieve the lower MSE (mean squared error). Ψ and Δ are related by Eq. (3.4b). Fit model set of layered optical model in terms of in terms of wavelength (figure (4.8a)) and energy (figure (4.8b)) is given as:



(a) In nm



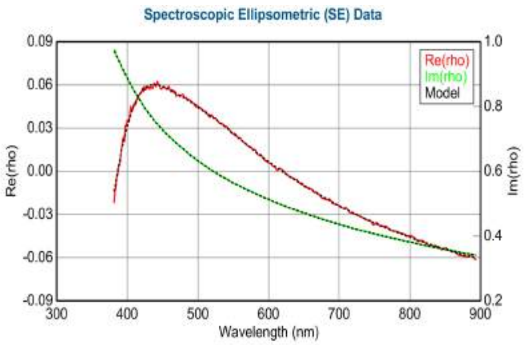
(b) In eV

Figure 4.8: Fit model set of layered optical model

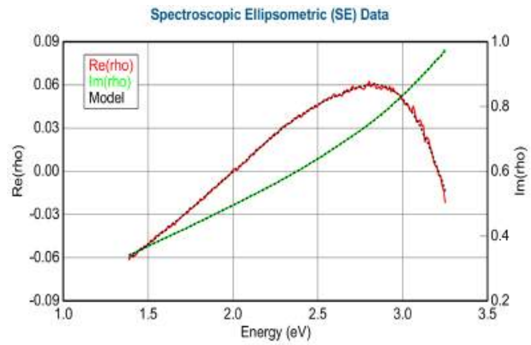
Since we are dealing with a bulk sample with no oxide, so we are aiming to directly determine the optical constants. Such optical constant are termed as 'pseudo optical constant'. They can be calculated by:

$$\langle n_3 \rangle = \tan\theta_1 \sqrt{1 - \frac{4\rho}{(1+\rho)^2}\sin^2\theta_1}$$

There behavior in terms of wavelength (figure (4.9a)) and energy (figure (4.9b)) is:



(a) In nm



(b) In eV

Figure 4.9: Real and imaginary parts of ρ

Fit model data set is shown below.

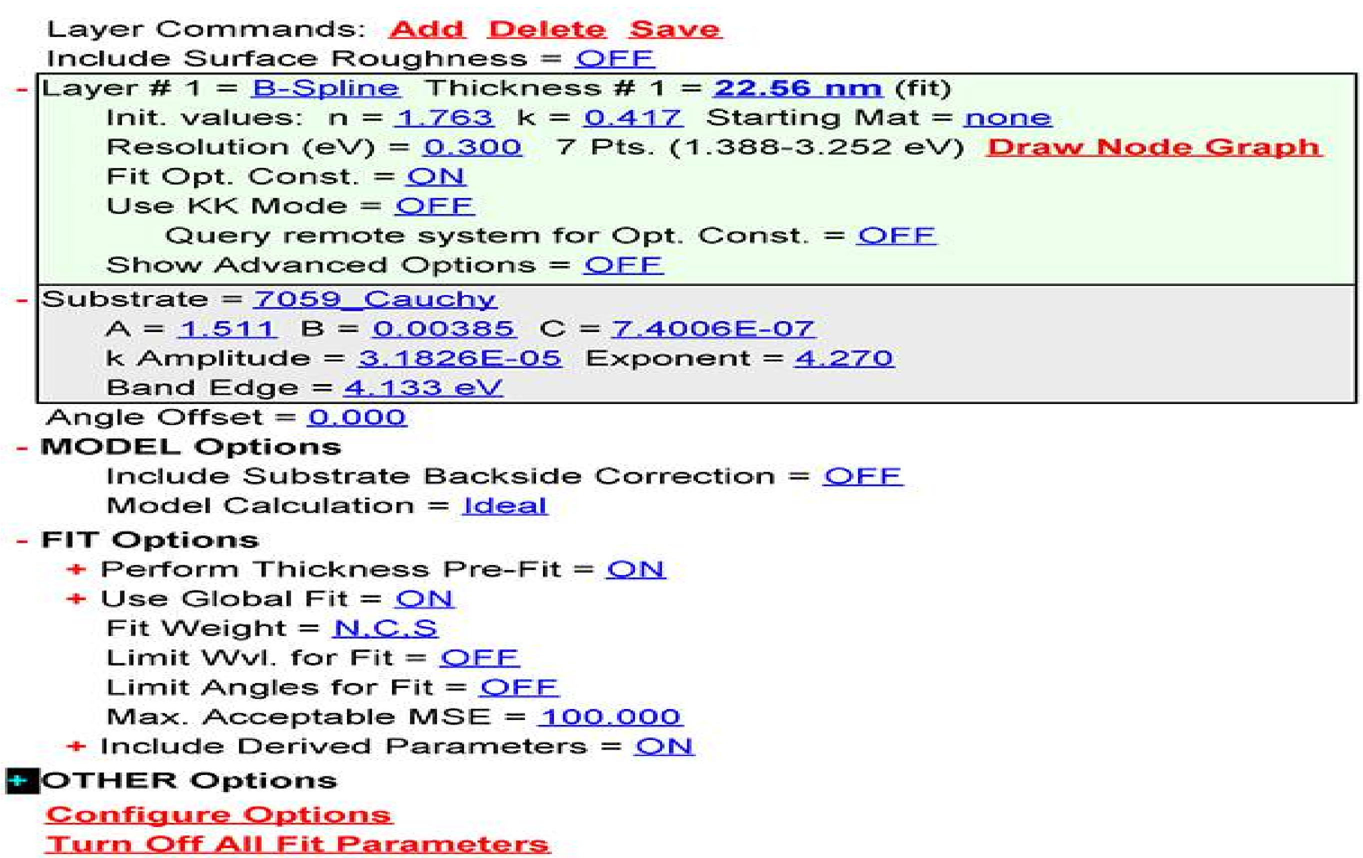


Figure 4.10: Fit model set

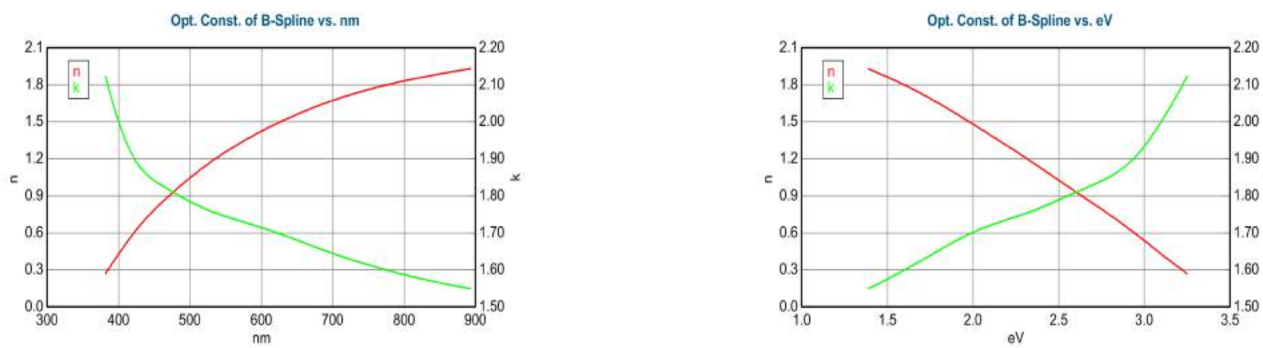
4.2.1.2.0 Optical Constants n and κ

According to Cauchy‘s equation

$$n(\lambda) = A + \frac{B}{\lambda^2} + \frac{C}{\lambda^4} + \dots \tag{4.1}$$

Here, n is the index of refraction, or just index, λ is the wavelength and A, B, C are constants. It shows the inverse relation between index and wavelength.
In our case, index of the material (n) is going to increase towards higher energy (eV) or shorter wavelength which indicates that optical constant ‘index’ for glass is real, physical and acceptable. While negative extinction coefficient (κ) (i.e. loss of energy in wave) is also positive which is an indication of physically acceptable solution. It should be remembered that these optical constant together called complex refractive index.

$$\widetilde{n}(\lambda) = n(\lambda) + \iota\kappa(\lambda) \tag{4.2}$$

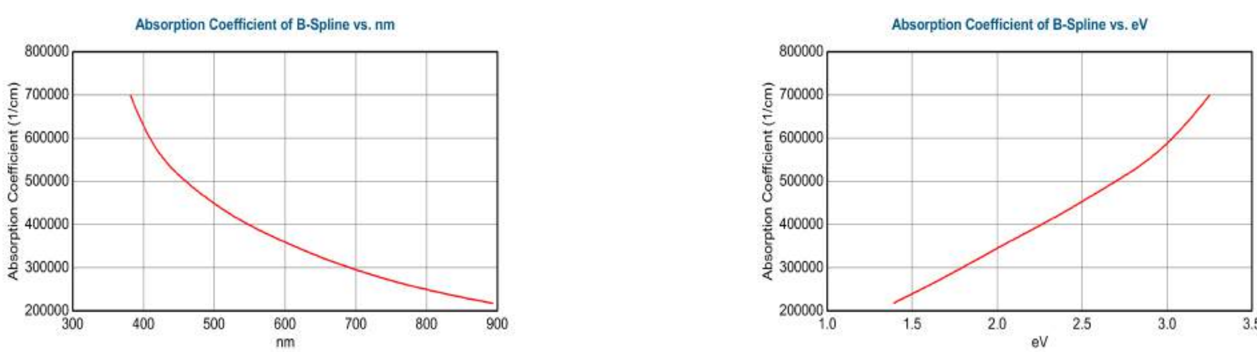


(a) n and k vs. nm (b) n and k vs. eV

Figure 4.11: Optical Constants of B-Spline

4.2.1.3.0 Absorption Coefficient of B-Spline

Study reveals that absorption coefficient of the material is positive which is physically acceptable.

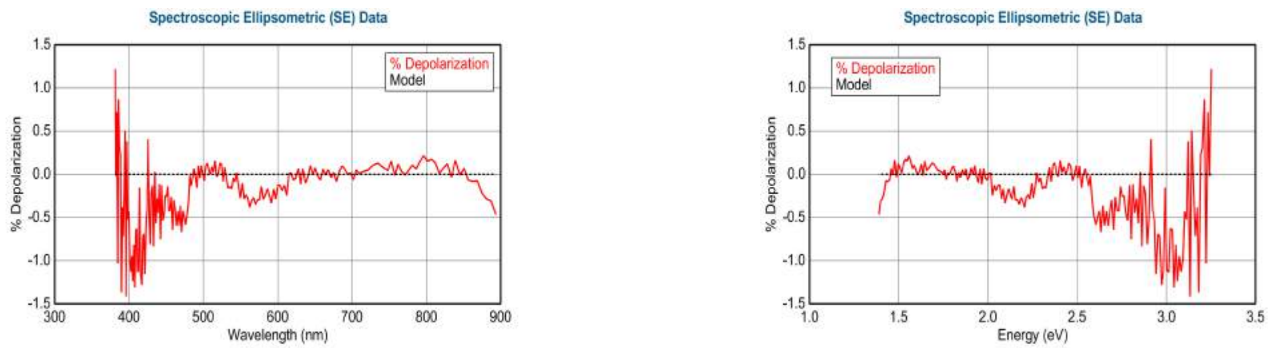


(a) In nm (b) In eV

Figure 4.12: Absorption Coefficient of B-Spline

4.2.1.4.0 Depolarization

Depolarization graph shows that as the energy increases, depolarization is going far away from zero or we can also interpret that as the wavelength increases, depolarization is going near to zero. It shows that material is not depicting depolarized behavior and the change in polarization can be studied by Ψ and Δ only.

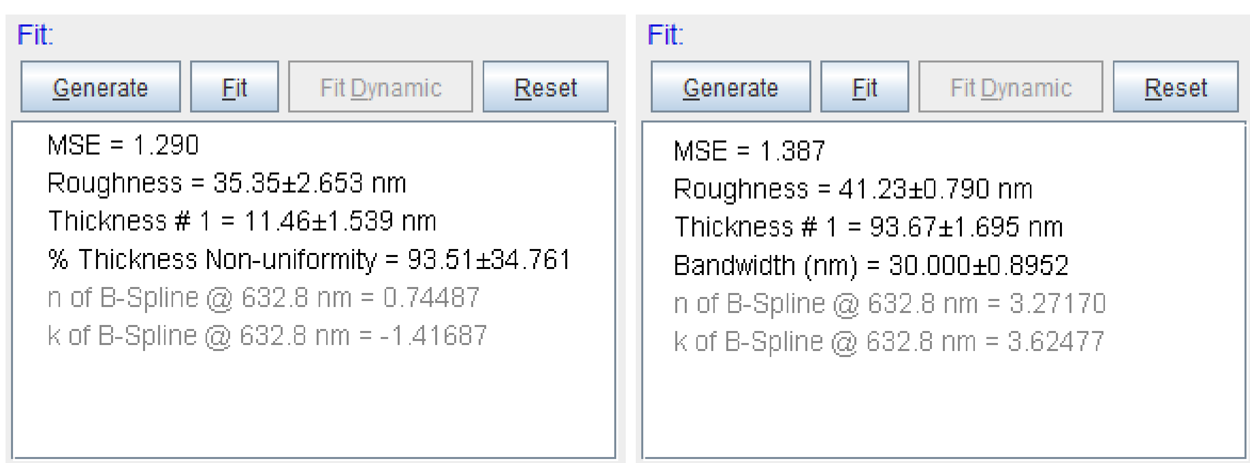


(a) In nm (b) In eV

Figure 4.13: Percentage Depolarization

4.2.1.5.0 Model Calculation – Thickness Non-Uniformity and Bandwidth

To calculate the thickness non-uniformity within measurement spot, we have changed the model calculation from 'ideal' to 'thickness non-uniformity' and for bandwidth calculation within measurement spot, again change the model calculation from 'ideal' to 'bandwidth'. It shows thickness non-uniformity of 6.04 ± 373.563 and bandwidth of 19.438 ± 1.0352 nm.



(a) Thickness non-uniformity (b) Bandwidth

Figure 4.14: Model calculations

4.2.1.6.0 Band Gap by using Tauc Plot

If the Direct transition is found at a lower transition energy then the direct one, we have an optically direct band material. It can be plotted[5][8], through MATLAB, as shown in figure(4.15) and its formula is:

$$\alpha E = B\left(E - E_g\right)^n$$

where for direct band gap $n = 1/2$ and for indirect band gap $n = 2$. From graph it is clear that our sample is optically indirect and has band gap between $\,\mathrm{eV}$.

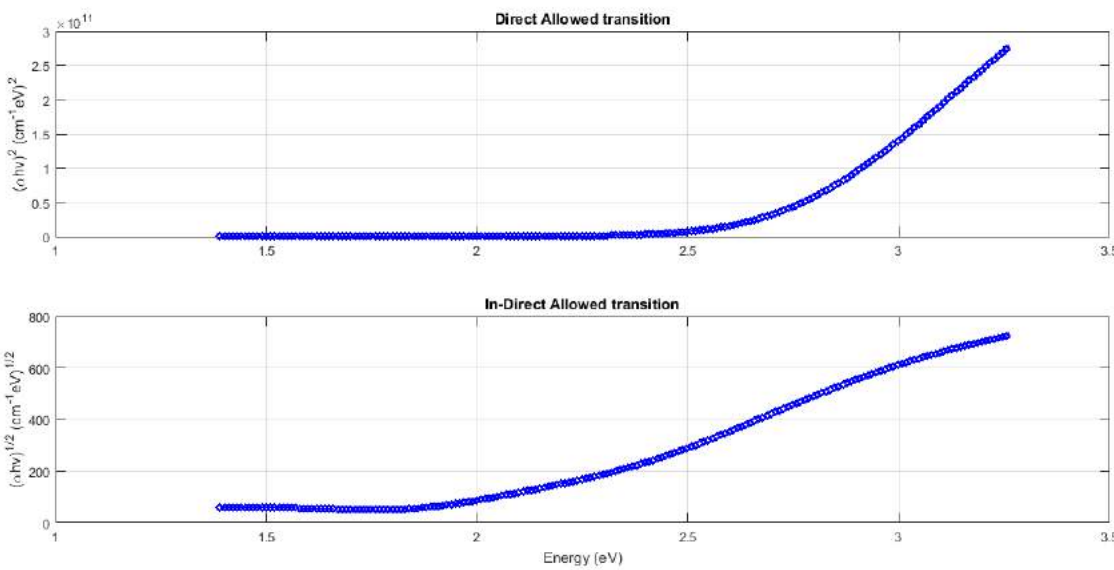
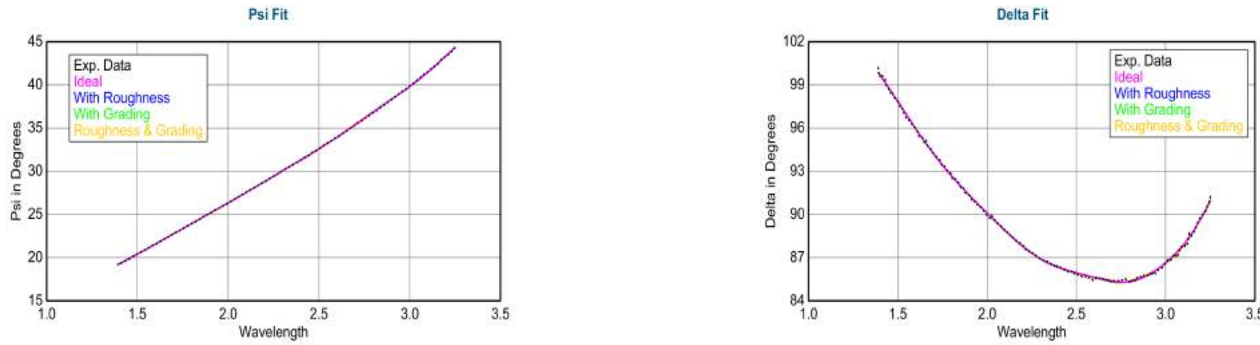


Figure 4.15: Tauc plot

4.2.1.7.0 Alternate Models

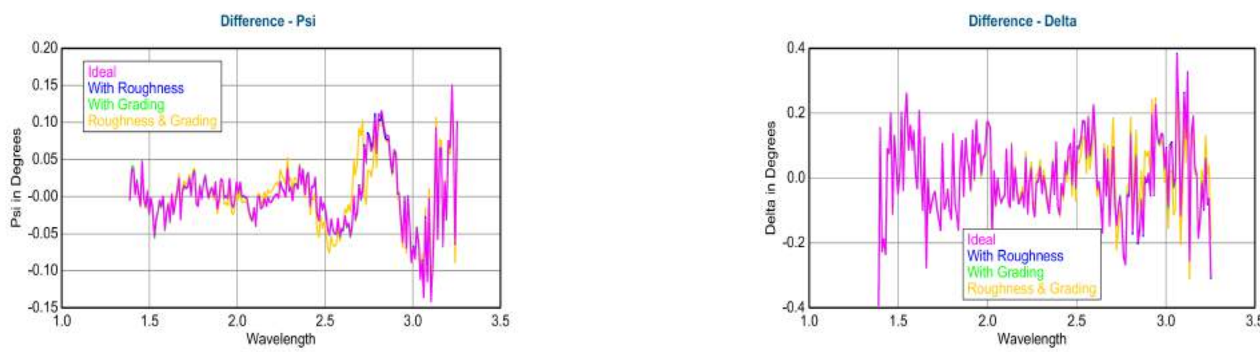
In the end, we have also studied it under ‘alternate models’ to automatically fit the data under ideal layered model. Graphical representation of alternate models is shown here.



(a) Psi fit

(b) Delta fit

Figure 4.16: Alternate models fit



(a) Differences - Psi

(b) Differences - Delta

Figure 4.17: Alternate models differences

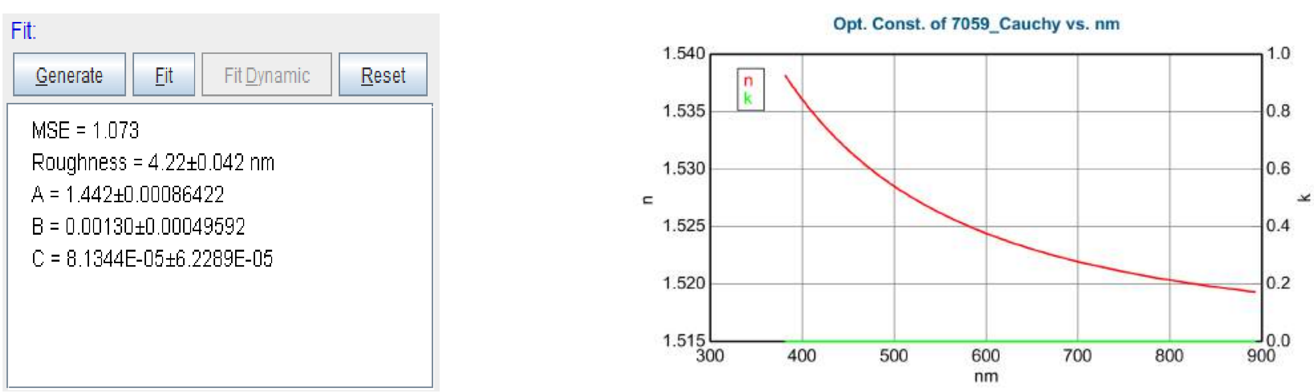
And results are tabulated here:

Parameter	Ideal	Roughness	Grading	Roughness & Grading
MSE	1.444	1.445	1.433	1.376
Roughness	N/A	-0.01 ± 0.035 nm	N/A	-0.16 ± 0.038 nm
spline_e1(1.388)	-4.6892 ± 0.11801	-4.6607 ± 0.12199	-5.4284 ± 2.19427	-5.8276 ± 1.58684
spline_e2(1.388)	7.8695 ± 0.03657	7.8579 ± 0.04080	7.9195 ± 0.07787	7.9997 ± 0.06437
spline_e1(1.699)	-4.5262 ± 0.09995	-4.5013 ± 0.10375	-5.1048 ± 1.63654	-5.4330 ± 1.18412
spline_e2(1.699)	5.4974 ± 0.01617	5.4948 ± 0.01885	5.3912 ± 0.33717	5.3299 ± 0.24540
spline_e1(2.009)	-4.4152 ± 0.07644	-4.3941 ± 0.08111	-4.8357 ± 1.15148	-5.0593 ± 0.83130
spline_e2(2.009)	3.8909 ± 0.02951	3.8951 ± 0.02957	3.6949 ± 0.55941	3.5723 ± 0.40761
spline_e1(2.320)	-4.1948 ± 0.05955	-4.1783 ± 0.06315	-4.4558 ± 0.67981	-4.6280 ± 0.49054
spline_e2(2.320)	2.3536 ± 0.05138	2.3622 ± 0.05157	2.1155 ± 0.63769	1.9085 ± 0.46377
spline_e1(2.631)	-4.3214 ± 0.03233	-4.3079 ± 0.04113	-4.4502 ± 0.32853	-4.4634 ± 0.22523
spline_e2(2.631)	1.1743 ± 0.05600	1.1904 ± 0.06013	0.9356 ± 0.61206	0.7515 ± 0.45066
spline_e1(2.942)	-4.1885 ± 0.02886	-4.1831 ± 0.02876	-4.1630 ± 0.11205	-4.3030 ± 0.10416
spline_e2(2.942)	-0.9863 ± 0.11581	-0.9672 ± 0.11576	-1.1338 ± 0.31821	-1.7258 ± 0.22335
spline_e1(3.252)	-6.9229 ± 0.06668	-6.9024 ± 0.07281	-6.9488 ± 0.08717	-7.1578 ± 0.09001
spline_e2(3.252)	-3.1152 ± 0.09118	-3.0986 ± 0.09201	-3.0688 ± 0.20030	-3.4831 ± 0.14399
% Inhomogeneity	N/A	N/A	52.97 ± 157.507	47.15 ± 112.844
Thickness # 1	22.56 ± 0.292 nm	22.63 ± 0.303 nm	21.86 ± 1.757 nm	20.79 ± 1.278 nm
n of B-Spline @ 632.8 nm	0.90722	0.90939	0.84235	0.80485
k of B-Spline @ 632.8 nm	2.29025	2.28639	2.36165	2.40026

Figure 4.18: Alternate models

4.2.2 Glass Substrate

We have also studied another different sample i.e. glass substrate for further verification of our mathematical formulation and the deductions are quite exact to expectations. Model fit is done by selecting ‘glass substrate (Cauchy model for glass substrate, with surface roughness)’ to achieve best fit model and lowest MSE. In reference to Eqs. (4.1) and (4.2), we have measure the optical constants and Cauchy constants which are shown below.



(a) Cauchy constants

(b) Graph

Figure 4.19: Glass substrate

Clearly, we can see from figure (4.19b) that for red light $632.8\ \mathrm{nm}$, the value of refractive index is in the range of , which is very close to the value obtained by using Michelson Interferometer with He-Ne Gas laser (PhysLab experiment code 2.9) done by us.
MATLAB program to calculate refractive index using Michelson Interferometer is:

```
% Experimental data and physical constants are:
lambda = 627*10^-9 ;
t = 1.2*10^-3;
N = 20;
theta = 9.5;
th = (theta*3.14)/180;
% n is refractive index
n' = (2*t - (N*lambda))*(1-cos(th))/(2*t*(1-cos(th))-(N*lambda))
n' = 1.51
```

And theoretically it is calculate by

$$n_3 = \tan\theta_1 \sqrt{1 - \frac{4\rho}{(1+\rho)^2}\sin^2\theta_1}$$

This formula is basically derived for air-substrate system (considering there is no thin film).

Chapter 5

MATLAB Code Verification

We have determined all the properties by J. A. Woollam's Alpha-SE and now we will verify these by using MATLAB environment.

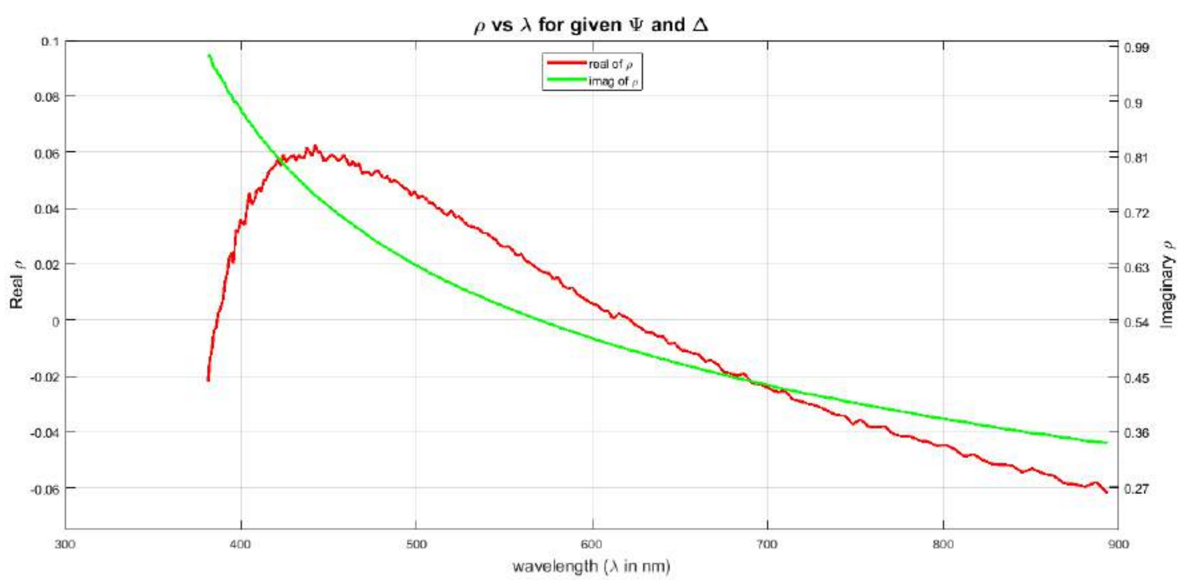


Figure 5.1: ρ and λ generated by Ψ and Δ

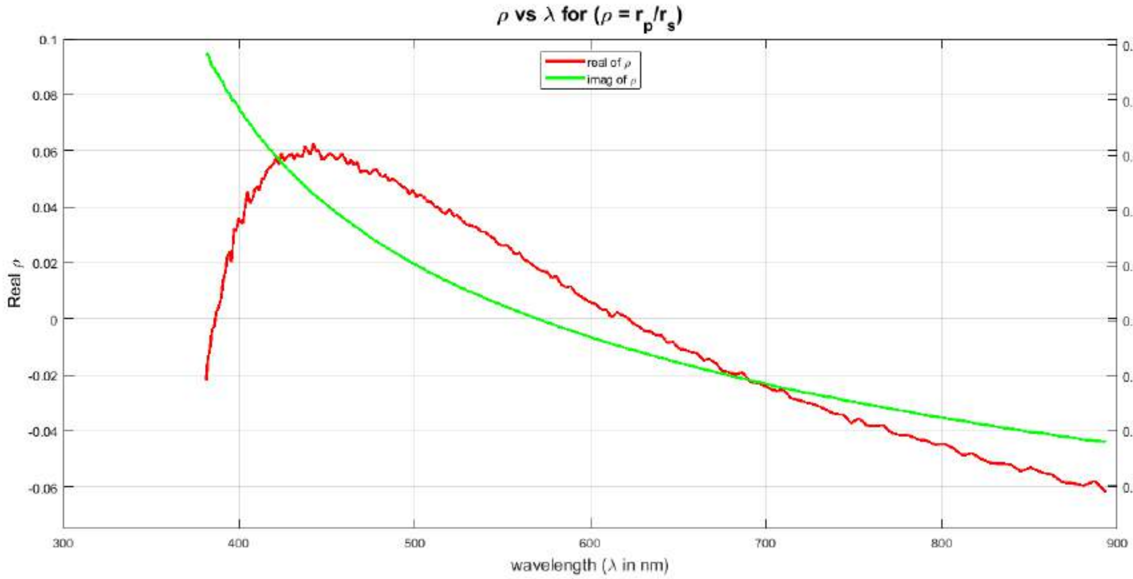


Figure 5.2: ρ by using the ratio of reflection coefficients

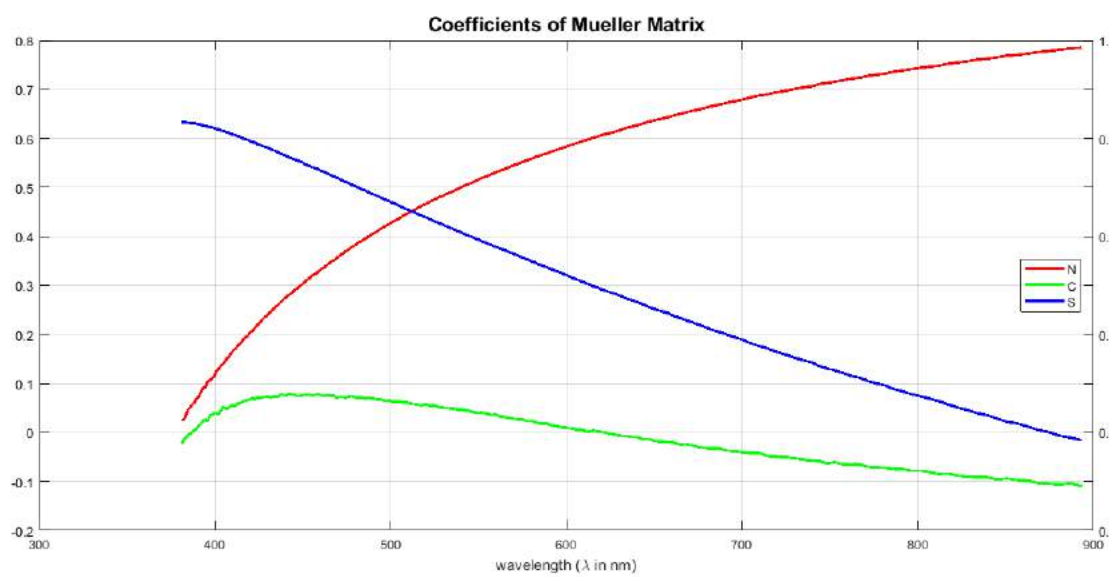


Figure 5.3: Coefficients of Mueller matrices

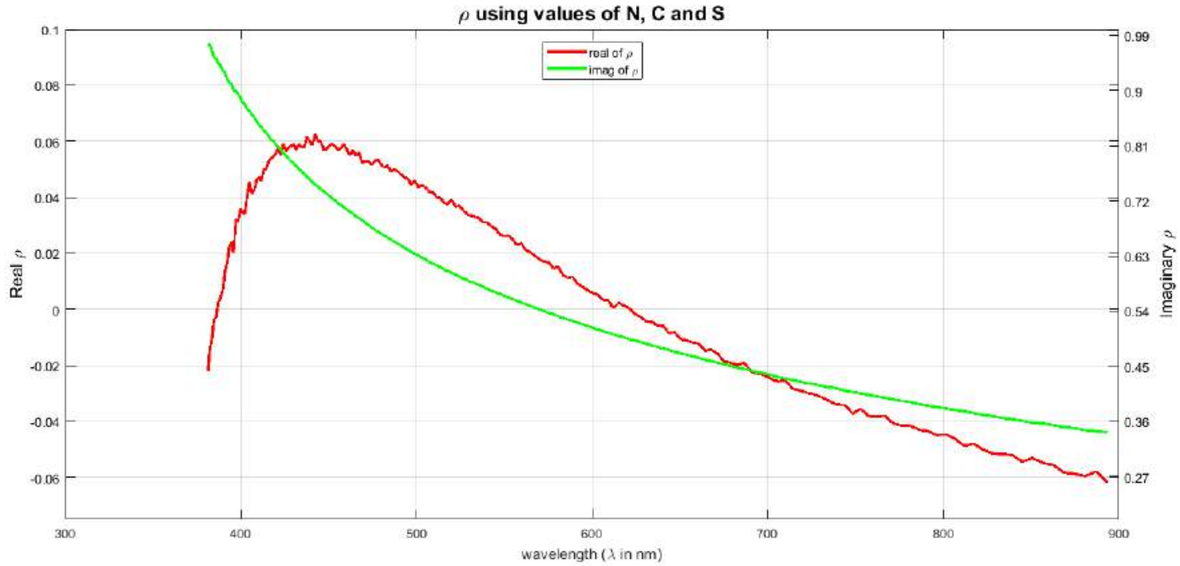


Figure 5.4: ρ by using N, C and S

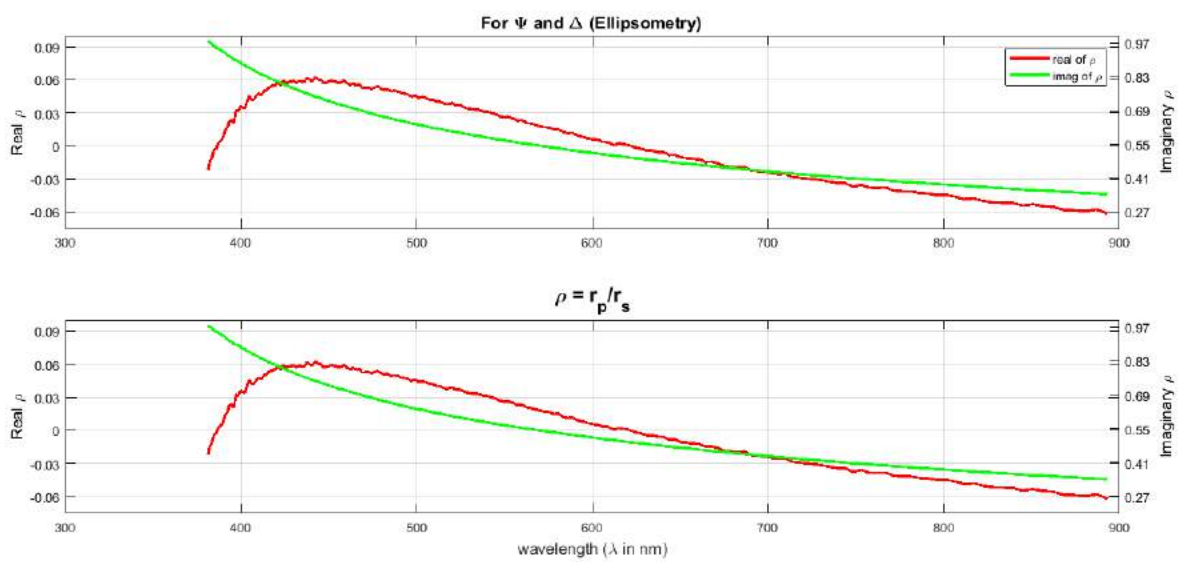


Figure 5.5: Comparison of ρ by two different methods i.e. by alpha-SE and by ratio of reflection coefficients matrix through MATLAB

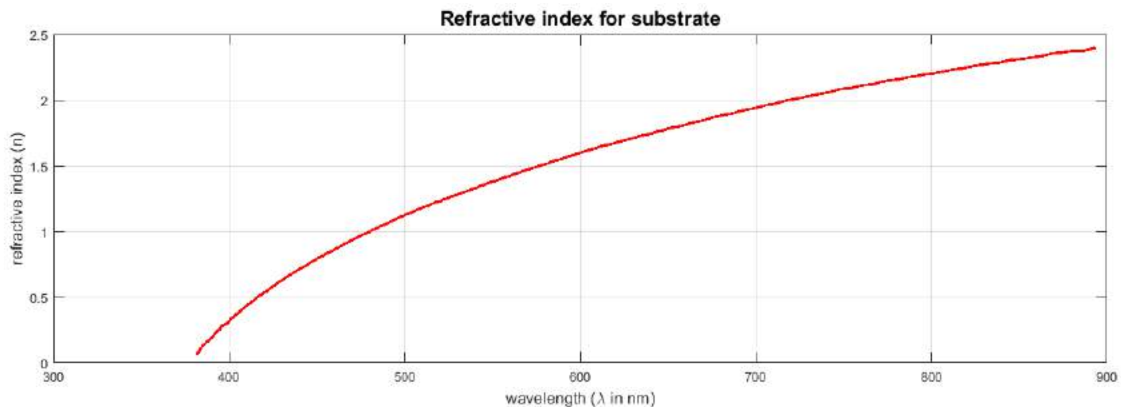


Figure 5.6: Refractive index for substrate (n_3 vs. λ)

Conclusion

Ellipsometry is a good technique to measure optical properties, thickness, roughness of thin films. But one has to be very careful about the model fitting as this is the crucial part of all the calculations and measurements. We measured

- real and imaginary part of refractive index,
- absorption coefficient,
- depolarization graphs,
- band gap using Tauc plot,
- refractive index for glass substrate.

All the results was very much comparable to those obtained by Woollam's Alpha-SE and theory.

Future Work

Research is to explore more and more and being physicists, we wish to pursue it more. We have some future intentions to work on ellipsometry that will include:

- regression analysis,
- to study anisotropic materials by using Mueller matrix coefficients (N, C, S),
- to study dielectric properties and its associatives,
- fabrication of thin films on different substrates.

Appendix A

MATLAB Code for Ellipsometric Parameters

```
clc, clear all, close all
%% data loading
a = load('psi_delta.txt');
b = load('n-k.txt');
lamda = a(:,1);
psi = a(:,2);
delta = a(:,3);
%% figure_1
rho_1 = tan(psi*pi/180).*exp(1j.*delta*pi/180);
[ax,h1,h2] = plotyy(lamda,real(rho_1),lamda,imag(rho_1));
set(ax(1),'YLim',[-0.075 0.1])
set(ax(1),'ycolor',[0 0 0])
set(ax(1),'YTick',[-0.06 : 0.02 : 1])
set(ax(2),'YTick',[0.27 : .09 : 1])
set(ax(2),'ycolor',[0 0 0])
title('\rho vs \lambda for given \Psi and \Delta','FontSize',15)
xlabel('wavelength (\lambda in nm)','FontSize',13)
legend('real of \rho' , 'imag of \rho','location','north')
ylabel(ax(1),'Real \rho','FontSize',13)
ylabel(ax(2),'Imaginary \rho','FontSize',13)
grid on

%% for verification
d = 40.07*10^-9;
n2 = b(:,2) + 1i * b(:,3);

%% Initial Calculation
n1 = 1;                                                % refractive index for air
th_i = 70 * (pi/180);                                  % Angle of incidence
```

```matlab

% Substitution
x = cos(th_i);
y = sin(th_i);
x1 = sqrt(1 - (y.^2).*(n1./n2).^2);             % equivalent to cos(th_2)

% Refractive Index for substrate calculation
n3 = n1.*tan(th_i).*sqrt(1 - (4*rho_1.*y.^2)./(rho_1+1).^2);
y1 = sqrt(1 - (y.^2).*(n1./n3).^2);             % equivalent to cos(th_3)

%% S and P polarization

% Delta Calculation
del = (2 * pi * n2 * d * cos(th_i))./lamda ;

% TM Case
rp_12 = (n2.*x - n1.*x1) ./ (n2.*x + n1.*x1);
rp_23 = (n3.*x1 - n2.*y1)./ (n3.*x1 + n2.*y1);
rp = (rp_12 + (rp_23.*exp(-1i*2*del)))./(1 + (rp_12.*rp_23.*exp(-1i*2*del)))
    ;

% TE Case
rs_12 = (n1.*x - n2.*x1) ./ (n1.*x + n2.*x1);
rs_23 = (n2.*x1 - n3.*y1)./ (n2.*x1 + n3.*y1);
rs = (rs_12 + (rs_23.*exp(-1i*2*del)))./(1 + (rs_12.*rs_23.*exp(-1i*2*del)))
    ;

% Rho calculation (Using TE,TM cases)
%[figure_2]
figure
rho_2 = rp./rs;
[axh,l1,l2] = plotyy(lamda,real(rho_2),lamda,imag(rho_2));
xlabel('wavelength (\lambda in nm)','FontSize',13)
title('\rho vs \lambda for (\rho = r_p/r_s)','FontSize',15)
legend('real of \rho' , 'imag of \rho','location','north')
grid on
set(axh(1),'YLim',[-0.075 0.1])
set(axh(1),'ycolor',[0 0 0])
set(axh(1),'YTick',[-0.06 : 0.02 : 1])
set(axh(2),'YTick',[0.27 : .09 : 1])
set(axh(2),'ycolor',[0 0 0])
ylabel(axh(1),'Real \rho','FontSize',13)
ylabel(axh(2),'Imaginary \rho','FontSize',13)

%% Mueller matrix coefficients for Isotropic Material N,C,S
```

```
% Figure_3
figure
N = cos(2*psi*pi/180);
C = sin(2*psi*pi/180).*cos(delta*pi/180);
S = sin(2*psi*pi/180).*sin(delta*pi/180);
plot(lamda,N,'r');
hold on
[axp,p1,p2] = plotyy(lamda,C,lamda,S);
grid on
xlabel('wavelength (\lambda in nm)','FontSize',11)
set(axp(1),'YLim',[-0.2 0.8])
set(axp(1),'ycolor',[0 0 0])
set(axp(1),'YTick',[-0.2 : .1 : .8])
set(axp(2),'YLim',[0.5 1.1])
set(axp(2),'YTick',[0.38 : .12 : 1.1])
set(axp(2),'ycolor',[0 0 0])
ylabel(axh(1),'N = cos(2*\Psi) ; C = sin(2*\Psi)*cos(\Delta)','FontSize',11)
ylabel(axh(2),'S = sin(2*\Psi).*sin(\Delta)','FontSize',11)
legend('N','C','S','location','east')
title('Coefficients of Mueller Matrix','FontSize',15)

%% rho in terms of C,S,N
figure
rho_3 = (C + 1i*S )./(1+N);
[axl,h11,h22] = plotyy(lamda,real(rho_3),lamda,imag(rho_3));
xlabel('wavelength (\lambda in nm)','FontSize',11)
title('\rho using values of N, C and S','FontSize',15)
legend('real of \rho' , 'imag of \rho','location','north')
grid on
set(axl(1),'YLim',[-0.075 0.1])
set(axl(1),'ycolor',[0 0 0])
set(axl(1),'YTick',[-0.06 : 0.02 : 1])
set(axl(2),'YTick',[0.27 : .09 : 1])
set(axl(2),'ycolor',[0 0 0])
ylabel(axl(1),'Real \rho','FontSize',13)
ylabel(axl(2),'Imaginary \rho','FontSize',13)

%% Combining all
subplot(2,1,1)
[ax,h1,h2] = plotyy(lamda,real(rho_1),lamda,imag(rho_1));
set(ax(1),'YLim',[-0.075 0.1])
set(ax(1),'ycolor',[0 0 0])
set(ax(1),'YTick',[-0.06 : 0.03 : .9])
set(ax(2),'YTick',[0.27 : .14 : 1])
set(ax(2),'ycolor',[0 0 0])
```

```
title('For \Psi and \Delta (Ellipsometry)','FontSize',13)
ylabel(ax(1),'Real \rho','FontSize',12)
ylabel(ax(2),'Imaginary \rho','FontSize',12)
legend('real of \rho' , 'imag of \rho')
grid on

subplot(2,1,2)
[axh,l1,l2] = plotyy(lamda,real(rho_2),lamda,imag(rho_2));
xlabel('wavelength (\lambda in nm)','FontSize',12)
title('\rho = r_p/r_s','FontSize',15)
grid on
set(axh(1),'YLim',[-0.075 0.1])
set(axh(1),'ycolor',[0 0 0])
set(axh(1),'YTick',[-0.06 : 0.03 : .9])
set(axh(2),'YTick',[0.27 : .14 : 1])
set(axh(2),'ycolor',[0 0 0])
ylabel(axh(1),'Real \rho','FontSize',12)
ylabel(axh(2),'Imaginary \rho','FontSize',12)
legend('real of \rho' , 'imag of \rho','location')

%% Refractive index for Substrate
plot(lamda,real(n3),'b','linewidth',2.5)
xlabel('wavelength (\lambda in nm)','FontSize',12)
ylabel('refractive index (n)','FontSize',12)
title('Refractive index for substrate','FontSize',15)
grid on

%% Refractive index for Thin Film
[a,b,c]=plotyy(lamda,real(n2),lamda,imag(n2))
xlabel('wavelength (\lambda in nm)','FontSize',12)
title('Refractive index for Thin Film','FontSize',15)
grid on
set(a(1),'YLim',[2 3]);
set(a(1),'YTick',[2 : 0.2 : 3]);
set(a(1),'Ycolor',[0 0 0]);
set(a(2),'YTick',[0 : 0.1 : 0.5]);
set(a(2),'Ycolor',[0 0 0]);
ylabel(a(1),'refractive index (n)','FontSize',12);
ylabel(a(2),'Attenuation Coefficient ( \kappa)','FontSize',12);
legend('n','\kappa')
```

Appendix B

MATLAB Code for Tauc Plot

```
    %% Tauc plot
% Input Parameters
z = load('n-k.txt');
h = 6.63 * 10^-34;
c = 3 * 10^8;
lamda = z(:,1)*10^-9;
k = z(:,3);
% absorption coefficient
alpha = (4*pi * k)./(lamda);
alpha = alpha * 10^-2;              % m-1 to cm-1
% Energy
E = ((h*c)./lamda)*(6.242*10^18);    % joule to eV

%% Indirect allowed transition
subplot(2,1,2)
y = (alpha.*E).^(1/2);
plot(E,y,'bo','linewidth',2)
grid on
xlabel('Energy (eV)')
ylabel('(\alphahv)^1^/^2 (cm^-^1eV)^1^/^2')
title('In-Direct Allowed transition')

%% Direct allowed transition
subplot(2,1,1)
z = (alpha.*E).^(2);
plot(E,z,'bo','linewidth',2)
grid on
ylabel('(\alphahv)^2 (cm^-^1eV)^2')
title('Direct Allowed transition')
```

Appendix C

Mueller-Matrix Formalism

Mueller-matrix formalism[1][9] provides another approach to study ellipsometric measurements. Actually, it is one of the most complete and most general descriptions of ellipsometry in both reflection and transmission configurations. By disregarding non-linear effects, optical properties of the materials are characterized by polarized light-matter interaction. It is used for both isotropic and anisotropic materials. Mueller matrices are defined by Stokes vector through a linear relationship as:

$$S_r = MS_i$$

where S_r and S_i are the Stokes vectors of the reflected and incident beam respectively and $M = (m_{ij})_{1\leq ij\leq 4}$ is a 4×4 Mueller matrix.
For isotropic materials

$$M_{iso} = \begin{bmatrix} 1 & -N & 0 & 0 \\ -N & 1 & 0 & 0 \\ 0 & 0 & C & S \\ 0 & 0 & -S & C \end{bmatrix}$$

Here

$$\begin{aligned} N &= \cos(2\Psi) \\ C &= \sin(2\Psi)\cos(\Delta) \\ S &= \sin(2\Psi)\sin(\Delta) \end{aligned}$$

Some of the advantages to use this notation are:

1. NCS will be non-zero for all,
2. they are bounded between -1 to 1,
3. they are well-defined always.

And following information can be extracted from Mueller matrix in reflection mode:

1. Ψ and Δ can be measured,

2. isotropic ellipsometric parameters,
3. anisotropic ellipsometric parameters,
4. Fresnel coefficients
5. reflectance for s- and p- polarized plane wave,
6. depolarization.

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