INDUSTRIAL APPLICATIONS OF ELLIPSOMETRY

By

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Abstract

Ellipsometry is generally a non-invasive, non-destructive measurement technique to obtain optical properties of a sample material by studying the state of polarization of the reflected light waves. Light polarization is a rich source of information and its measurement is important in many applications. In ellipsometry, which is a branch of optical polarimetry, fast measurement of the state of polarization of reflected light is making possible contineous, in-situ, and non-destructive monitoring and control of industrial processes. Basic concepts of these fast polarimetric sensors, along with thier applications in different industries, are briefly discussed.

Acknowledgements

First and formost, I thank the almighty GOD for helping me finish my work. I would like to express my sincere thanks to my advisor and instructor Prof. A.V.Gholap for his guidance, assistance, supervision and contribution of valuable suggestions. Finally, I thank my family and friends for their encouragement and support.

Introduction

Ellipsometry is a technique that has been studied for several centuries. However, it has recently found much favor in the non-destructive characterization of solids, particularly, semiconductors. Ellipsometry can generally be defined as the process of measurement and analysis of the elliptical polarization of light. Ellipsometry (reflection) measures the change in the state of polarization of light upon reflection from a surface. The fact changes are measured rather than the absolute intensity of the light renders ellipsometry sensitive to sub mono layer surface coverage.

The name ellipsometry comes from the fact that polarized light often becomes elliptical upon reflection. The change in light polarization upon reflection carries information of the optical properties of the medium under consideration.

Nowadays, there are two major kinds of ellipsometry widely used. These are spectroscopic ellipsometry (SE) and multiple angle of incidence (MAI) ellipsometry. In SE, the complex reflection ratio is measured over a range of wavelength at a fixed angle of incidence. In MAI Ellipsometry the angle of incidence is varied over range of angles which are particularly grouped around the principal angle. MAI system, generally, but necessarily, employs lasers as the light source. Lasers are highly monochromatic and have a much higher intensity at specific wavelength than conventional sources. Furthermore, the beam divergence is minimum. This reduces systematic errors in MAI systems.

Ellipsometry was developed first by Drude in 1887. He also derived the equations of ellipsometry, which are used even today. Most ellipsometers were operated manually and the ellipsometery measurment was very time consuming. In 1975, however, Aspens realized the complete atomization of spectroscopic ellipsometry measurements. The development of this instrument improved not only the measurement time, but also the measurement precision significantly. Recently, optical anisotropic materials have been studied extensively by applying Mueller Matrix ellipsometry that allows the complete characterization of optical behavior in an anisotropic materials. For the characterization of the conventional isotropic sample, current spectroscopic ellipsometry instruments are highly satisfactory. Thus, most of recent ellipsometry studies have been made on a material characterization rather than the development of ellipsometry instruments.

Objective of the Project

The main objective of this project is:

This project gives the basic introduction to the theory of ellipsometry and typical ellipsometry applications in industries such as: Semiconductor, Optical Coatings, Data Storage, and Flat Panel Display industries.

Project Structure

The project is structured as follows:

Chapter one introduces the theory of light. In this chapter, concepts of polarized and unpolarized light waves are briefly treated. Different approaches for representation of polarization of light waves are thoroughly considered.

Under chapter two the basic theory of ellipsometry is described and experimental technique for ellipsometry is presented.

Chapter three is the main frame of the project. It describes the applications of ellipsometry in industries.

Finally, conclusions from the preceding chapters are made.

Chapter 1

Theory of Light

1.1 Historical Development of the Concept of Light

The question what is light? immutably remains while the answer subtly changes through time. The search for the explanation of the property of light dates back to remote antiquity. The rectilinear propagation of light, as well as laws of reflection, were explained by Euclid in 300 B.C. [1]

From seventeenth century onward, a number of laws and theories are proposed for light. The discovery of the law of refraction by Willebroad Snell in 1621 was one of the greatest moment in optics.

The actual nature of light, particle or wave comes to the picture of contemporary physicists in the seventeenth century. Sir Isaac Newton, proposed a corpuscular theory of light. He concluded that white light is composed of a mixture of particles. Contrary to Newton, C. Huygens advocated the wave theory of light. Using wave theory, he was able to derive laws of reflection and refraction.

The wave theory of light was reborn at hands of Pr.Thomas Young. He was able to explain colored fringes of thin films and determined wavelength of various colors using Newtons data. This is an interference phenomena. A.J. Fresnel, unaware of the efforts of Young, also independently developed wave theory of light. He was able to calculate the diffraction patterns. Fresnel went on to evolve to calculate a mechanistic description of aether oscillation, which led to his famous formulas for amplitudes of reflected and transmitted light. The polarization phenomenon demands that the light wave phenomenon as described by transverse waves with this breaking discovery, by 1825 corpuscular theory had only a few tenacious advocates.

One of the fascinating problems of measurement in experiment was determination of the speed of light. The first terrestrial determination of speed of light was performed by A.H.L. Fizeau in 1849. Using rotating mirror arrangement in order to measure the duration of an electric spark, Arago reported to the academy of science that the speed of light in water is less than the speed in air. This surprising result at that time shocked strongly held Newton's formulation of the corpuscular theory. Quite independently, the magnetism and electricity was studied thoroughly by experimentalist Michael Faraday. Faraday established an interrelationship between electromagnetism and light when he found that polarization direction of a beam could be allowed by a strong magnetic field applied to the medium.

One of the greatest breakthrough of Electricity and Magnetism is achieved by James Clerk Maxwell. He elegantly summarized the behavior of electric and magnetic fields in a single set of mathematical equations. From this equation, he successfully solved the speed of light. He predicted that the electromagnetic wave propagates as a transverse wave in the luminiferous aether. This conclusion leads to the fact that light was electromagnetic disturbance in the form of waves propagating through aether.

The acceptance of the wave theory of light seemed to necessitate an equal acceptance of the existence of all pervading substrum, the luminiferous aether. If there were waves, it seemed obvious that there must be a supporting medium. The corpuscular model of light could explain stellar aberration rather handily. Alternatively, the wave theory also offers a satisfactory explanation provided that aether totaly undisturbed as earth plows through it. The Michelson-Morley experiment refuted the concept of aether.

In twentieth century new concepts of explanation of light arose, Quantum mechanics. In 1905, Einstein proposed a new form of corpuscular theory in which he asserted that light consisted of globs or particles of energy. Each quantum of radiant energy is called photon. It gradually, using quantum mechanics, become evident that concept of particle and wave, which in the macroscopic world seem so obviously mutually exclusive must be merged in submicroscopic domain.

Many properties of matter are probed by interaction of matter with light. This branch of physics is spectroscopy. With this tool, many optical properties of a given material are analyzed. The invention of laser greatly enhanced research undergoing on spectroscopy. There are number of techniques used depending on the information required reflectance, RAS, ellipsometry, transmission, Raman scattering etc. A far-reaching revolution in the methods of processing and community information is quietly taking, a revolution that will continue to change our lives in the years ahead. On other side theoretical explanation of mysterious light is still of keen interest for many scientists.

1.2 Maxwell Equations and Boundary Conditions

Maxwell expressed the results of his theoretical investigation in the form of four fundamental equations which have since become famous as Maxwell's Equations. They were based on the earlier experimental researches of Oersted, Faraday and Joseph Henry concerning the the relations between electricity and magnetism. They summarize these relations in concise mathematical form and constitute a starting point for the investigation of all electromagnetic phenomena. The four Maxwell equations can be expressed in the following way for the case of free space:

$$\nabla.\mathbf{D} = \rho_f \tag{1.2.1}$$

$$\nabla.\mathbf{B} = 0 \tag{1.2.2}$$

$$\nabla \times \mathbf{E} = \frac{-\partial \mathbf{B}}{\partial t} \tag{1.2.3}$$

$$\nabla \times \mathbf{H} = J_f \tag{1.2.4}$$

The above four equations are sufficient to determine the electromagnetic field completely if ρ_f and $\mathbf{J}_f$ are given and the electric properties of the medium are known. For isotropic linear medium, $\mathbf{B} = \mu\mathbf{H}$ and $\mathbf{D} = \epsilon\mathbf{E}$.

Maxwell equations become

$$\nabla.\mathbf{E} = \frac{\rho_f}{\epsilon} \tag{1.2.5}$$

$$\nabla.\mathbf{B} = 0 \tag{1.2.6}$$

$$\nabla \times \mathbf{E} = \frac{-\partial \mathbf{B}}{\partial t} \tag{1.2.7}$$

$$\nabla \times \mathbf{B} = \mu J_f + \mu\epsilon\frac{\partial \mathbf{E}}{\partial t} \tag{1.2.8}$$

For no external charge densities and currents

$$J_f = \sigma_c \mathbf{E}$$

$$\nabla \times \mathbf{B} = \mu\sigma_c\mathbf{E} + \mu\epsilon\frac{\partial \mathbf{E}}{\partial t} \tag{1.2.9}$$

where σ_c is conductivity of the material

μ is permeability of the material

ϵ is the permittivity of the material

This relations yield to a three-dimensional wave equations which are expressed by

$$\nabla^2\mathbf{E} = \mu\sigma_c\frac{\partial \mathbf{E}}{\partial t} + \mu\epsilon\frac{\partial^2 \mathbf{E}}{\partial t^2} \tag{1.2.10}$$

$$\nabla^2\mathbf{B} = \mu\sigma_c\frac{\partial \mathbf{B}}{\partial t} + \mu\epsilon\frac{\partial^2 \mathbf{B}}{\partial t^2} \tag{1.2.11}$$

The solution of the above equations have septile complex form

$$\mathbf{E} = \hat{E}e^{-i(\omega t - \mathbf{k}.\mathbf{r})}, \qquad \mathbf{B} = \hat{B}e^{-i(\omega t - \mathbf{k}.\mathbf{r})} \tag{1.2.12}$$

where **E** and **B** are complex vector amplitudes independent of **r** and t. When light r passes from one medium in to another, EMF vectors must satisfy boundary condition. The boundary condition is the continuity of the tangential components of **E** and **H** vectors on the interface between the two isotropic dielectric media. The incident electric field **E** can be decomposed into two orthogonal components. The component perpendicular to the plane of incidence is S-component, and the component parallel to the plane of incidence is P-component. From boundary condition, the Fresnel reflection and transmission coefficients for S- and P-polarization can be derived.

$$r_p = \frac{E'_{op}}{E_{op}} = \frac{N_1 \cos\Phi_i - N_0 \cos\Phi_t}{N_1 \cos\Phi_i + N_0 \cos\Phi_t} \tag{1.2.13}$$

$$t_p = \frac{E_{1p}}{E_{op}} = \frac{2N_0 \cos\Phi_i}{N_1 \cos\Phi_i + N_0 \cos\Phi_t} \tag{1.2.14}$$

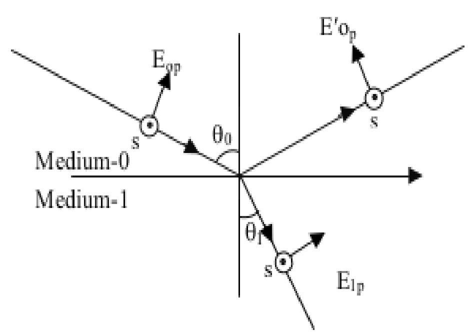


Figure 1.1: Reflection and transmission of a plane wave at the planar interfaces between two semi-infinite media 0 and 1.

$$r_s = \frac{E'_{os}}{E_{os}} = \frac{N_0 \cos\Phi_i - N_1 \cos\Phi_t}{N_0 \cos\Phi_i + N_1 \cos\Phi_t} \tag{1.2.15}$$

$$t_s = \frac{E_{1s}}{E_{os}} = \frac{2N_0 \cos\Phi_i}{N_0 \cos\Phi_i + N_1 \cos\Phi_t} \tag{1.2.16}$$

and Snells law for the two systems,

$$N_o \sin\Phi_i = N_1 \sin\Phi_t \tag{1.2.17}$$

where N_o and N_1 are indices of refraction of the two media.

When a P-polarized light wave is incident on the interface between two transparent media, the reflected wave entirely disappears at a particular angle of incidence called the Brewster angle ϕ_B, and the incident beam is totally refracted into the second medium. Setting $r_p = 0$ and using equation (1.2.17),

$$\tan\phi_B = (N_1/N_0) \tag{1.2.18}$$

1.3 Polarization of Light Wave

An oscillating vector field must instantaneously have a unique direction. For the plane electromagnetic wave in an isotropic medium this direction must be perpendicular to the wave normal; if it remains constantly in the same direction, the wave is said to be Plane polarized. On the other hand, if the direction changes randomly, the wave is said to be unpolarized.

Depending on the phase difference between two oscillating electric field vectors, we can have a linear, circular or elliptical polarization. Two plane polarized waves combine to produce another wave which is also plane polarized.

If the phase difference is a multiple of $\pi/2$, the resultant oscillating vector now rotates following a circle or ellipse depending on the amplitudes of the two vectors. Linearly polarized light is a surprisingly common phenomenon in everyday circumstances. Light reflected from any smooth surfaces such as a wet road or a polished table top, partially linearly polarized; this is easily demonstrated by turning the polaroid glass which gives a change in brightness according to the change in angle between the plane of polarization and the transmission axis of the polaroid. The maximum effect is found for reflection at a particular angle of incidence, the Brewster angle.

1.3.1 Formal Description of Polarized Light

When light interacts with matter, the force exerted on the electron by the electric field of the light wave is much greater than the magnetic field. That is why the polarization is determined by the direction of electric field.

Let us consider an electromagnetic wave propagating along x̂ direction. The orthogonal electric fields are along ŷ and ẑ axes. These components are the two plane polarized waves. There is a phase difference ϕ between the two components.

$$\mathbf{E}_y = E_{0y} \exp i(\omega t - kx)\hat{y} \tag{1.3.1}$$

$$\mathbf{E}_z = E_{0z} \exp i(\omega t - kx + \phi)\hat{z} \tag{1.3.2}$$

If we take the real component of the above equations, and take the electric field at a fixed space x = 0

$$\mathbf{E}_y = E_{0y} \cos(\omega t)\hat{y}$$

$$\mathbf{E}_z = E_{0z} \cos(\omega t + \phi)\hat{z}$$

Taking the magnitude of E_y and E_z

$$\frac{\mid \mathbf{E}_y \mid}{E_{oy}} = \cos(\omega t)$$

$$\frac{\mid \mathbf{E}_z \mid}{E_{oz}} = \frac{\mid \mathbf{E}_y \mid}{E_{oy}} \cos(\phi) - \sin(\omega t)\cos(\phi)$$

Squaring both side and simplifying,

$$\frac{\mid \mathbf{E}_z \mid^2}{E_{oz}^2} + \frac{\mid \mathbf{E}_y \mid^2}{E_{oy}^2} - 2\frac{\mathbf{E}_z \mathbf{E}_y}{E_{oz}E_{oy}} \cos(\phi) = \sin^2(\phi) \tag{1.3.3}$$

This is the general equation of ellipse. Depending on the values of ϕ, the equation can represent line, circle or ellipse. The sign of ϕ determines the sense of rotation.

Case I. When the phase difference is an integral multiple of π, equation(1.3.3) becomes

$$Ey = \pm \frac{A_y}{A_z} E_z$$

The wave is linearly polarized. The negative sign is when it is an odd multiple of π and

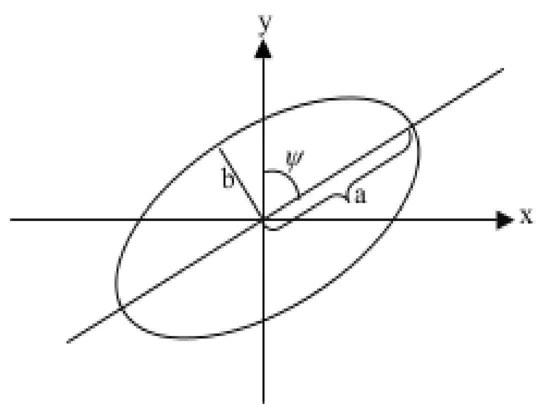


Figure 1.2: Elliptically polarized light for arbitrary phase shift.

the positive sign is when it is an even multiple of π.

Case II. When phase difference is an odd multiple of $\pi/2$ and $E_{oy} = E_{oz}$, equation(1.3.3) represents an equation of a circle.

$$E_y^2 + E_z^2 = A^2$$

This is a circularly polarized light, a given vector precesses with a constant angular speed with constant magnitude. When z-component electric field leads y-component, we have clockwise rotation which is called right handed polarization.

Case III. When the phase difference is an odd multiple of $\pi/2$ and $E_{oz} \neq E_{oy}$, the polarization becomes elliptic whose major axis lies either on y or x axis.

Case IV. For a general case, when ϕ is not an integral multiple of $\phi/2$, elliptical polarization whose major axis does not lie along z or y will result. The tilting angle ψ is defined as:

$$\tan(2\psi) = \frac{2ab\cos(\phi)}{a^2 - b^2}$$

Ellipticity e is the ratio of the length of the semi-minor axis of the ellipse b to the length of semi-major axis a. The right-handed and left-handed circularly polarized states correspond to e = 1 and e = -1 respectively. Linearly polarized light has ellipticity of zero magnitude.

1.3.2 Modern Description of Polarized and Unpolarized Light

Poincar'e Sphere

The Poincar'e sphere is a unit radius spherical surface each point of which signifies a different polarization state [3]. It is a polarization space in the form of a spherical surface whose points are one to one correspondence with different states of polarizations of light. The state of polarization of light can be described by using different kinds of polarization space. The complex plane representation of polarized light gives another space whose points are in one to one correspondence with different possibilities of polarization.

Consider a sphere of radius S_0. Any point on the sphere is represented by longitude 2θ and latitude 2ϵ. The following properties of polarized light can be associated with a point P on a sphere.

1. The north and the south pole stands for the left and right circular polarization respectively.

2. Every point on the equator represents a linear polarization form; each point implies different oscillation direction.

3. The northern hemisphere excluding the north pole represents right handed elliptical polarization and the southern hemisphere excluding the south pole represents left handed elliptical polarization.

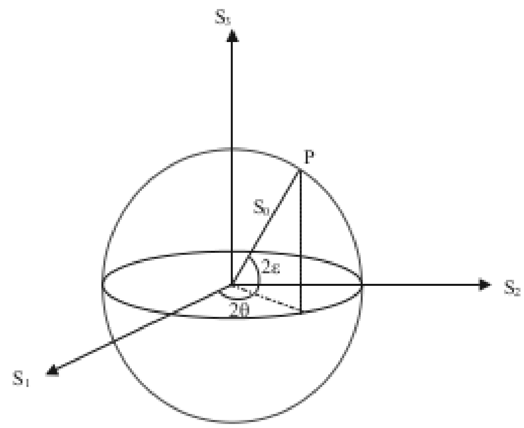


Figure 1.3: Poincar'e sphere.

4. The latitude whose common axis is polar axis from south to north pole represents an equiellipticity contour.

In general, the state of polarization is described by azimuthal ψ and ellipticity angle as described in the previous section. These two quantities represent a point on the Poincar'e sphere with a coordinate of latitude 2ϵ and the longitude 2θ. A bilinear transformation can be produced from the Poincar'e sphere representation to a cartesian coordinate system. A given point P is represented with a spherical coordinate (S_0, $\pi/2 - 2\epsilon$, 2θ). This can be expressed in a new cartesian coordinate system (see figure 1.3).

$$S_0^2 = S_1^2 + S_2^2 + S_3^2 = E_x^2 + E_y^2, \tag{1.3.4}$$

$$S_1 = S_0 \cos(2\epsilon) \cos(2\theta) = E_x^2 - E_y^2, \tag{1.3.5}$$

$$S_2 = S_0 \cos(2\epsilon) \cos(2\theta) = 2E_x E_y \cos(\phi), \tag{1.3.6}$$

$$S_3 = S_0 \sin(2\epsilon) = 2E_x E_y \sin(\phi), \tag{1.3.7}$$

where ϕ is the phase shift between the horizontal and the vertical components of the electric field **E** propagating in z direction.

If the radius of the Poincar'e sphere is unity, the above equations represent Stokes parameters.

1.3.3 Stokes Vectors

In 1852 G.C. Stokes introduced four quantities, Stokes parameters, which are functions of the observable electromagnetic waves. It equally applies well to polarized light, partially polarized light and unpolarized light. Stokes vector is a 4 x 1 column of vector consisting of Stokes parameters. In order to exploit the use of compact matrix formalism to investigate the interaction between the light wave and the optical components, Stokes vectors is preferred to Poincar'e sphere representation. It is often written horizontally to save space. Stokes parameters are a set of four real quantities with dimension of intensity given by equations(1.3.4-1.3.7)

The first parameter S_0 is the total intensity of the light waves. S_1 gives the difference between x and y components and can be either positive, negative or zero. It reduces to positive when the vibration is horizontal and reduces to negative when the vibration is vertical. It becomes zero when the beam is circularly polarized, elliptically polarized with major axis is at $\pm\pi/4$ or unpolarized. Thus it does indicate preference of x polarization to y polarizations. Stokes parameter S_3 represents the preference of the wave to either right or left handed circularly polarized component. The third component S_2 represents a preference for $\pm\pi/4$ linear polarization.

When a given light is completely polarized, the following relation holds.

$$S_0^2 = S_1^2 + S_2^2 + S_3^2.$$

For partially polarized light, the relation becomes,

$$S_0^2 > S_1^2 + S_2^2 + S_3^2.$$

The degree of polarization is the ratio of the intensity of totally polarized light to the total intensity of the light. Mathematically, it is given as,

$$P = \frac{S_1^2 + S_2^2 + S_3^2}{S_0^2}$$

It is important to remember that Stokes vectors may be added only when the beams concerned are incoherent [12].

1.3.4 Jones Vectors and Matrices

Jones vector is an abstract mathematical space formed by all vectors that are obtained by considering all possible pairs of complex numbers for $\mathbf{E}_x$ and $\mathbf{E}_y$. It is a two elements column vector. Each element describes one component of electric field $\mathbf{E}$. It is superior to the Stokes vector in some ways and inferior in others. It is superior in that, it is applicable to the addition of coherent beams; also it is more compact. But it can not handle unpolarized or partially polarized light.

Consider a uniform transverse electric elliptically polarized plane wave. If such a wave is assumed to propagate in z-direction, $\mathbf{E}$ is given by

$$\mathbf{E}(z,t) = \hat{E}_x \cos(\omega t - \frac{2\pi z}{\lambda} + \delta_x)\hat{x} + \hat{E}_y \cos(\omega t - \frac{2\pi z}{\lambda} + \delta_y)\hat{y}, \tag{1.3.8}$$

where E_x and E_y represent amplitudes of the linear, simple harmonic oscillation of the electric field components along the x and y axes, and δ_x and δ_y represent the respective phases of the oscillation.

A more compact mathematical description of the wave can be obtained from equation(1.3.8). This compact description is sufficient enough to fully explain the wave polarization and its modification after interacting with optical devices. The concise description is the Jones vector of a wave represented by the following matrix.

$$\mathbf{E} = \begin{pmatrix} \tilde{E}_x e^{i\sigma_x} \\ \hat{E}_y e^{i\sigma_y} \end{pmatrix} \tag{1.3.9}$$

From the above equation, the Jones vectors for different polarization can be obtained.

1. For linearly polarized light wave, the normalized Jones vector is

$$\mathbf{E} = \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}$$

where θ is the angle the vector makes with the x-axis.

Particularly for x-polarization and y-polarization, the Jones vectors become

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad and \qquad \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

2. For left and right circularly polarized light, the normalized Jones vectors are respectively

$$\mathbf{E}_l = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}$$

$$\mathbf{E}_r = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}$$

The main use of Jones vector is in computing the effect of inserting optical devices like polarizer, analyzer and retarder in a given system. This effect is easily computed by multiplying Jones vectors of incident beam by the respective Jones matrices of the optical devices. The optical elements are represented by 2 x 2 Jones matrix.

Consider an incident wave on a non depolarizing optical system that consists of a single optical device. Due to the interaction, a modified wave will emerge from the system. This is shown below in schematic diagram. The incident and the out going plane waves can be described by their appropriate Jones vectors $\mathbf{E}_1$ and $\mathbf{E}_0$. These two plane waves are related by a linear relation,

$$E_{ox} = T_{11}E_{1x} + T_{12}E_{1y}, \tag{1.3.10}$$

$$E_{oy} = T_{21}E_{1x} + T_{22}E_{1y}, \tag{1.3.11}$$

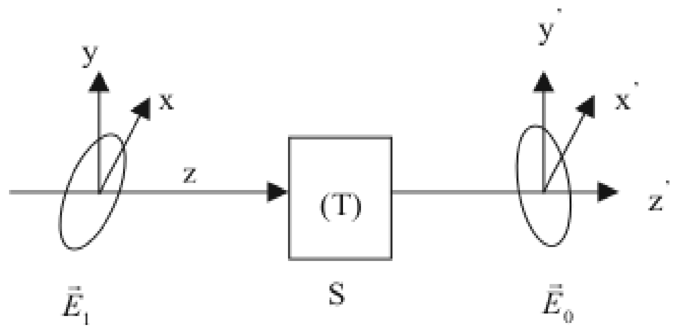


Figure 1.4: Schematic diagram for incident and output plane waves of Jones vectors

This can be written in a more compact form by matrix,

$$E_0 = TE_1, \quad where \qquad T = \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix}$$

The 2 x 2 transformation matrix T is called Jones matrix of the optical device. [12] It includes the overall effect of optical devices on the incident wave.

This result can be generalized for a series of successive optical devices. The out going light is given for such system simply as,

$$E_0 = T_n T_{n-1} ... T_1 T_0 E_1,$$

where T_n represents Jones matrix of the nth optical device.

Chapter 2

Ellipsometry

2.1 Ellipsometry Theory

Ellipsometry can be generally defined as the measurement of polarization of a polarized vector wave. The mathematical theory of ellipsometry is based on the Fresnels equations which are derived from Maxwells boundary conditions discussed under chapter 1. Although measurement of the state of polarization of light wave is important in its own right, ellipsometry is generally conducted in order to obtain information about an optical system that modifies the state of polarization [8].

2.1.1 Basic mathematical Tools

Basic mathematical tools of ellipsometry are built on the Maxwell's wave equations at the boundaries of the interface.

$$r_p = \frac{N_1 \cos\Phi_i - N_0 \cos\Phi_t}{N_1 \cos\Phi_i + N_0 \cos\Phi_t} \tag{2.1.1}$$

$$r_s = \frac{N_0 \cos\Phi_i - N_1 \cos\Phi_t}{N_0 \cos\Phi_i + N_1 \cos\Phi_t} \tag{2.1.2}$$

$$t_p = \frac{2N_0 \cos\Phi_i}{N_1 \cos\Phi_i + N_0 \cos\Phi_t} \tag{2.1.3}$$

$$t_s = \frac{2N_0 \cos\Phi_i}{N_0 \cos\Phi_i + N_1 \cos\Phi_t} \tag{2.1.4}$$

Φ_i and Φ_t are the incident and refracted (transmitted) angles respectively. They are related by snells law.

$$N_0 \sin \Phi_i = N_1 \sin \Phi_t \tag{2.1.5}$$

The reflection ellipsometry employs the Fresnels coefficients for the reflection ellipsometry is usually written as

$$r_p = |r_p| e^{i\delta_{rp}} \tag{2.1.6}$$

$$r_s = |r_s| e^{i\delta_{rs}} \tag{2.1.7}$$

where δ_{rp} and δ_{rs} are the phase shifts upon reflection for p and s polarized light respectively.

As it has been stated in the introduction part, reflection ellipsometry is a technique based on measurement of the states of polarization of incident and reflected waves, leading to the determination of the ratio ρ of the complex Fresnel reflection coefficients for p and s polarizations.

$$\rho = \frac{r_p}{r_s} \tag{2.1.8}$$

It is often convenient to write ρ in the form

$$\rho = \tan \Psi e^{i\Delta} \tag{2.1.9}$$

From equations (2.1.6), (2.1.7) and (2.1.8), it is readily seen that

$$\tan \Psi = \left| \frac{r_p}{r_s} \right| \tag{2.1.10}$$

$$\Delta = \delta_{rp} - \delta_{rs} \tag{2.1.11}$$

Ψ and Δ are ellipsometric angles determining the differential changes in amplitude and phase, respectively, experienced upon reflection by component vibrations of the electric field vector parallel and perpendicular to the plane of incidence[9].

If we substitute for r_p and r_s of equations (2.1.1) and (2.1.2) in equation (2.1.8), and using snell's law (2.1.5), the complex refractive index of the second medium/film N_1 in terms of ρ and Φ_i are solvable and given in the following equation.

$$N_1 = N_0 \sin \Phi_i \left[1 + \left(\frac{1-\rho}{1+\rho} \right)^2 \tan^2 \Phi_i \right]^{\frac{1}{2}} \tag{2.1.12}$$

Let an electromagnetic wave of p and s polarized wave incident at the upper surface of thin film of thickness d at angle[10] of incidence Φ_i shown in figure 2.1. As the wave enters

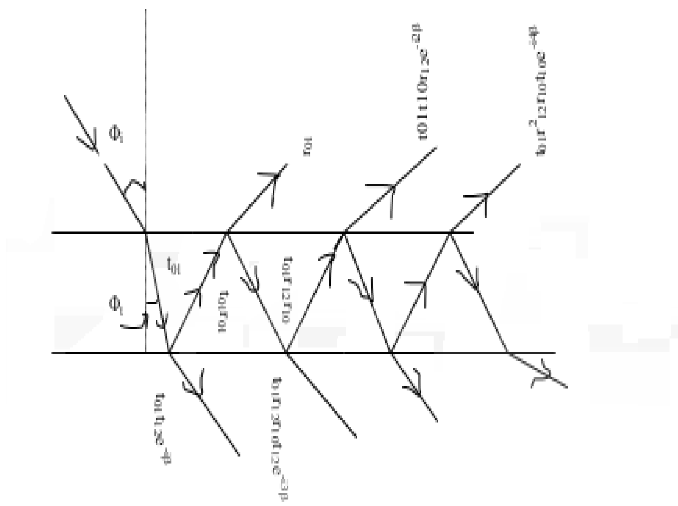


Figure 2.1: Multiple Reflections from Thin film

the film, the propagated wave reflected inside the film and transmitted to the surrounding media of the film. Inside the film the propagation wave makes a zigzag path. The phase angle β or the the film phase thickness is given by[17, 25]

$$\beta = 2\pi \frac{d}{\lambda} N_1 \cos \Phi_t \tag{2.1.13}$$

or,

$$\beta = 2\pi \frac{d}{\lambda} (N_1^2 - N_0^2 \sin^2 \Phi_t)^{\frac{1}{2}} \tag{2.1.14}$$

From figure 2.1: the total reflected amplitude R is computed from an infinite geometric series for the waves coming from the upper face of the film.

$$R = r_{01} + t_{01}t_{10}r_{12}e^{-i2\beta} + t_{01}t_{10}r_{10}r_{12}^2e^{-i4\beta} + t_{01}t_{10}r_{10}^2r_{12}^3e^{-i6\beta} \tag{2.1.15}$$

This summation gives:

$$R = r_{01} + \frac{t_{01}t_{10}e^{-i2\beta}}{1 - r_{10}r_{12}e^{-i2\beta}} \tag{2.1.16}$$

From the principle of reversibility[25]: $r_{10} = r_{01}$ and $t_{01}t_{10} = 1$ - r_{01}^2. Therefore,

$$R = \frac{r_{01} + r_{12}e^{-i2\beta}}{1 + r_{01}r_{12}e^{-i2\beta}} \tag{2.1.17}$$

Similarly, the total transmitted amplitude from the lower part of the film is computed in the following equation.

$$T = \frac{t_{01}t_{12}e^{-i\beta}}{1 + r_{01}r_{12}e^{-i2\beta}} \tag{2.1.18}$$

Reflection Ellipsometry utilizes equation (2.1.17) by introducing p and s subscripts as follows:

$$R_p = \frac{r_{01p} + r_{12}e^{-i2\beta}}{1 + r_{01p} + r_{12p}e^{-i2\beta}} \tag{2.1.19}$$

$$R_s = \frac{r_{01s} + r_{12}e^{-i2\beta}}{1 + r_{01s} + r_{12s}e^{-i2\beta}} \tag{2.1.20}$$

The ellipsometric angles Ψ and Δ are related to equations (2.1.19) and (2.1.20) by finding their ratio as follows:

$$\rho = \tan\Psi e^{i\Delta} = \frac{R_p}{R_s} = \frac{r_{01p} + r_{12p}e^{-i2\beta}}{1 + r_{01p}e^{-i2\beta}} \times \frac{1 + r_{01s}r_{12s}e^{-i2\beta}}{r_{01s} + r_{12s}e^{-i2\beta}} \tag{2.1.21}$$

The corresponding amplitude reflection coefficients for p and s from the upper and lower surface of the film is given by:

$$r_{01p} = \frac{N_1\cos\Phi_i - N_0\cos\Phi_t}{N_1\cos\Phi_i + N_0\cos\Phi_t} \tag{2.1.22}$$

$$r_{12p} = \frac{N_2\cos\Phi_t - N_1\cos\Phi_t}{N_2\cos\Phi_t + N_1\cos\Phi_{t^1}} \tag{2.1.23}$$

$$r_{01s} = \frac{N_0 \cos\Phi_i - N_1 \cos\Phi_t}{N_1 \cos\Phi_i + N_0 \cos\Phi_t} \tag{2.1.24}$$

$$r_{12s} = \frac{N_1 \cos\Phi_t - N_2 \cos\Phi_{t^1}}{N_1 \cos\Phi_t + N_2 \cos\Phi_{t^1}} \tag{2.1.25}$$

By relating equations (2.1.13) and (2.1.21), one can obtain the film thickness d.

2.2 The Fourier Coefficients a and b, and Ellipsometric Parametrs Ψ and Δ

Non polarized source emits, an electromagnetic wave of intensity[11]

$$I(\lambda) = E.E^* \tag{2.2.1}$$

Let the first a polarizer select a beam with components

$$E_p = E_0 \cos\alpha, \qquad\qquad E_s = E_0 \sin\alpha \tag{2.2.2}$$

Which after reflection becomes:

$$E_{ref} = r_p E_p + r_s E_s = E_0 \mid r_p \mid \cos(\alpha) e^{i\delta_p} + E_0 \mid r_s \mid \sin(\alpha) e^{i\delta_s} \tag{2.2.3}$$

And finally, it is filtered by the second rotating analyzer rotating by w, and the emerging electric field becomes

$$E_{out} = r_p E_p \cos(\omega t) + r_s E_s \sin(\omega t) \tag{2.2.4}$$

$$E_{out} = E_0 \mid r_p \mid \cos(\omega t)\cos(\alpha) e^{i\delta_p} + E_0 \mid r_s \mid \sin(\omega t)\sin(\alpha) e^{i\delta_s} \tag{2.2.5}$$

The intensity detected by photo detector becomes now

$$I_D = E_{out}.E^*_{out} = \mid E_0 \mid^2 [\mid r_p \mid]^2 \cos^2(\omega t)\cos^2(\alpha) + \mid r_s \mid^2 \sin^2(\omega t) \tag{2.2.6}$$

$$+2 \mid r_p \mid\mid r_s \mid \cos(\omega t)\cos(\alpha)\sin(\omega t)\sin(\alpha)\cos(\delta_p - \delta_s)]$$

$$I_D = \frac{\mid E_0 \mid^2}{2} \mid r_p \mid^2 \cos^2(\alpha) + \mid r_s \mid^2 \sin^2(\alpha) + [\mid r_p \mid^2 cos^2(\alpha) - \mid r_s \mid^2 \sin^2(\alpha)]\cos(2\omega t) \tag{2.2.7}$$

$+\frac{1}{2} \mid r_p \mid\mid r_s \mid \sin(2\alpha)\cos(\Delta)\sin(2\omega)$

By rearranging the terms in the equation we can obtain,

$$I_D(\lambda) = g\Bigg[1 + \frac{s_1}{s_0}\cos\Bigg(2\omega t\Bigg) + \frac{s_2}{s_0}\sin\Bigg(2\omega t\Bigg)\Bigg] \tag{2.2.8}$$

Angle α is a fixed angle for the polarizer. This angle is usually chosen as 45^0

$$s_2 = \frac{\mid r_p \mid\mid r_s \mid \sin(\alpha)}{\mid r_p \mid^2 \cos^2(\alpha) + \mid r_s \mid^2 \sin^2(\alpha)}$$
$$s_1 = \frac{\mid r_p \mid^2 \cos^2(\alpha) - \mid r_s \mid^2 \sin^2(\alpha)}{\mid r_p \mid^2 \cos^2(\alpha) + \mid r_s \mid^2 \sin^2(\alpha)}$$
$$s_0 = \mid r_p \mid^2 \cos^2(\alpha) + \mid r_s \mid^2 \sin^2(\alpha)$$
$$\tan\Psi = \frac{\mid r_p \mid}{\mid r_s \mid}$$
$$a = \frac{s_1}{s_0}$$
$$b = \frac{s_2}{s_0}$$

'g' is the the reflected intensity amplitude detected by the photodetector. Where as 'a' and 'b' are the Fourier coefficients which are determined during the experiment by fitting to non linear curve. They depend on $\tan\Psi$ and $\cos\Delta$. Now:

$$a = \frac{s_1}{s_0} = \frac{\tan^2\Psi - \tan^2\alpha}{\tan^2\Psi + \tan^2\alpha} \tag{2.2.9}$$

$$b = \frac{s_2}{s_0} = \frac{\tan\Psi\tan\alpha}{\tan^2\Psi + \tan^2\alpha}\cos\Delta \tag{2.2.10}$$

$$\tan\Psi = \sqrt{\frac{1+a}{1-a}}, \qquad \cos\Delta = \frac{b}{\sqrt{1-a^2}} \tag{2.2.11}$$

Therefore:

$$I_D = g\Bigg[1 + a\cos\Bigg(2\omega t\Bigg) + b\sin\Bigg(2\omega t\Bigg)\Bigg] \tag{2.2.12}$$

2.3 Ellipsometry Measurement

2.3.1 Calibration of Ellipsometer

Reliable operation of any ellipsometer stands or fails with the accurate determination of the position of all of its component relative to the plane of incidence. [19] During calibration procedure, the position of all components relative to the plane of incidence of the sample under investigation, are determined. If this step is not taken under careful consideration, the resulting Ψ and Δ spectra are strongly affected. Hence, calibration is very critical step in the experiment.

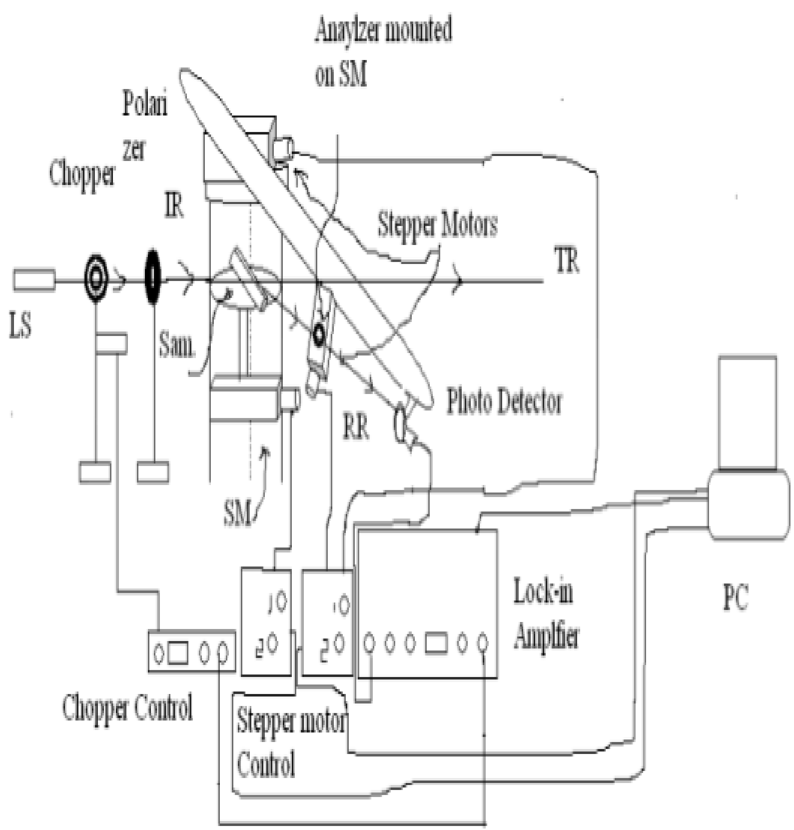


Figure 2.2: Systematic Set up of Ellipsometry

In calibration, the correct azimuthal angle of the analyzer and the polarizer is sought.

Figure 2.2 gives the azimuthal angle of the analyzer versus the intensity of the reflected light for the glass substrate. The polarizer is set at 0^0 i.e. the incident light is S-polarized. The reflected light is also S-polarized. The correct position of the analyzer gives maximum transmission at 0^0 and 180^0, and the minimum transmission at 90^0 and 270^0. This calibration is repeated for a number of times.

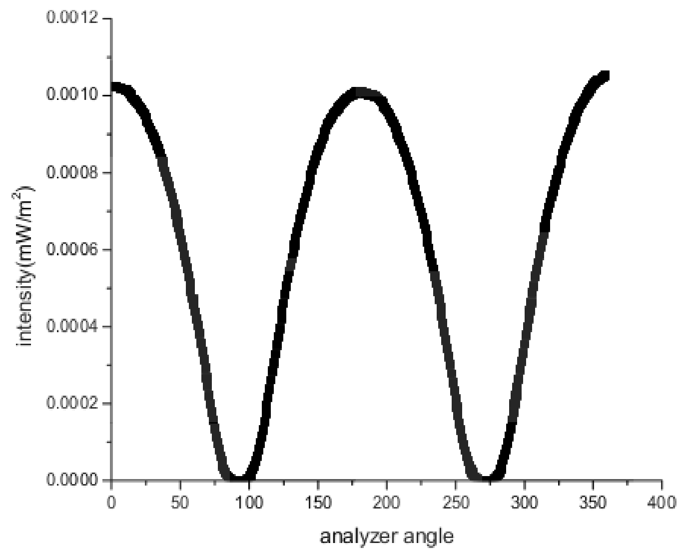


Figure 2.3: Reflected intensity for S-polarized incident light versus analyzer angle for glass.

2.3.2 Measurement

Once the calibration is made, different measurements can be made using reflection or transmission ellipsometry. For a given substrate, the Brewster angle is measured. The procedure for the Brewster angle measurement is given below.

1. Set the polarizer at azimuthal angle P, this angle must be different from 0^0 i.e. the incident light must not be perpendicular to the plane of incidence.

2. Set the analyzer angle at 0^0

3. Rotate the sample. Here the APT(Advanced Positioning Technology) stepper motor controller user interface software that controls the stepper motors and the LabVIEW that acquires data from the lock-in-amplifier must run simultaneously.

4. Plot a graph of the intensity versus angle of incidence.

The Brewster angle is the angle where the S-component of the reflected light vanishes. Therefore, the angle where the intensity becomes zero or minimum is sought. For glass, the index of refraction can easily be determined from Brewster angle measurement. In the case of a thin film substrate system, the index of refraction, obtained from the Brewster angle, can be used as an initial guess in the simulation programme. The other measurement made is multiple angle of incidence rotating analyzer ellipsometry. For a fixed angle of incidence, the analyzer is rotated through 360^0. The intensity versus the analyzer angle is plotted. The Fourier coefficient is obtained by fitting the curve and the ellipsometric quantities Ψ and Δ are computed. This is repeated for different angles of incidence and wavelengths.

Chapter 3

Applications

Ellipsometry has applications in many different fields, from semiconductor physics to microelectronics and biology, from basic research to industrial applications. Under this chapter industrial applications of ellipsometry are breifly discussed. The source for data and figures used in this chapter is '[18]'.

3.1 Semiconductor Industry

ONOPO/Si stacks

A common material system in the Si-based semiconductor industry with important metrology consists of a thin-film stack of oxide on nitride on oxide on poly-silicon on oxide on crystalline silicon: ONOPO/Si. An ellipsometry measurement can determine thicknesses of all five layers, as well as the poly-Si optical constants. Ellipsometry data and analysis are given in figure 3.1. Ellipsometry data are aquired and fit is saught at four angles of incidence.

(a)

5	SiO2	12.73 nm
4	Si3N4	10.49 nm
3	SiO2	17.65 nm
2	Poly-Si	262.2 nm
1	SiO2	8.838 nm
0	Si Substrate	2 mm

(b)

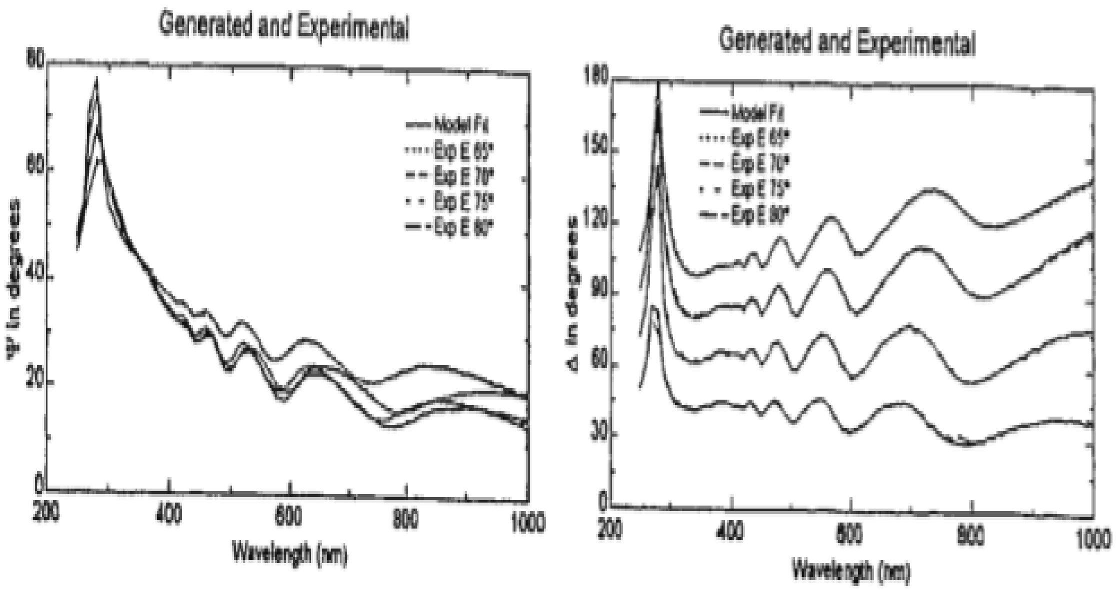


Figure 3.1: Optical model (a) and ellipsometry data fits (b) from a ONOPO/Si stack.

The optical constants of poly-silicon depend strongly on crystallinity, which in turn depends on process conditions.

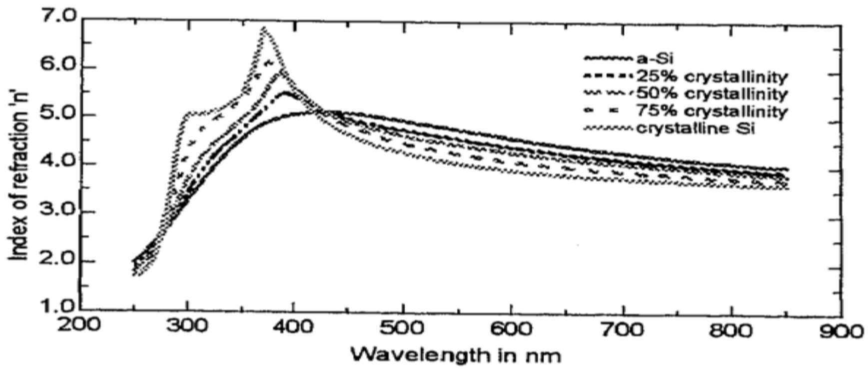


Figure 3.2: Index of Refraction of poly-Si as a function of crystallinity.

Optical Constants of Photoresist

Ellipsometry is used reguraly in optical characterization of new photoresists, and for process control of photoresists on the production line. In figure 3.3 the optical constants for a typical photoresist are shown, both before and after 'bleaching' (i.e., 'exposing' the resist by UV light), which induces large changes in the optical properties of the resist. To prevent exposure of the photoresist by the measurement beam, it is extremely important to have the monochromator placed before the sample in the ellipsometry system. Another photoresist example (figure 3.4) involves a multilayer of photoresist with an antireflective coating (ARC) beneath it. Both layer thicknesses can be extracted from the ellipsometry data, but only by including UV data in the analysis, as this spectral region exhibits optical contrast between two materials.

Compound Semiconductors: Al_xGa_{1-x}As Multilayer Structure

The thickness and compositions of complex compound semiconductor structures can also be determined by ellipsometry measurements. Figure 3.5 shows an example in which ellipsometry unambiguously determined the surface oxide thickness, three layer compositions, and light layer thicknesses. ellipsometric data at multiple angles (three in this case) helped to extract the many thicknesses and alloy ratios with high precision and accuracy.

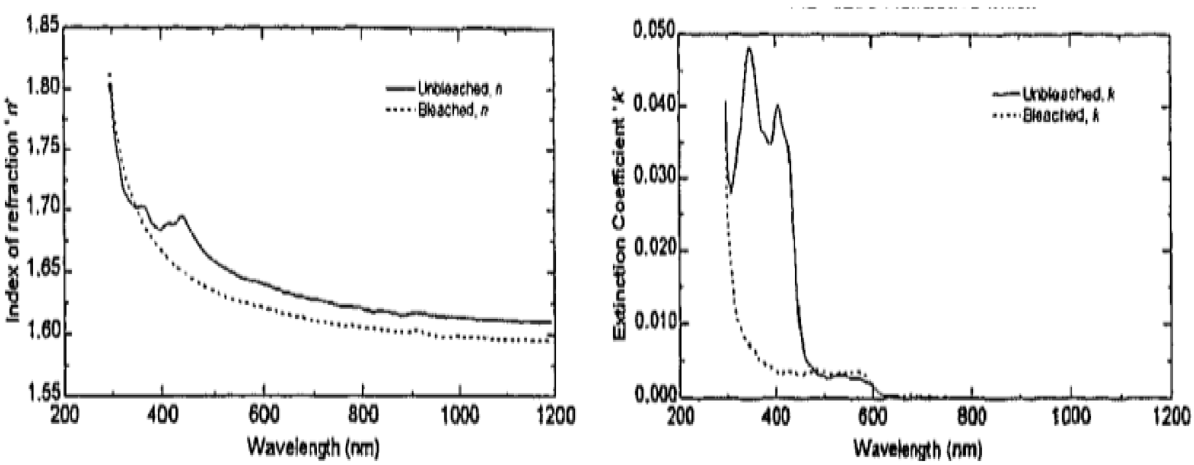


Figure 3.3: Optical constants of photoresist determined by ellipsometry measurement, before and after bleaching(by exposure to UV light).

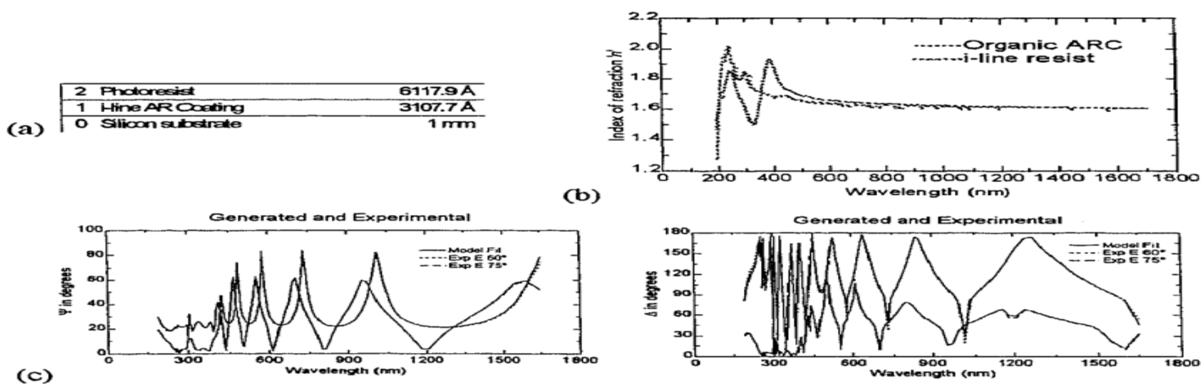


Figure 3.4: Multilayer photoresist on anti-reflective coating(ARC) example: (a) optical model, (b) optical properties of the resist and ARC films(note the contrast in the UV spectral range), and (c) ellipsometry data fits.

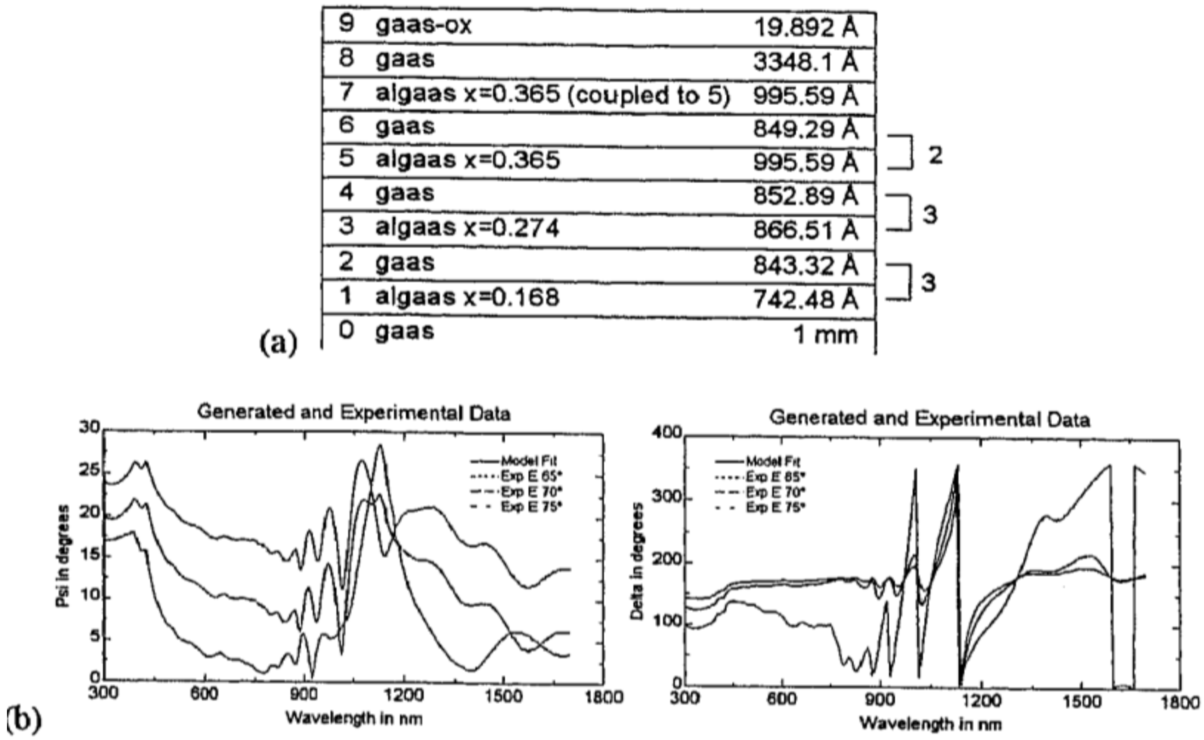


Figure 3.5: Ellipsometry analysis of Al_xGa_{1-x}As Mutilayer structure: (a) optical model, and (b) data fits. Note the near perfect fits to all of the structure in the data, which were essential to simultaneously and accurately extract all the layer thickness and compositions.

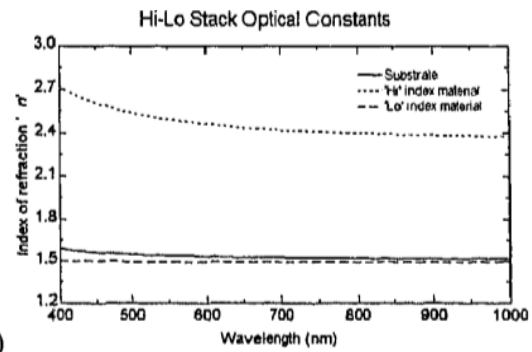
3.2 Optical Coatings Industry

Five Layer Hi-Lo Index Stack

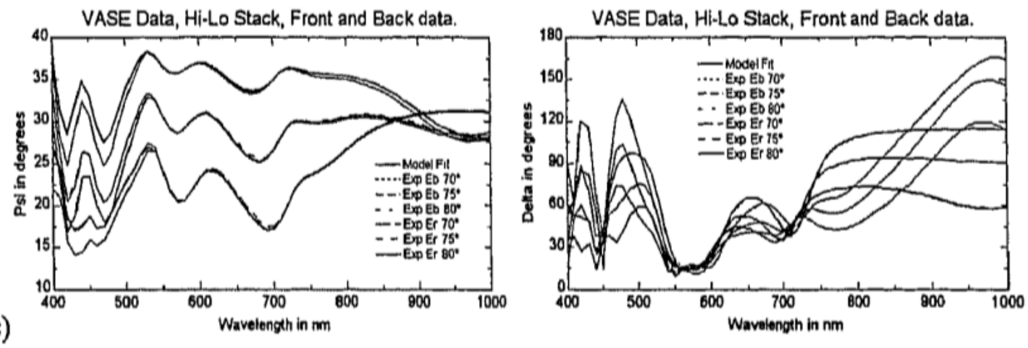
Five layer thickness and three sets of optical constants in 'Hi-Lo' index multilayer stack were simultaneously determined. To achieve this result, multiple data types were included in the analysis: Ellipsometry data acquired from front side and back side of the sample (both of which included the reflections from the opposite side of the trnsparent substrate), and spectroscopic transmission aquired at normal incidence. The cauchy dispersion formula was used to model the dispersion in index of refraction for the three materials in the stack. From a simultaneous analysis of all the data, anambiguous results for this multilayer structure were obtained: five layer thickness (plus a surface roughness thickness), and the indices of refraction for three materials

Surface Roughness	1.7 nm
High Index	119.4 nm
Low Index	188.2 nm
High Index	120.6 nm
Low Index	201.7 nm
High Index	121.2 nm
Substrate	-

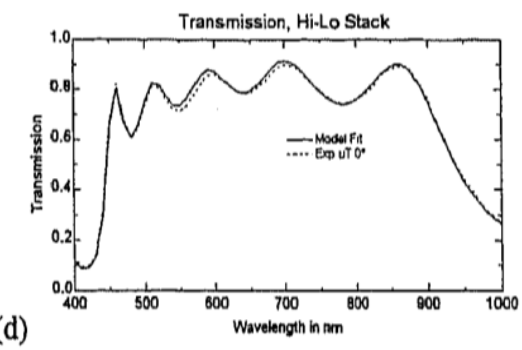
(a)



(b)



(c)



(d)

Figure 3.6: Analysis of a 5 layer Hi-Lo index optical stack using multiple data types: (a) best fit optical model, (b) extracted indices of refraction for the three constituent materials in the stack, (c) ellipsometric data fits, in which the 'Eb' curves correspond to ellipsometric data acquired on the front side of the sample (including the 'backside' reflection), and the 'Er' curves correspond to ellipsometric data acquired in the 'reverse' direction. i.e. from the backside of the sample (including the 'frontside' reflection), and (d) fit to normal incidence transmission data.

Variation in Optical Coating Index Vs. Depth

While trying to determine the film thickness and index of refraction for a Si_3N_4 coating on glass, the first modeling attempt of the ellipsometry data (shown in figure 3.7a) was not successful, as evidenced by the poor data fits and high Mean Squared Error(MSE) value. A second model, which included a surface roughness layer, was also tried (figure 3.7b), but this optical model did not adequately fit the experimental ellipsometry data either. An optical model was found which provided excellent fits to the data (figure 3.7c). This best fit model had an optically less dense 'interfacial' layer embedded in the film, the optical properties of which where modeled by a 50 percent Bruggeman EMA mixture of the Si_3N_4 film index and void (similar to the optical modeling of surface roughness). The ellipsometry analysis of this sample is deposited in two passes, thus explaining the double layer embedded interface solution. It demonstrates the sensetivity of ellipsometry measurements to non-uniformity (gradients) in film optical properties as a function of depth in the film.

3.3 Data Storage Industry

Diamond-Like Carbon (DLC)

Due to their excellent protective and lubricative properties, DLC films are commonly applied to hard disk media and read-write heads. DLC films are usually made by plasma CVD using a mixture of hydrocarbon gasses, such that a wide range of film mechanical properties can be obtained by adjusting the process conditions. As there is a correlation between variations in the DLC mechanical and optical properties (see figure 3.8), ellipsometry is very useful in the monitoring of DLC processes. The sensetivity of ellipsometry to ultra-thin film is also advantageous when characterizing DLC coatings, which are typically < 1000 Å (figure 3.9)

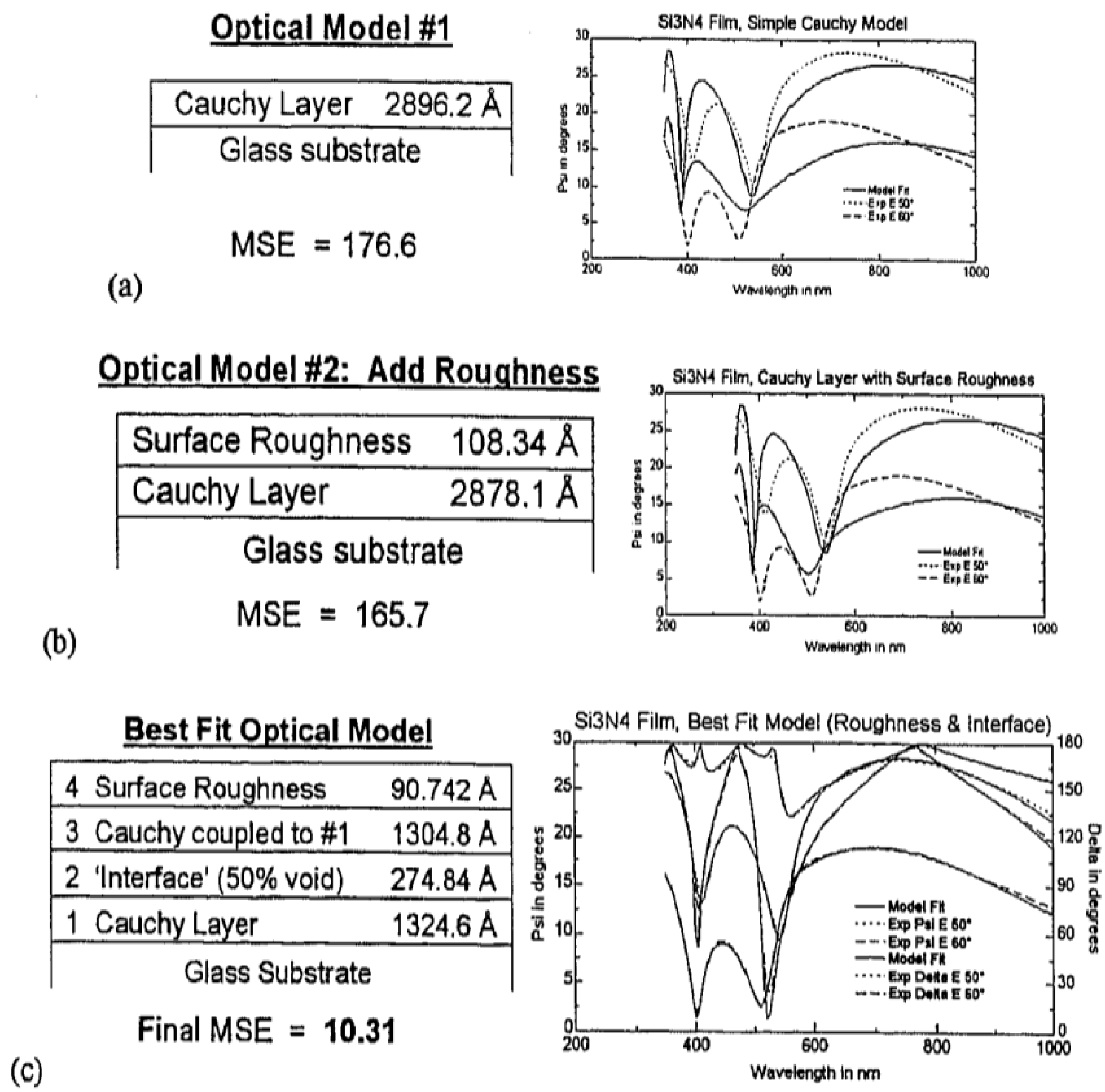


Figure 3.7: Progression of optical models used to analyze a Si_3N_4 coating on glass sample: (a) simple single film model, (b) single film with surface roughness, and (c) best fit optical model, which included a less dense 'interfacial' layer within the film (this was introduced by the two-pass deposition of the film).

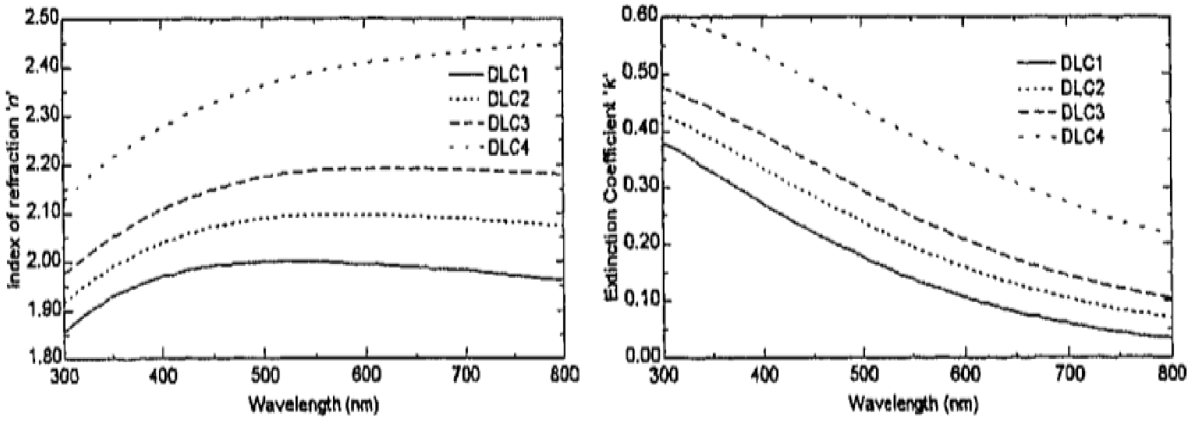


Figure 3.8: Variation in DLC optical constants, these optical constants were extracted from an ellipsometry analysis of four different samples, in which the DLC deposition conditions were systematically varied.

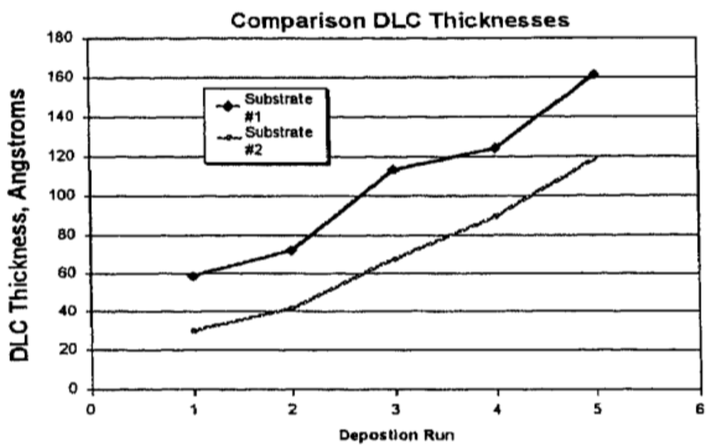


Figure 3.9: Systematic study of DLC films coated on two different substrates; the high sensitivity of ellipsometry to ultra-thin films enable precise thickness determination in this application.

Thickness of Thin Magnetic Films

The performance of advanced read heads is critically dependent on the thickness of thin magnetic films. Accurate characterization of such films requires thin film optical constants for the metallic layers of interest, which may differ significantly from the bulk optical constants found in the literature. By performing ellipsometry analysis on a thin magnetic layer deposited on a thick dielectric film, it is possible to simultaneously and accuratly extract optical constants of the metallic layer, along with the metal and dielectric film thickness.

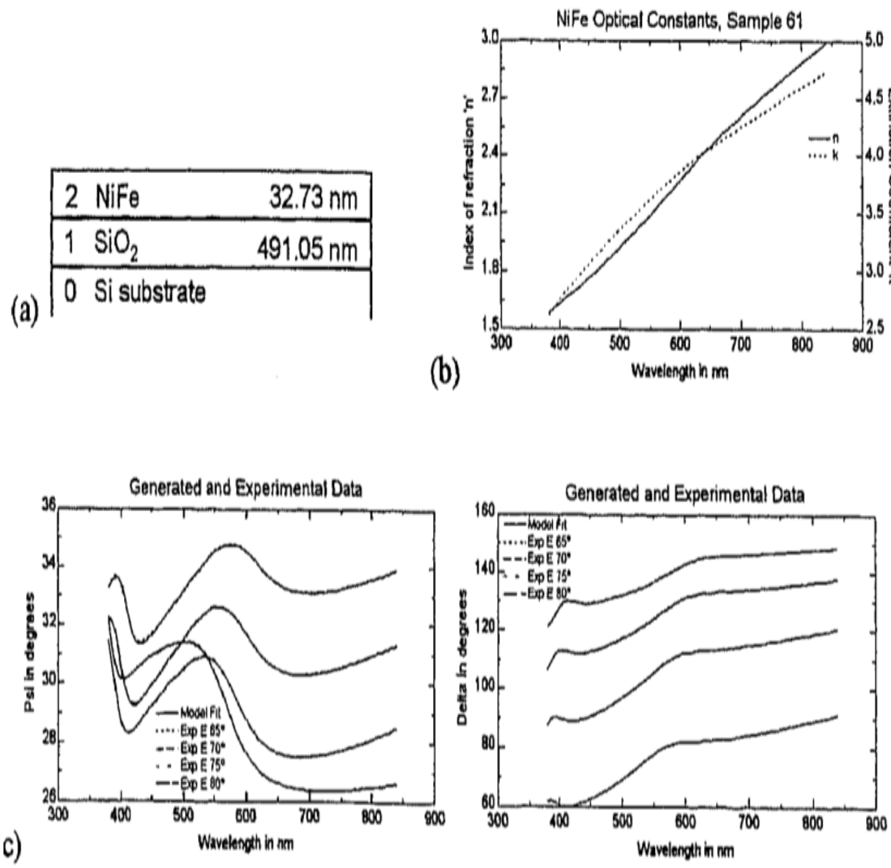


Figure 3.10: Simultaneous thickness and optical constant determination for a thin NiFe layer deposited on a thick SiO_2 film on Si: (a) optical model, (b) resulting NiFe optical constants, and (c) ellipsometry data fits.

3.4 Flat Panel Display Industry

Indium Tin Oxide (ITO) Films

Indium tin oxide (ITO) is a transparent electrically conducting film used extensively in the flat panel display industry as a large-area electrode. Optical characterization of ITO films is challenging, as the ITO optical properties are highly dependent on the film deposition and annealing process. Furthermore, siginificant gradients in the optical constants (Vs. depth in the film) are commonly observed in ITO films. An ellipsometry analysis of a typical ITO sample is presented and described in figure 3.11. To adequately fit the experimental ellipsometry data and properly characterize the ITO film, a complex graded optical model is required.

Thin-Film Transistors (TFT) Structures

Thin-Film Transistors (TFT) are important in active matrix liquid crystal display technology. Ellipsometry can be used to characterize important TFT layer thickness, as shown below (figure 3.12). By aquiring ellipsometry data in to the NIR spectral range, the ability to characterize thicker amorphous silicon (a-Si) films is generally enhanced, as a-Si becomes essentially transparent in this spectral range.

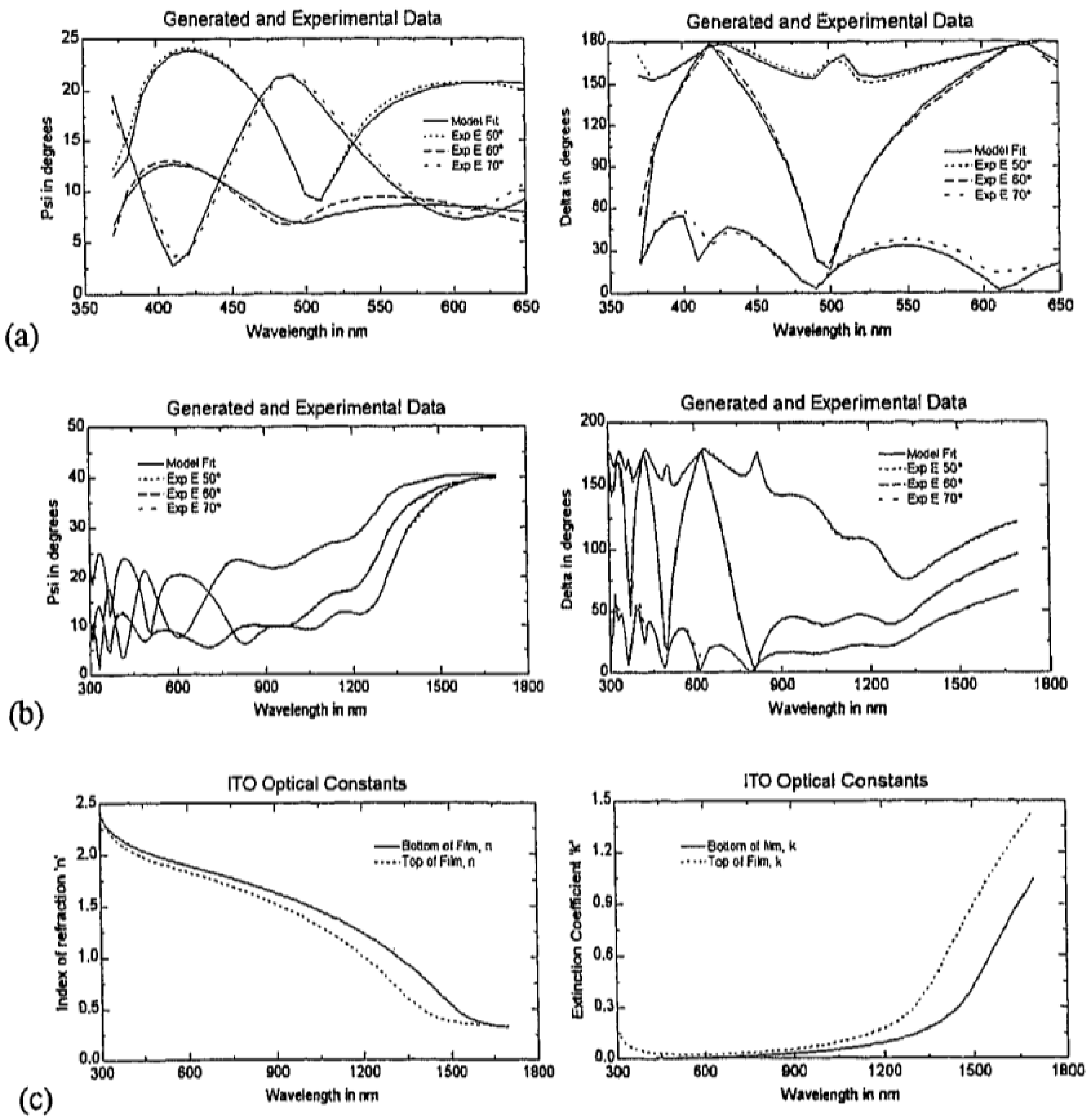
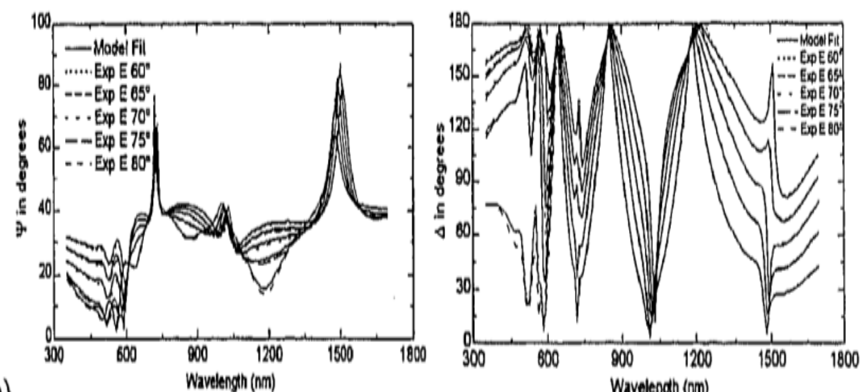


Figure 3.11: Ellipsometry characterization of an ITO film. (a) Data analysis using a single cauchy film optical model results in poor data fits, even over the limited spectral range shown here. (b) A graded- film optical model (using Lorenz oscillators to model the dispersion in the ITO film) results in excellent fits the ellipsometry data over a wide spectral range. (c) The ITO optical constants at the top and bottom of the film are compared in this plot; the amplitude and shape of the free-carrier absorption tail (see the 'k' plot at the longer wavelength) is directly related to the electrical conductivity of the film.

(a)

4	sio2	**22.994 Å**
3	a-si	**1837.3 Å**
2	si3n4	**3315.5 Å**
1	cr	3700 Å
0	1737 glass	1 mm



(b)

Figure 3.12: Ellipsometry analysis of a TFT structure: (a) optical model(only the top 3 layers were determined in this analysis, as the Cr metal layer was optically thick and therefore fixed at its nominal value), and (b) data fits.

Chapter 4

Conclusion

The ability to accurately acquire and quantitatively analyze ellipsometry data on a wide range of samples is presented. Ellipsometry is now well-established as an important metrology tool in several different industries, and as an important technique for industrial research on new materials and processes.

Most of the ellipsometry applications require a time-consuming and sometimes subjective process of 'fine tuning' the optical model to achieve acceptable data fits which accurately characterize the sample properties. However, once an appropriate optical model has been developed, it is very straightforward to apply it to the ellipsometry data analysis of similar samples.

Finally, in this project basic concepts and examples of industrial applications of ellipsometry are given. The description of some models and results in a simplified form are presented which emphasizes the potential of ellipsometry as an experimental tool.

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Declaration

This project is my original work, has not been presented for a degree in any other University and that all the sources of material used for the project have been dully acknowledged.

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Place and time of submission: Addis Ababa University, June 2013

This project has been submitted for examination with my approval as University advisor.

Name: Prof. A.V. Gholap

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