A Report on

Ellipsometry and its application to measure thickness of Al and Ag thin films

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For the One month Internship at Korea Institute of Science and Technology, KIST, South Korea

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Abstract

This report sums up the work done during the one month Summer Internship at Korea Institue of Science and Technology, KIST, South Korea.
Ellipsometry is non-invasive, non-destructive measurement technique to obtain optical properties of a sample material by means of the reflected light waves.
The report contains a brief overview of ellipsometry and its applications.
A study of the topic is presented along with its application to measure thickness of Aluminium thin film on glass and Silver thin film on glass.
The analysis of the data obtained from the ellipsometer was done and parameters were fit using regression. The result and conclusion are presented both in tabular and in graphical representation.

Chapter 1

Ellipsometry

1.1 Definition

Ellipsometry is non-invasive, non-destructive measurement technique to obtain optical properties of a sample material by means of the reflected light waves.
The technique measures a relative change in the polarisation and is therefore not dependent on absolute intensity as long as it is sufficient.

1.2 Principle

It is a method based on measurement of the change of the polarisation state of light after reflection at non normal incidence on the surface under study.
Measurement gives two independent angles: Ψ and Δ.
It is an absolute measurement does not need any reference.
It does not give directly the physical parameters of the sample.
It is necessary to always use a model to describe the sample.

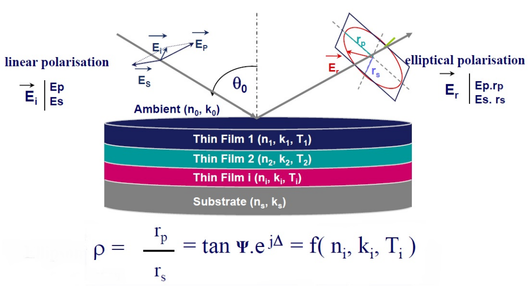

Figure 1.1: Ellipsometry

Ellipsometry is typically done only in reflection setup. The exact nature of polarisation change is determined by the sample's properties. Ellipsometry exploits the phase information and can achieve sub-nanometer resolution.
Assumptions in most models, Sample is composed of number of discrete, well defined layers that are optically homogeneous and isotropic.

1.3 Ellipsometer

Construction -

1. A light source
2. The linear polariser
3. The compensator
4. The surface
5. The analyser
6. The detector

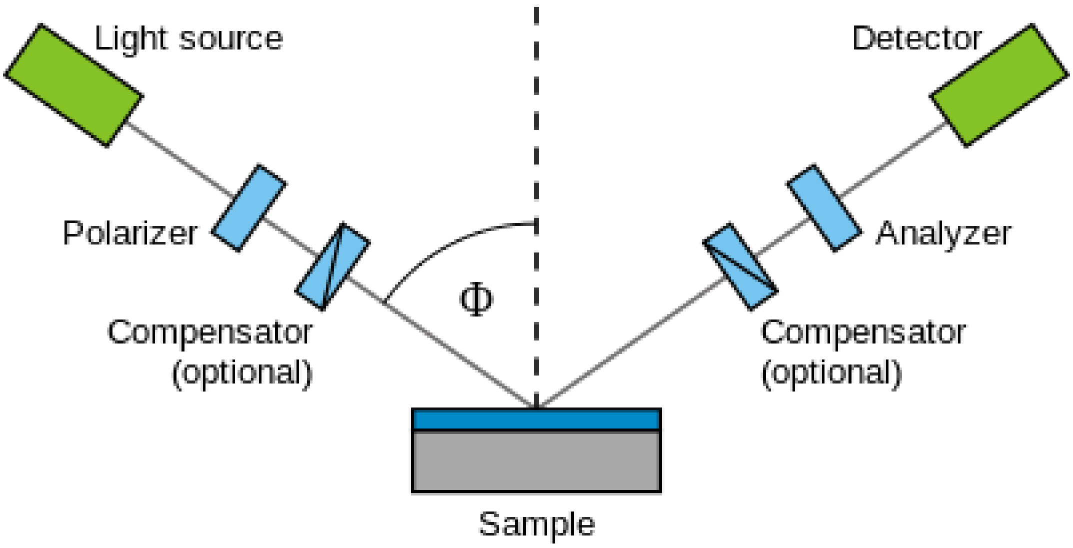

Figure 1.2: Ellipsometer

Chapter 2

Ellipsometry Parmeters

2.1 Parameters

Ellipsometry measure the complex reflectance ration, ρ which is parametrised by

1. ψ – Amplitude ratio

2. δ - Phase difference

These parameters give all the relevant information about the polarisation state of the light at a given wavelength. Ellipsometry measures - ψ and δ
Model based analysis is required to extract the quantities of interest.
Quantities of interest are -

1. Film Thickness

2. Refractive Index

3. Surface Roughness

4. Composition

5. Anisotropy etc.

2.2 Relating ψ and δ to Physical parameters

The incident polarised light is split into s and p polarised light.
Incident and reflected light propagate in the same medium and make equal angle with the normal.
Frensel's Equations -

$$\rho_\pi = \frac{\tilde{n}_1 \cos(\theta_0) - \tilde{n}_0 \cos(\theta_1)}{\tilde{n}_1 \cos(\theta_0) + \tilde{n}_0 \cos(\theta_1)}$$
$$\rho_\sigma = \frac{\tilde{n}_0 \cos(\theta_0) - \tilde{n}_1 \cos(\theta_1)}{\tilde{n}_0 \cos(\theta_0) + \tilde{n}_1 \cos(\theta_1)}$$

Figure 2.1: Frensel's Equations

Consider Ex and Ey electrical feild vectors parallel and perpendicular to the surface respectively. Main equation in ellipsometry -

$$P = \frac{P_\pi}{P_\sigma} = \tan(\psi) e^{j\Delta}$$

Figure 2.2: Ellipsometry Equations

The system that we are considering for the derivation is as follows -

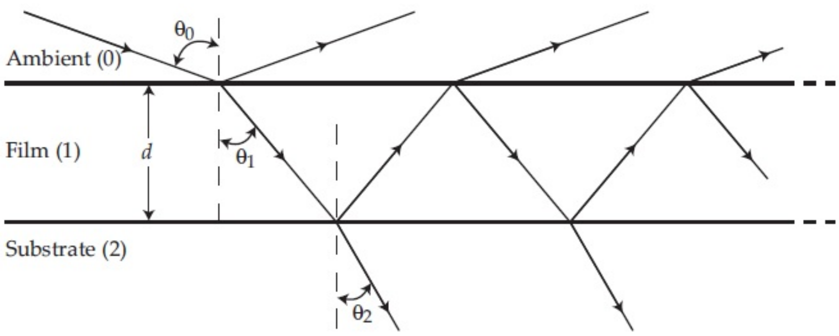

Figure 2.3: System under consideration

Assuptions -
System is considered to have parallel boundaries.
Medium 1(material film) has lateral dimensions much greater than its thickness, medium 0(ambient),medium 2(substrate) have infinite thickness compared to medium 1.
All three medium are homogeneous and isotropic.
Incident wave is monochromatic.

Total reflection coefficients -

$$P_\sigma = \frac{\rho_{01,\sigma} + \rho_{12,\sigma} e^{-j2\beta}}{1 + \rho_{01,\sigma}\rho_{12,\sigma} e^{-j2\beta}}$$
$$P_\pi = \frac{\rho_{01,\pi} + \rho_{12,\pi} e^{-j2\beta}}{1 + \rho_{01,\pi}\rho_{12,\pi} e^{-j2\beta}}$$

Figure 2.4: Total reflection coefficients

By substituting these reflection coefficients in the main ellipsometric formula we can get the Relation between ψ and δ and the Physical parameters.

$$P = P_\pi \cdot \frac{1}{P_\sigma} = \frac{\rho_{01,\pi} + \rho_{12,\pi} e^{-j2\beta}}{1 + \rho_{01,\pi}\rho_{12,\pi} e^{-j2\beta}} \cdot \frac{1 + \rho_{01,\sigma}\rho_{12,\sigma} e^{-j2\beta}}{\rho_{01,\sigma} + \rho_{12,\sigma} e^{-j2\beta}}$$
$$= \frac{\rho_{12,\pi}\rho_{01,\sigma}\rho_{12,\sigma} e^{-j4\beta} + (\rho_{01,\pi}\rho_{01,\sigma}\rho_{12,\sigma} + \rho_{12,\pi})\, e^{-j2\beta} + \rho_{01,\pi}}{\rho_{01,\pi}\rho_{12,\pi}\rho_{12,\sigma} e^{-j4\beta} + (\rho_{01,\pi}\rho_{12,\pi}\rho_{01,\sigma} + \rho_{12,\sigma})\, e^{-j2\beta} + \rho_{01,\sigma}}$$
$$P = \frac{AX^2 + BX + C}{DX^2 + EX + F} \qquad X = e^{-j2\beta}$$
$$(PD - A)X^2 + (PE - B)X + (PF - C) = 0$$
$$X = \frac{-(PE - B) \pm \sqrt{(PE - B)^2 - 4(PD - A)(PF - C)}}{2(PD - A)}$$

Figure 2.5: Relation to physical parameters

The equation obtained is an equation of 11 parameters, where ψ and δ are related to 9 real parameters -
3 complex indices(real + imaginary part), Angle of incidence, Wavelength in free space of incident light, Film thickness

Solving for film thickness

$$\beta = 2\pi \frac{d}{\lambda} \tilde{n}_1 \cos(\theta_1)$$
$$X = e^{-j2\beta}$$
$$\ln(X) = -j4\pi \frac{d}{\lambda} \tilde{n}_1 \cos(\theta_1)$$
$$d = \frac{j \ln(X) \lambda}{4\pi \tilde{n}_1 \cos(\theta_1)}$$

Figure 2.6: Solving for film thickness

Chapter 3

Experimentation

3.1 Flow Chart

A general flow chart of the experimentation is as below -

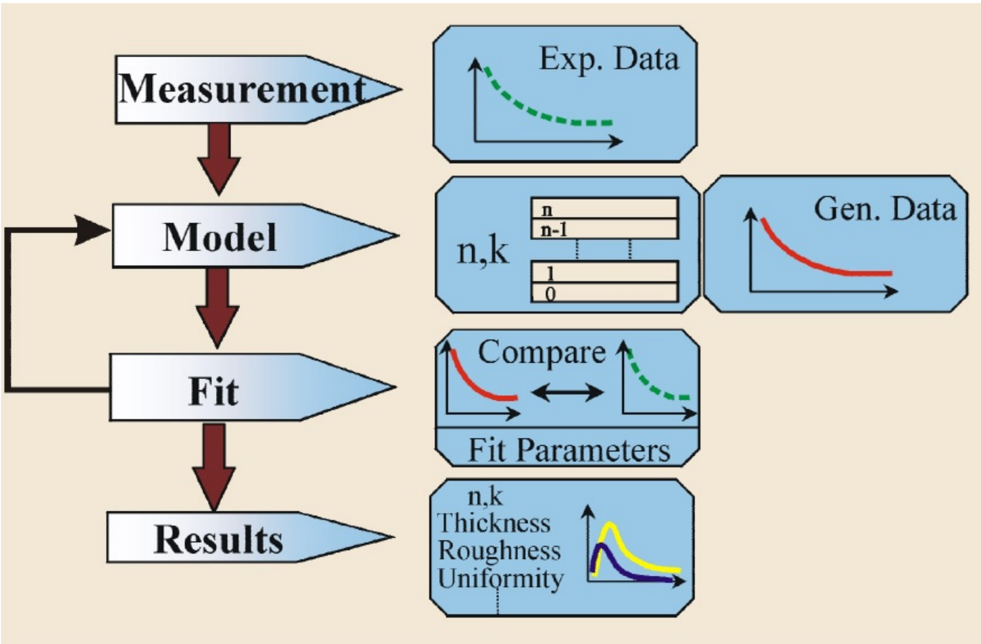

Figure 3.1: Flow Chart

3.2 Build a Model

A model is nothing but a description of a layered structure that describes sample that light interacted with. Basic types of models -

1. 2 media model : substrate alone
2. 3 media model : one layer on known substrate
3. Multilayer stack

Spectroscopic ellipsometry is a technique based on the measurement of the relative phase change of the reflected and polarised light in order to characterize thin film optical functions and other properties
The measured data are used to describe a model where each layer refers to a given material
The model uses mathematical relations called dispersion formulae that help to evaluate the thickness and optical properties of the material adjusting the specific fit parameters

1. Cauchy dispersion formula
2. Sellmeier dispersion formula
3. Drude dispersion formula
4. Lorentz dispersion formula
5. Tauc-Lorentz dispersion formula

3.2.1 Cauchy dispersion

Cauchy transparent -
Works best with material with no optical absorption in visible spectral range.
Generally has a monotonous decreasing refractive index with increasing wavelength.

$$n(\lambda) = A + \frac{10^4 \cdot B}{\lambda^2} + \frac{10^9 \cdot C}{\lambda^4}$$
$$k(\lambda) = 0$$

Figure 3.2: Cauchy Transparent

Cauchy absorbent -

More suitable for describing the optical properties of weakly absorbing materials.

$$n(\lambda) = A + \frac{10^4 \cdot B}{\lambda^2} + \frac{10^9 \cdot C}{\lambda^4}$$
$$k(\lambda) = 10^{-5} \cdot D + \frac{10^4 \cdot E}{\lambda^2} + \frac{10^9 \cdot F}{\lambda^4}$$

Figure 3.3: Cauchy Absorbent

Parameters of the Equations -

A is dimensionless parameter, as λ-¿ inf : n(λ) -¿A

B(nm2) – affects the curvature and amplitude of the refractive index at medium wavelength

C(nm2) – affects the curvature and amplitude of the refractive index at smaller wavelength in the UV

D is analogous to A

E is analogous to B

F is analogous to C

Limitations of the model -

Cannot be applied to metals and semiconductors.

Real and imaginary part of the refractive index are not related to each other.

Parameters do not have any physical meaning.

Application -

Transparent materials like insulators, glasses exhibiting low optical absorption.

3.2.2 Lorentz Dispersion Model

The Lorentz classical theory is based on the classical theory of interaction between light and matter and is used to describe frequency dependent polarisation due to bound charge.

The Lorentz dispersion formula comes from the solution of the equation of the solution of the equation of an electron bound to a nucleus driven by an oscillating electric field E.

The response is equivalent to classical mass-spring system, it generates damped harmonic oscillations.

Single Lorentz oscillator dielectric function -

$$\tilde{\varepsilon}(\omega) = \varepsilon_\infty + \frac{(\varepsilon_s - \varepsilon_\infty) \cdot \omega_t^2}{\omega_t^2 - \omega^2 + i \cdot \Gamma_0 \cdot \omega} \quad (9)$$

where ε_s is defined as: $\varepsilon_s = \varepsilon_\infty + \frac{\omega_p^2}{\omega_t^2}$

Figure 3.4: Single Lorentz Model

Multiple Lorentz oscillators dielectric function -

$$\tilde{\varepsilon}(\omega) = \varepsilon_\infty + \frac{(\varepsilon_s - \varepsilon_\infty) \cdot \omega_t^2}{\omega_t^2 - \omega^2 + i \cdot \Gamma_0 \cdot \omega} + \sum_{j=1}^{2} \frac{f_j \cdot \omega_{0j}^2}{\omega_{oj}^2 - \omega^2 + i \cdot \gamma_j \cdot \omega}$$

Figure 3.5: Multiple Lorentz Model

The single lorentz oscillator model is for a material which has only one resonance, the e-e and atom-atom interaction is ignored.
Real materials have many such sources of resonance and all these must be added together.
If we consider all these types of vibrations/resonances that can be caused by the applied Electro-Magnetic wave then, we get the multiple Lorentz Model.
This allows any no. of resonances to be accouned for through a simple summation.
At macroscopic level, all resonance mechanisms can be characterised by using the Lorentz model.

3.2.3 Drude dispersion Model

Drude's Model is based on the kinetic theory of electrons in a metal which assumes that the material has motionless positive ions and a non-interacting electron gas.
The simple model uses classical mechanical theory of free electron.

$$\tilde{\varepsilon}(\omega) = \varepsilon_\infty + \frac{\omega_p^2}{-\omega^2 + i \cdot \Gamma_d \cdot \omega}$$

Figure 3.6: Drude dispersion Model

The Drude's oscillator describes well the optical properties of metals but does not take into account the notion of optical energy band gap Eg semiconductors and the quantum effects.
This model fits well the optical properties of metallic samples and heavily doped semiconductors.
The spectral range used for fitting depends on the material.

3.3 Data Analysis

After the sample is measures a model is constructed to describe the sample. The model is used to calculate the predicted response from Fresnel's equations, which describe each material with thickness and optical constants.
If values are not known an estimate is given for the preliminary calculation. The calculated values are compared to experimental data.
The best match between the model and the experiment is typically achieved through regression.
An estimator like mean squared error(MSE), is used. The unknown parameters are allowed to vary until the minimum MSE is reached. The best answer corresponds to the minimum MSE.
Each of the involved steps is important, but parametrisation of the model and fitting of the data is most important, if the goodness of the fit parameter is not calculated there is no quantifiable measure of whether or not the model fits the data.

3.3.1 Regression MSE

Finding the best match between the model and the experiment is typically achieved through regression.
An estimator, like the Mean square Error(MSE) is used to quantify the difference between curves.
Unknown parameters are allowed to vary until minimum MSE is reached.
The best answer corresponds to the lowest MSE.
It is possible that the regression algorithm will mistakenly fall into a "local" minima depending on the starting thickness and the MSE conditions.
What can be done is we can obtain a graph of the thickness vs MSE value and can verify the global minimum of MSE and get the correct thickness.

Comparing the results in the form of a graph for the lowest MSE and a local minima allows us to distinguish the true global minimum easily.

3.3.2 Evaluating Fit Results

Evaluating the fit results is the most important aspect of SE data analysis. For a model fit to be acceptable the following requirements should be simultaneously met -

1. The model generated data must fit the measured data

2. The model should be unique

3. The model and fit parameters must be physical

Chapter 4

Application and Advantages

4.1 Application

1. Measurement of optical properties of materials in visible, IR, and near-UV spectral ranges.
2. Thin film thickness measurement, especially in semiconductor industry.
3. Study of the oxidation kinetics of semiconductor and metal surfaces.
4. Measurement of barrier layer thickness in food packaging industry.

4.1.1 Areas of application

1. Semicinductors
2. Flat panel displays
3. Material Science
4. Optical coatings
5. Photovoltaics
6. Biotechnology and surface Chemistry
7. Optoelectronic

4.2 Advantages

1. Non-invasive and non-destructive measurement technique
2. Very high precision
3. No reference measurement needed
4. By using polarised light, normal ambient unpolarised stray light does not significantly influence the measurement, no dark box is necessary
5. Both real and imaginary part of the dielectric function can be extracted
6. Ellipsometry measures an intensity ratio instead of pure intensity instabilities of the light source or atmospheric absorption
7. Spectroscopic Ellipsometry(SE), Increased sensitivity to multiple layer film stacks and measures data at wavelengths of interest
8. Variable angle Spectroscopic ellipsometry, New information(different path length) with each angle optimizes sensitivity.

Chapter 5

Silver on Glass thin film

5.1 Optained data ψ and δ

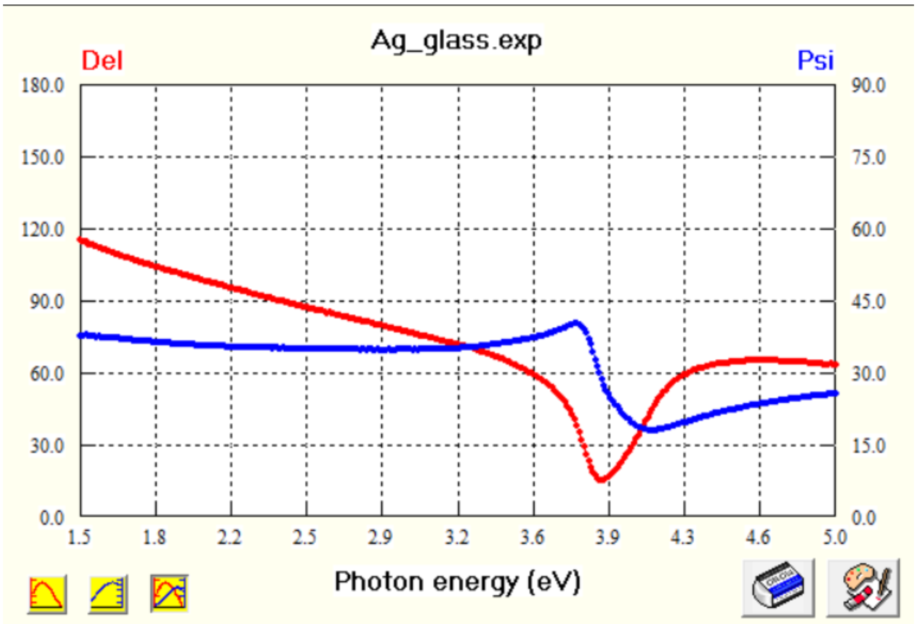

Figure 5.1: Optained data Ag on glass

5.2 Different Models used for fitting

Table 5.1: Different models for Ag on glass

Model used	Standard Deviation	Thickness (nm)
Standard reference Model	5.731	13.585
Lorentz Model N = 1	11.893	34.056
Drude's Model	17.265	51.9
Lorentz Model N = 2	4.838	15.5
Lorentz Model N = 4	3.232	13.5
Lorentz Model N = 4	3.615	22.991
Lorentz Model N = 4	2.843	17.218
Lorentz Model N = 6	1.91	18.053
Lorentz Model N = 6	1.646	18.594
Lorentz Model N = 7	0.967	15.948

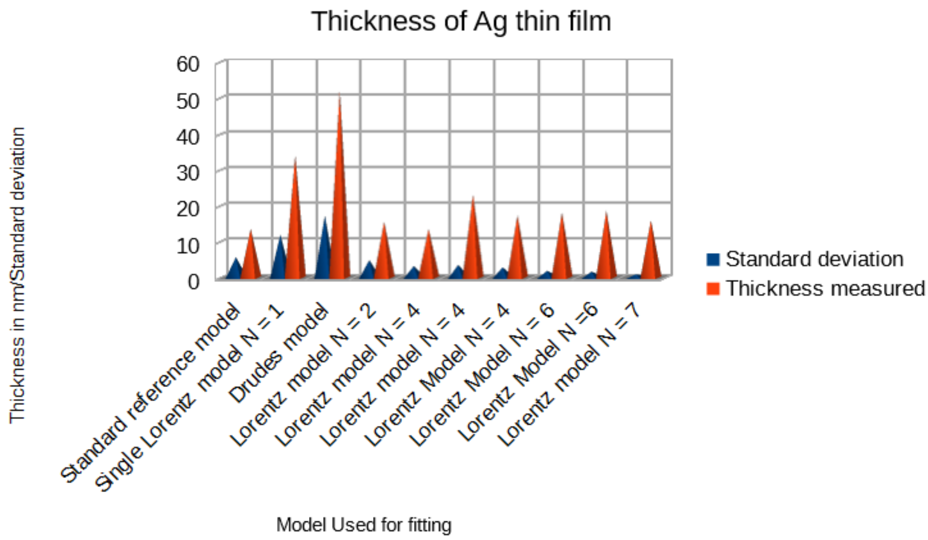

Figure 5.2: Standard deviation and thickness for Ag

5.3 Result (Best fit)

From the graph we can infer that the best fit was obtained with a minimum standard deviation of 0.967.

The corresponding thickness concluded is 15.948nm.

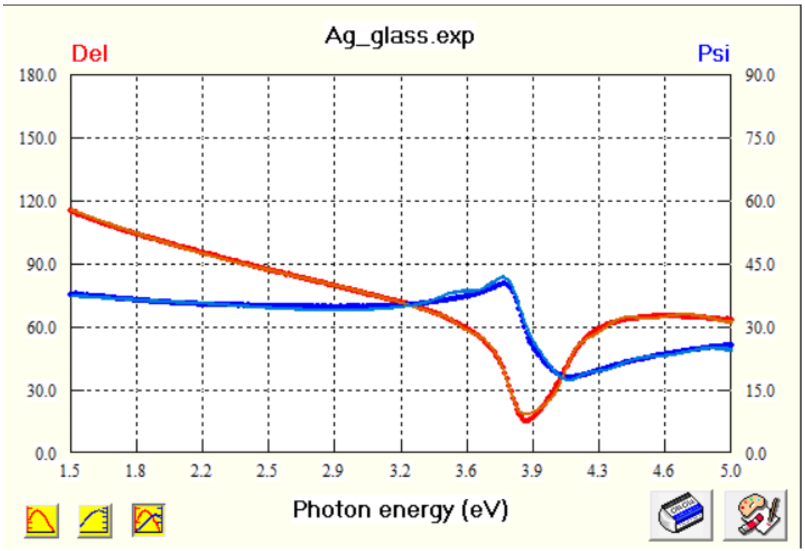

Figure 5.3: Ag - Result (Best fit)

Chapter 6

Aluminium on glass thin film

6.1 Optained data ψ and δ

Obtained data is as follows -

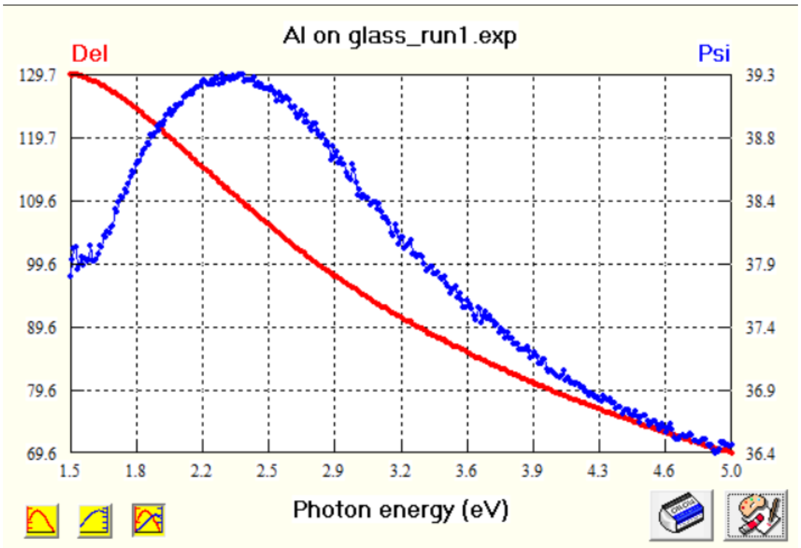

Figure 6.1: 10s integration time, 1.45-5ev range

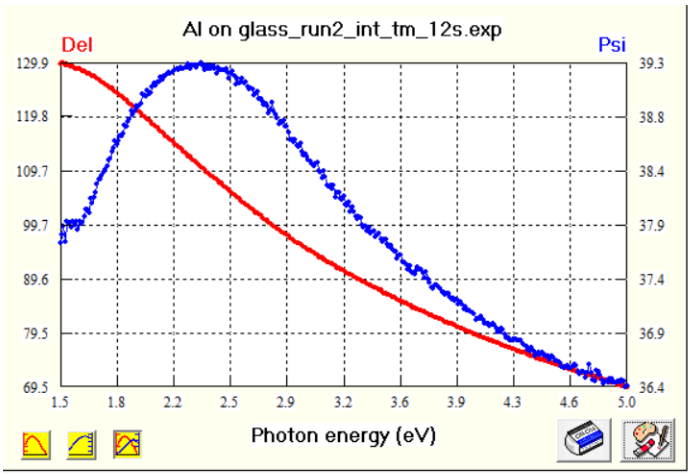

Figure 6.2: 12s integration time, 1.45-5ev range

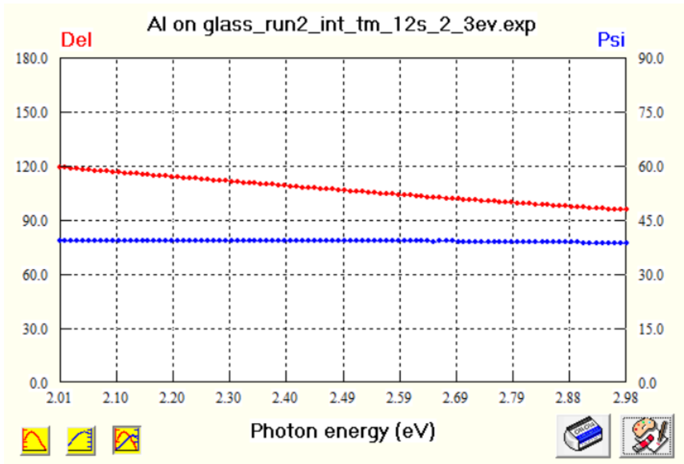

Figure 6.3: 2-3ev visible range

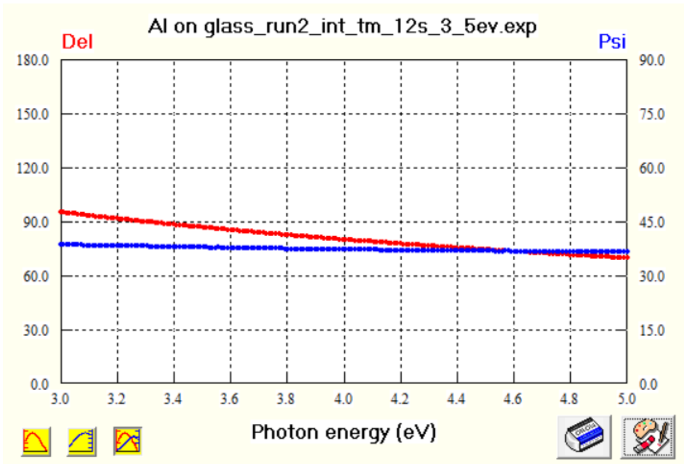

Figure 6.4: 3-5ev UV range

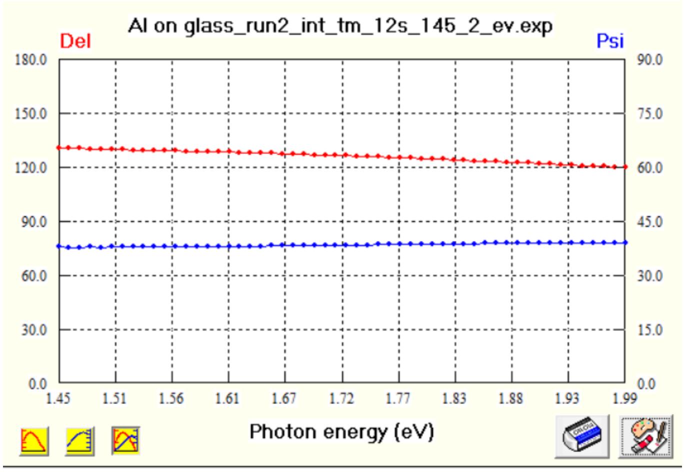

Figure 6.5: 1.45-2ev IR range

6.2 Different Models used for Al on glass

Table 6.1: Different models used

Model	Standard deviation	Thickness(nm)	Integration time and range
Standard Al Palik	13.994	4.589	10s 1.45-5ev
Lorentz Model N = 1	2.583	20.153	
Lorentz Model N = 2	2.268	17.235	
Lorentz Model N = 2	0.856	21.465	
Lorentz Model N = 2	0.861	21.473	12s 1.45-5ev
Lorentz Model N = 2	0.110	20.891	12s 2-3ev visible range
Lorentz Model N = 2	0.198	20.628	12s 3-5ev UV range
Lorentz Model N = 2	0.189	21.473	
Lorentz Model N = 2	0.499	21.473	12s 1.45-2ev IR range
Lorentz Model N = 2	0.828	21.066	
Lorentz Model N = 1	1.066	21.079	
Lorentz Model N = 1	0.787	21.033	

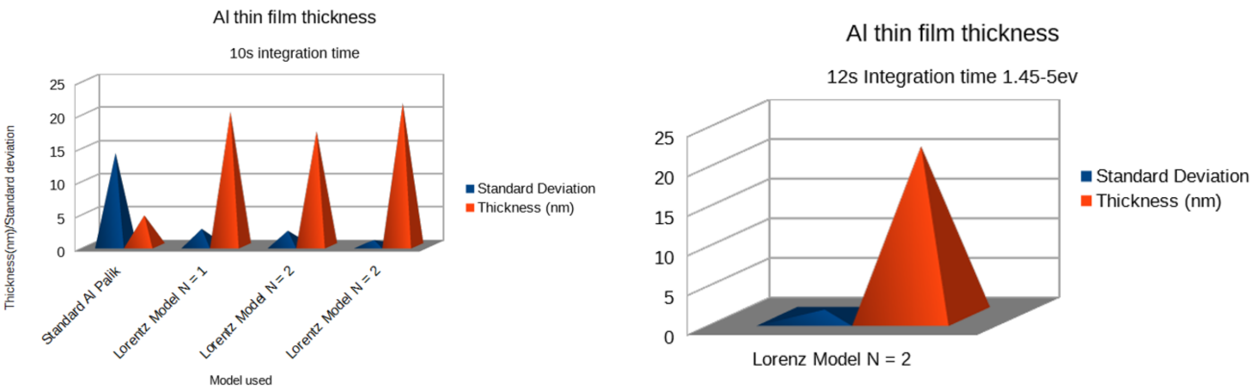

Figure 6.6: Standard deviation and thickness

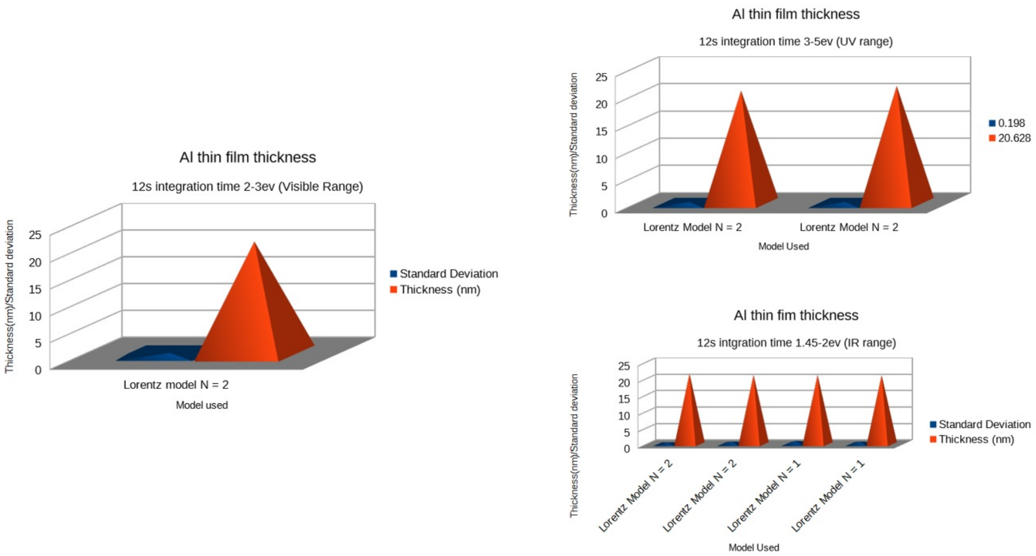

Figure 6.7: Standard deviation and thickness in respective regions

6.3 Result (Best fit)

The results suggests that the film thickness is approximately 21nm.
As we have standard deviation 0.861 at thickness 21.473nm.
Also standard deviation 0.856 at thickness 21.465nm.
The fitting of parameters in the visible range indicates a standard deviation of 0.110 at thickness 20.891nm.
In the UV region the standard deviation is 0.198 at thickness 20.628.
In the IR region the fit is obtained at one particular thickness, there is an slight uncertainty in concluding the thickness as if regression is continued the thickness goes on increasing with decrease in standard deviation.

Chapter 7

Conclusion

In the course of one month, ellipsometry as a method for measuring thin film thickness was studied and practicle measurements of Al thin fim on glass and Ag thin film on Glass were taken.
The thickness of the Silver on glass thin film was found to be 15.948nm with a standard deviation of 0.967. Lorentz model with N = 7 was used to fit this data.
The thickness of the Aluminium on glass thin film was found to be 21.473nm with a standard deviation of 0.861. The fit was performed using the Lorentz model with N = 2. Data was taken in different wavelength ranges. Applicability of the Lorentz model was tested in different wavelength regions and the thickess was measured. For the Visible range (2-3 ev) and UV range (3-5 ev) the thickness a match to the full range result, with thickness 20.89nm and 21.47nm from visible and UV range data respectively.

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