1 Introduction to Ellipsometry

Ellipsometry is generally a 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 polarization and is therefore not dependent on absolute intensity as long as the absolute intensity is sufficient. This makes ellipsometric measurement very precise and reproducible.

Ellipsometry uses the fact that linearly polarized light at an oblique incidence to a surface changes polarization state when it is reflected. It becomes elliptically polarized, thereby the name ”ellipsometry”. In some cases elliptically polarized light is used as the incident light wave. The idea of ellipsometry is shown in general in Figure 1.1.

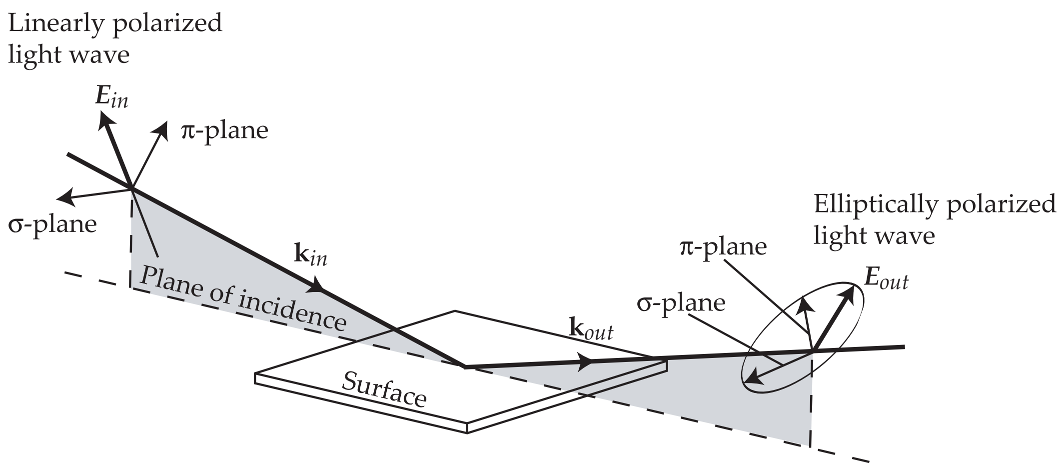


Figure 1.1: The general principle in ellipsometry. [Jawoollam 2004]

When a monochromatic, plane light wave is directed at a surface at oblique incidence, the plane of incidence is defined as a plane perpendicular to the surface and containing the vector which points in the direction of propagation of the light wave. This vector is called the wavevector $\mathbf{k}_{in}$. Perpendicular to $\mathbf{k}_{in}$ are the two mutually perpendicular vectors for the electric field **E** and the magnetic field **B** of the light wave. The **E**-vector is chosen as the vector defining the polarization of the light wave and is therefore the only one shown in Figure 1.1. The **E**-vector is decomposed into two components, which are mutually perpendicular and perpendicular to $\mathbf{k}_{in}$. The two components of **E** are respectively parallel and perpendicular to the plane of incidence as seen in Figure 1.1. The vectors are named from their German names, ”Parallel” and ”Senkrecht”, and are from this given the corresponding Greek letters π and σ, respectively.

The incident light wave is linearly polarized. Polarization will be described in depth later, but for now the π- and σ-component of **E** can be seen as oscillating with an amplitude and mutual phase causing the endpoint of **E** to move in a straight line in the plane of the π- and σ-components. When the light wave reflects off the surface, the polarization changes to elliptical polarization. This means that the amplitude and mutual phase of the π- and σ-component of **E** are changed causing the endpoint of **E** to move in an ellipse.

The form of the ellipse can be measured by a detector and data processing can relate this to the ellipsometric parameters ψ and Δ. The ellipsometric parameters can be related to the reflection coefficients of the light polarized parallel and perpendicular to the plane of incidence ρ_π and ρ_σ, respectively. The relation is the basic equation in ellipsometry and is given by the complex ratio ρ of the two reflection coefficients

$$\rho = \frac{\rho_\pi}{\rho_\sigma} = \tan(\psi)e^{j\Delta} \tag{1.1}$$

The ellipsometric parameters ψ and Δ are given by a measurement with an ellipsometer and the two reflection coefficients are functions of the complex refractive index of the material.

Ellipsometry is often used to measure the thickness of thin films on top of a substrate. A simplified model of this is shown in Figure 1.2 where an incident light wave is reflected off and transmitted through the surface of a thin film. If the refractive indexes of the film and the substrate are known, it is possible to calculate the thickness d of the thin film by ellipsometry. This application of ellipsometry is widely used to investigate materials and surfaces.

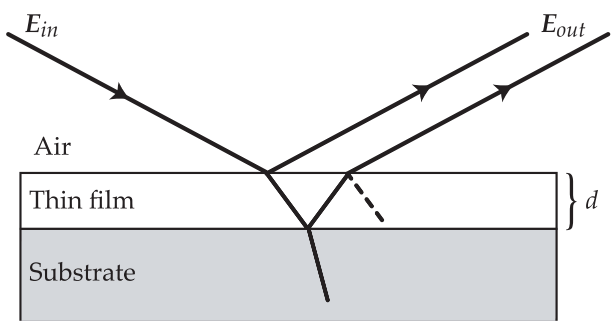


Figure 1.2: Illustration of a thin film on top of a crystal.

2 Problem Description

There are two overall objectives in this project. These are to determine the refractive index of various materials and to determine the thickness of various films by ellipsometry. The materials at hand in this project for measuring the index of refraction are silicon, aluminum, copper and silver. The materials with a film on a substrate are silicon with a silicon dioxide film and silicon with a polymer film.

The following requirements are to be met in this project.

1. **Theoretical**
   (a) Modelling of the optical system under investigation in order to enable calculation of refractive index and film thickness.
2. **Simulation**
   (a) Simulation of the refractive index of silicon, aluminum, copper and silver.
3. **Experiments**
   (a) Refractive Index — Use ellipsometry to measure the refractive index of silicon, aluminum, copper and silver.
   (b) Thickness of thin SiO_2 film — Measurement of the thickness of a thin film of silicon dioxide on a silicon wafer.
   (c) Thickness and uniformity of polymer film — Measurement of the thickness of two optically thick polymer films on substrates of silicon. Furthermore, several measurements of the thickness of the polymers should be performed in order to illustrate the uniformity of the surfaces.

All materials except the SiO_2 and polymer films are provided by the Institute of Physics and Nanotechnology at Aalborg University. The SiO_2 film sample is a test wafer from Sentech. The test wafer has a known film thickness. Two polymer films are imposed on silicon wafers by NanoNord A/S. The polymers are spin coated on the wafers and afterwards baked at high temperature as prescribed by the manufacturer of the polymer. The polymer is manufactured by HD MicroSystems and is called PI-5878G. The two samples differ only in the angular speed of the spin coating which should yield different thicknesses of the polymer. Estimates from NanoNord suggest that the polymers are 2 and 5 μm, but these estimates are very loose.

Part II

Ellipsometry Theory

This part contains three chapters. The first concerns polarization of light, where elliptically polarized light is of special interest. Also treated in this chapter is the correlation between the ellipsometric parameters and the Fresnel reflection coefficients. The second chapter concerns ellipsometer systems. In this chapter a description of different ellipsometer configurations is given. The ellipsometer used in the tests is also described in this chapter. The last chapter in this part concerns calculation of refractive index and film thickness by use of measured ellipsometric parameters.

3 Polarization of Light

This chapter describes the polarization of light. Three types of polarization will be introduced. These are linearly, circularly and elliptically polarized light. The descriptions of these polarization types will be limited to treat monochromatic plane waves only. Apart from this, a description of unpolarized light will be given. Finally, the ellipsometric parameters ψ and Δ will be introduced.

This chapter is mainly based on [Klein & Furtak 1986, pp. 585-596] and the definitions derived in Appendix A.

3.1 Definition of Polarization

From the description of monochromatic plane light waves, treated in Appendix A, it can be seen that light consists of an electric field **E** and a magnetic field **B**. The connection between these and the direction of propagation is given by (A.28) and rewritten here

$$\mathbf{B} = \frac{\mathbf{k} \times \mathbf{E}}{\omega} \tag{3.1}$$

where the direction of propagation is the direction of **k**. It is seen that electromagnetic waves are transverse waves, i.e. **E** and **B** are mutually perpendicular and perpendicular to **k**. As a consequence, **E** can point in any direction perpendicular to **k**. Thus **E** has two degrees of freedom, i.e. it is "free" to move in a 2-dimensional coordinate system. This can be seen in opposition to longitudinal waves, which are bound to point in the direction of propagation. This extra degree of freedom implies the existence of different polarization states, which in the following will be divided into some basic types. But first, some general definitions will be stated.

The polarization direction of light is defined as the direction of **E**. When **E** is known, **B** can readily be deduced, direct or indirect from Maxwell's equations, e.g. from (3.1).

In the following, a right-handed system of coordinates is used, where the z-axis is defined as the direction of propagation. Thus, the E-field can be described as a linear combination of an x- and y-component

$$\mathbf{E}(z,t) = E_x \hat{\mathbf{x}} + E_y \hat{\mathbf{y}} \tag{3.2}$$

where

$$E_x(z,t) = A_x \cos(\omega t - kz + \phi_x) \tag{3.3a}$$
$$E_y(z,t) = A_y \cos(\omega t - kz + \phi_y) \tag{3.3b}$$

as described in (A.24).

If only the polarization state is of interest, the temporal and spatial dependencies can be omitted. Thus, by using the Jones formalism, which is described in Appendix D, (3.3) can be expressed by a Jones vector

$$\mathbf{E} = \begin{bmatrix} E_x \\ E_y \end{bmatrix} = \begin{bmatrix} A_x e^{j\phi_x} \\ A_y e^{j\phi_y} \end{bmatrix} \tag{3.4}$$

as described in (D.6) and (D.7). (3.4) entirely describes the polarization of light. Whether the light is described using the Jones formalism (3.4) or with the temporal and spatial information included (3.3), the essential parameters are the relative phase ϕ defined as

$$\phi = \phi_y - \phi_x \tag{3.5}$$

and the relative amplitude, which is a relation between A_x and A_y.

3.2 Polarization Types

In the following some basic polarization types will be defined.

3.2.1 Linearly Polarized Light

Linearly polarized (LP) light[1] is the most straightforward example of polarized light. Light is linearly polarized when $\mathbf{E}(z)$ and $\mathbf{E}(t)$ oscillates on a bounded straight line projected in the xy-plane, with the center at $(0,0)$. This occurs when

$$\phi = \pm p\pi \text{ , for } p = \{0, 1, 2, \cdots\} \tag{3.6}$$

which imply

$$E_y = \pm \frac{A_y}{A_x} E_x \tag{3.7}$$

Hence, E_y is a linear function of E_x, and vice versa, as both A_x and A_y are constants. An illustration of the projection of LP light in the xy-plane can be found in Figure 3.1(a). A depiction of $\mathbf{E}$ with respect to z, where the time is held constant, can be found in Figure 3.1(b).

Note

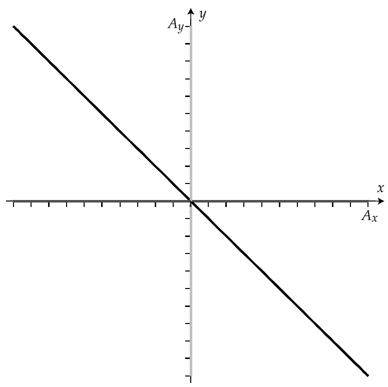
The requirement to the phase stated in (3.6) is only requisite when both $A_x \neq 0$ and $A_y \neq 0$. If $A_x = 0$ or $A_y = 0$, the light is linearly polarized.

3.2.2 Circularly Polarized Light

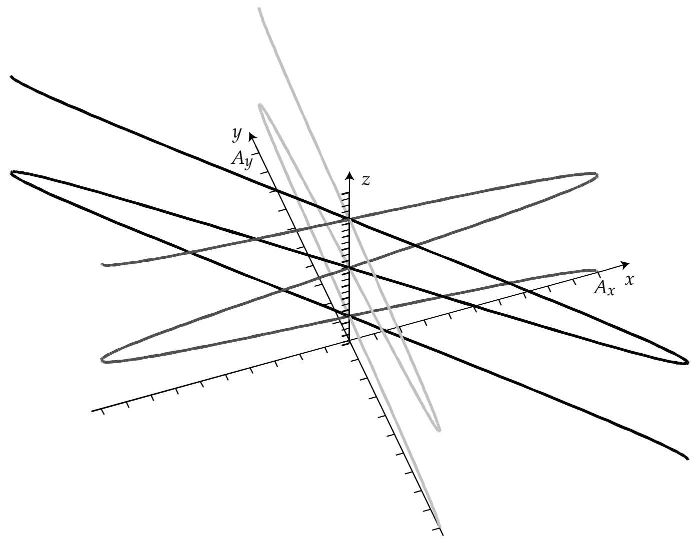
Light is circularly polarized (CP) when $\mathbf{E}$, with respect to t as well as z, defines a circle projected in the xy-plane. Thus, the following phase-relation must hold

$$\phi = \frac{\pi}{2} \pm p\pi \text{ , for } p = \{0, 1, 2, \cdots\} \tag{3.8}$$

[1] Linearly polarized light is also denoted plane polarized light.



(a) Depiction of $\mathbf{E}$ in the xy-plane.



(b) Illustration of $\mathbf{E}(z)$.

Figure 3.1: Illustration of linearly polarized light for $\phi = \pi$ and $A_x = A_y$. E_x and E_y are illustrated by the dark and light grey curve, whereas the total electric field is illustrated by the black curve.

and the following amplitude relation must be fulfilled

$$A_x = A_y \neq 0 \tag{3.9a}$$

or

$$A_x = -A_y \neq 0 \tag{3.9b}$$

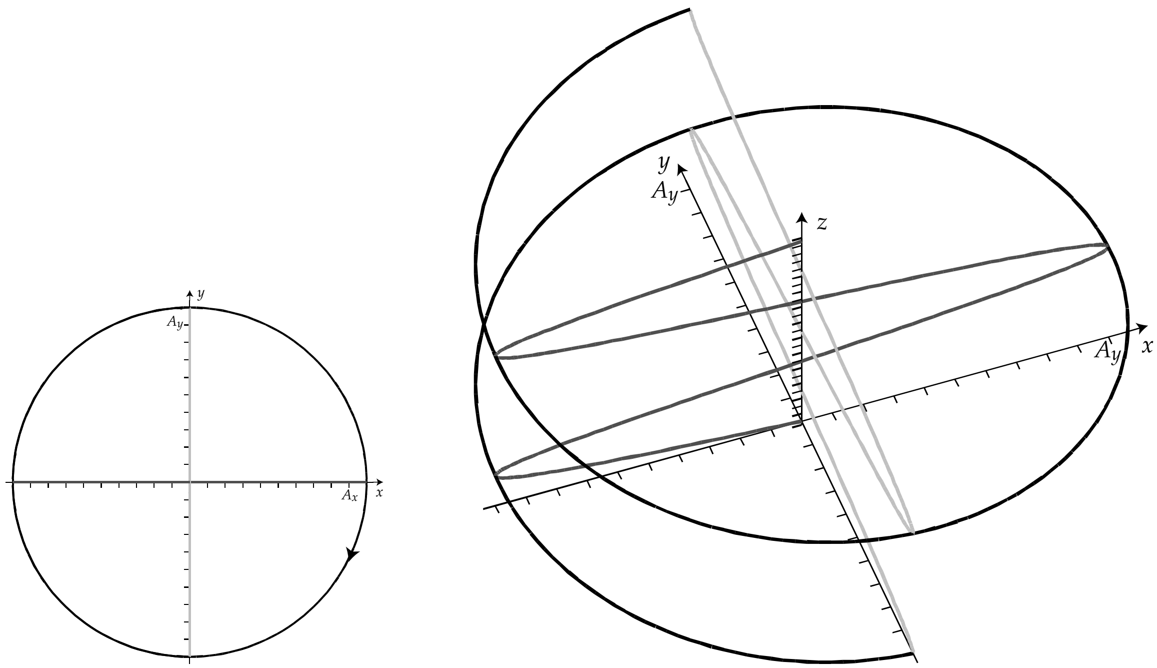
but the latter is not taken into account in the following, as (3.9b) can be expressed using (3.9a) with a extra phase difference of π. It is seen that the direction of rotation projected in the xy-plane depends of ϕ. The two directions are denoted RCP (Right Circularly Polarized)[2] and LCP (Left Circularly Polarized) respectively. LCP occurs when $\mathbf{E}$ rotates clockwise with respect to z when viewed along the negative direction of the z-axis. This can be seen in Figure 3.2(a). A spatial depiction of LCP light with respect to z can be found in Figure 3.2(b). When LCP light is described with respect to t, the rotation will consequently be in the counterclockwise direction. LCP occurs when $\phi = -\pi/2 \pm 2p\pi$, where $p = \{0, 1, 2, \cdots\}$. Naturally the direction of rotation of RCP is opposite to LCP both with respect to z and t. RCP occur when $\phi = \pi/2 \pm 2p\pi$, where $p = \{0, 1, 2, \cdots\}$.

The fact that $\mathbf{E}$ defines a circle in the xy-plane when (3.8) and (3.9) are met, can be seen from the following. If $\phi = \pm\pi/2$, and $A_x = A_y = A$, then (3.3) can be expressed as

$$E_x = A\cos(\omega t - kz + \phi_x) \tag{3.10a}$$

$$\begin{aligned} E_y &= A\cos(\omega t - kz + \phi_x \pm \frac{\pi}{2}) \\ &= \mp A\sin(\omega t - kz + \phi_x) \end{aligned} \tag{3.10b}$$

[2]The name RCP origins from the appearance of a normal screw, where the spiral groove has the same shape as RCP light with respect to z if the screw is placed in the z-axis [Klein & Furtak 1986, p. 588].



(a) Depiction of $\mathbf{E}(z)$ in the xy-plane.

(b) Illustration of $\mathbf{E}(z)$.

Figure 3.2: Illustration of LCP light ($\phi = -\pi/2$) and $A_x = A_y$. E_x and E_y are illustrated by the dark and light grey curve, whereas the total electric field are illustrated by the black curve.

Adding the squared of (3.10a) to the squared of (3.10b) yields

$$\begin{aligned} E_x^2 + E_y^2 &= (A\cos(\omega t - kz + \phi_x))^2 + (\mp A\sin(\omega t - kz + \phi_x))^2 \\ &= A^2(\cos^2(\omega t - kz + \phi_x) + \sin^2(\omega t - kz + \phi_x)) \\ &= A^2 \end{aligned} \tag{3.11}$$

where it is observed that (3.11) is the representation of a circle with the center in $(0,0)$.

3.2.3 Elliptically Polarized Light

If $\mathbf{E}$ with respect to z and t describes an ellipse projected in the xy-plane, the light is denoted elliptically polarized (EP). First, a simple description of EP light is considered.

Description of Elliptically Polarized Light Starting From Circularly Polarized Light

Starting from the description of CP light, the restriction to the phase given by (3.8) is kept, whereas the amplitude relation given by (3.9) is discarded. This is done in order to allow $A_x \neq A_y$. A_x and A_y must however still be nonzero. Similarly as in (3.11) it is seen that

$$\frac{E_x^2}{A_x^2} + \frac{E_y^2}{A_y^2} = 1 \tag{3.12}$$

which is the description of an ellipse with the major and minor axis along the x- and y-axis.

General description of Elliptically Polarized Light

In general, no restrictions to the relation between the amplitudes A_x and A_y or the phase difference ϕ exist for EP light. The general case of EP light can then be stated using (3.3) as

$$E_x = A_x \cos(\omega t - kz) \tag{3.13a}$$
$$E_y = A_y \cos(\omega t - kz + \phi) \tag{3.13b}$$

which can be written as

$$\frac{E_x}{A_x} = \cos(\omega t - kz) \tag{3.14a}$$
$$\frac{E_y}{A_y} = \cos(\omega t - kz)\cos(\phi) - \sin(\omega t - kz)\sin(\phi) \tag{3.14b}$$

Multiplying (3.14a) with $\cos(\phi)$ and subtracting the result from (3.14b) yields

$$\frac{E_y}{A_y} + \frac{E_x}{A_x}\cos(\phi) = -\sin(\omega t - kz)\sin(\phi) \tag{3.15}$$
$$= -\sin(\phi)\sqrt{1 - \cos^2(\omega t - kz)} \tag{3.16}$$

Squaring this, results in

$$\frac{E_y^2}{A_y^2} + \frac{E_x^2}{A_x^2}\cos^2(\phi) - 2\frac{E_x E_y}{A_x A_y}\cos(\phi) = [1 - \cos^2(\omega t - kz)]\sin^2(\phi) \tag{3.17}$$

Substituting the squared of (3.14a) into (3.17) yields

$$\frac{E_y^2}{A_y^2} + \frac{E_x^2}{A_x^2}\cos^2(\phi) - 2\frac{E_x E_y}{A_x A_y}\cos(\phi) = \left[1 - \left(\frac{E_x}{A_x}\right)^2\right]\sin^2(\phi) \tag{3.18}$$

or

$$\frac{E_y^2}{A_y^2} + \frac{E_x^2}{A_x^2} - 2\frac{E_x E_y}{A_x A_y}\cos(\phi) + \cos^2(\phi) = 1 \tag{3.19}$$

which defines an ellipse in the xy-plane. It is seen from (3.19) that if $\phi = p\pi$, for $p = \{\cdots, -2, -1, 0, 1, 2, \cdots\}$, then

$$E_y = ((-1)^p)\frac{A_y}{A_x}E_x \tag{3.20}$$

which, as expected results in the definition of LP light. Similarly if $\phi = p\pi/2$, then

$$\frac{E_y^2}{A_y^2} + \frac{E_x^2}{A_x^2} = 1 \tag{3.21}$$

which is EP light with the major axis along the x- or y-axis; or if $A_x = A_y$ it is CP light. Thus, LP and CP light are both special cases of EP light. It is clear that the ellipse described in the xy-plane will be inscribed in a rectangle given by A_x and A_y. An illustration of EP light projected in the xy-plane can be seen in Figure 3.3.

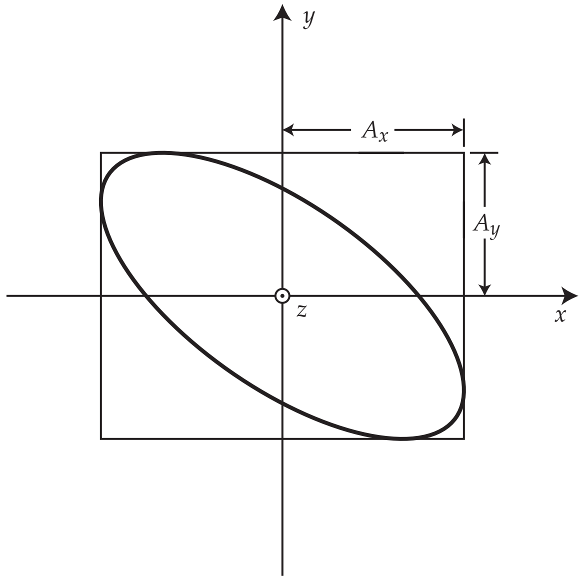


Figure 3.3: Illustration of elliptically polarized light.

3.2.4 Unpolarized Light

Unpolarized light is the term used for light that is not polarized in any defined pattern as the ones stated above. For unpolarized light, the electric field vector fluctuates in a random pattern. If **E** is divided into components described as in (3.2), E_x and E_y will be incoherent. That is, the phase relation of the components will be random. Furthermore, as the field vector fluctuates randomly, the mean value of the magnitude of the field will be the same in all directions perpendicular to the direction of propagation. Thus $\langle A_x^2 \rangle = \langle A_y^2 \rangle$.

3.3 Definition of the ellipsometric parameters ψ and Δ

ψ and Δ angles will in the following be defined as quantities describing the reflected light, when linearly polarized light is incident on a surface. A depiction of the orientations of the coordinate systems for the incident and the reflected E-field in relation to the surface can be seen in Figure 3.4. Using the definition of the Jones vector, a new term χ is defined as the ratio between the components in the Jones vector, namely

$$\chi = \frac{E_y}{E_x} \tag{3.22}$$

The surface can be viewed as a system with the incident E-field $\mathbf{E_i}$ as the input and the reflected E-field $\mathbf{E_o}$ as the output. This is illustrated in Figure 3.5 in terms of χ. The term of interest is the relation describing the optical system S, which is given as χ_i/χ_o, thus

$$\frac{\chi_i}{\chi_o} = \frac{\frac{E_{iy}}{E_{ix}}}{\frac{E_{oy}}{E_{ox}}} = \frac{E_{iy}E_{ox}}{E_{ix}E_{oy}} \tag{3.23}$$

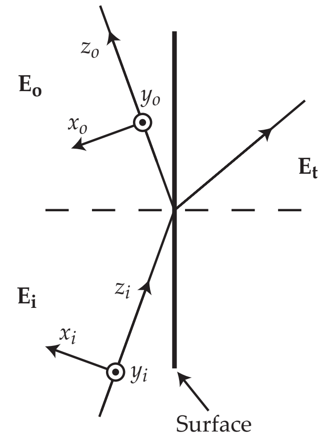


Figure 3.4: Illustration showing the orientation of the coordinate systems relative to the sample surface. $\mathbf{E_i}$ is the incident or input E-field, $\mathbf{E_o}$ is the reflected or output E-field and $\mathbf{E_t}$ is the transmitted E-field. y is parallel with the surface.

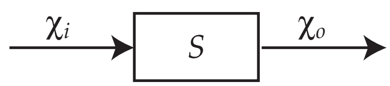


Figure 3.5: Input χ_i and output χ_o to an optical system S.

Rewriting this expression using the Jones vector, (3.4) yields

$$\frac{\chi_i}{\chi_o} = \frac{A_{iy}e^{j\phi_{iy}}}{A_{ix}e^{j\phi_{ix}}}\frac{A_{ox}e^{j\phi_{ox}}}{A_{oy}e^{j\phi_{oy}}} \tag{3.24}$$

$$= \frac{A_{iy}}{A_{ix}}e^{j(\phi_{iy}-\phi_{ix})}\frac{A_{ox}}{A_{oy}}e^{j(\phi_{ox}-\phi_{oy})} \tag{3.25}$$

If the incident light is linearly polarized with $\phi_i = 0$ and $A_{ix} = A_{iy}$, then (3.25) is given as

$$\frac{\chi_i}{\chi_o} = \frac{A_{ox}}{A_{oy}}e^{j(\phi_{ox}-\phi_{oy})} \tag{3.26}$$

which only contains information for the elliptically polarized reflected light. For the reflected light, the parameter ψ is defined in order to satisfy the following

$$\tan\psi = \frac{A_{ox}}{A_{oy}} \tag{3.27}$$

This is illustrated in Figure 3.6.

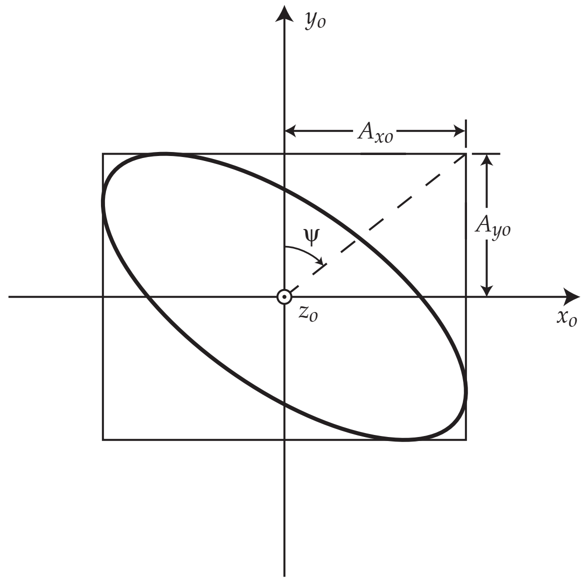


Figure 3.6: Illustration of ψ, which is defined for reflected elliptically polarized light.

Furthermore, the parameter Δ is defined as

$$\Delta = \phi_{ox} - \phi_{oy} \tag{3.28}$$

Using (3.27) and (3.28), (3.26) can be expressed as

$$\frac{\chi_i}{\chi_o} = \tan(\psi)e^{j\Delta} \tag{3.29}$$

which is a general ellipsometer equation [Azzam & Bashara 1977, p. 259].

3.3.1 Connecting ψ and Δ to ρ_π and ρ_σ

The Fresnel reflection coefficients are introduced in Appendix B as the reflected amount of the E-field in proportion to the incident amount. This is viewed either parallel (π) or perpendicular (σ) to the plane of incidence as

$$\rho_\pi = \left|\frac{\mathbf{E}_{o\pi}}{\mathbf{E}_{i\pi}}\right| \tag{3.30a}$$

$$\rho_\sigma = \left|\frac{\mathbf{E}_{o\sigma}}{\mathbf{E}_{i\sigma}}\right| \tag{3.30b}$$

where all **E**-vectors are Jones vectors. By fixing the xy-coordinate system to the sample surface so that x is parallel to the plane of incidence and y is perpendicular to the plane of incidence, (3.23) can be rewritten to

$$\frac{\chi_i}{\chi_o} = \frac{E_{iy}E_{ox}}{E_{ix}E_{oy}} \tag{3.31}$$

$$= \frac{|\mathbf{E}_{i\sigma}|\,|\mathbf{E}_{o\pi}|}{|\mathbf{E}_{i\pi}|\,|\mathbf{E}_{o\sigma}|} \tag{3.32}$$

$$= \frac{\frac{|\mathbf{E}_{o\pi}|}{|\mathbf{E}_{i\pi}|}}{\frac{|\mathbf{E}_{o\sigma}|}{|\mathbf{E}_{i\sigma}|}} \tag{3.33}$$

$$= \frac{\rho_\pi}{\rho_\sigma} \tag{3.34}$$

Inserting this expression into (3.29) yields

$$\frac{\rho_\pi}{\rho_\sigma} = \tan(\psi)e^{j\Delta} \tag{3.35}$$

which correlates the ellipsometric parameters to the Fresnel reflection coefficient of a surface. This correlation is utilized throughout the rest of the report to derive expressions for e.g. the refractive index of a material as a function of ψ and Δ.

4 Ellipsometer Systems

This chapter concerns the operational principle of ellipsometers. First a general introduction to ellipsometers is given which explains the different components encountered in an ellipsometer. After this introduction to ellipsometers, two different ellipsometer configurations are described, namely the null and the photometric ellipsometer. After this, the problem of measuring the ellipsometric parameters ψ and Δ with a photometric rotating analyzer ellipsometer is treated. Finally a description of the Sentech SE 850 ellipsometer used in this project is given.

4.1 Description of an Ellipsometer

Ellipsometry is generally defined as the task of measuring the state of polarization of a wave. In the case of an optical system the wave of interest would be a light wave. Although the polarization state of a light wave itself can be of interest, in reflection ellipsometry the change in polarization is the essential issue. This change in polarization as the light is reflected at a surface boundary is caused by difference in Fresnel reflection coefficients as described in Appendix B. These coefficients are different for π and σ polarized light. A general ellipsometer configuration is depicted in Figure 4.1. As can be seen from the figure an ellipsometer

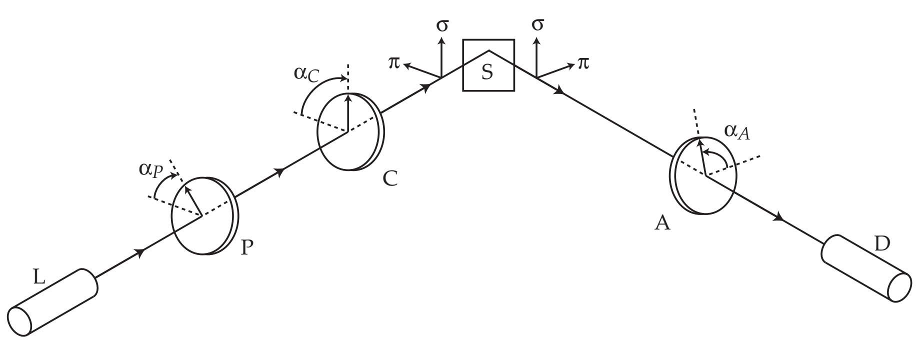


Figure 4.1: Illustration of a general ellipsometer setup. Light is emitted from the source L, passes through the linear polarizer P and the compensator C before it is reflected at the surface boundary S. After reflection the light again passes a linear polarizer denoted the analyzer A before it reaches the detector D. [Azzam & Bashara 1977, p. 159]

generally consists of six parts:

The light source which emits circularly or unpolarized light. This can be either a laser or some type of lamp. A laser has the advantage of emitting very intense and well collimated light which produces a very small spot size on the sample. It is however not possible to use a laser to perform spectroscopic measurements as the laser contains only one wavelength. However a lamp made of e.g. Xenon emits light at many different wavelengths enabling spectroscopic measurement.

The linear polarizer which converts the incoming light to linearly polarized light. The rotational azimuth angle of the polarizer relative to the direction of the π linear eigenpolarization is denoted α_P in the figure. This angle is the angle from the plane of incidence to the transmission axis of the polarizer.

The compensator or linear retarder, retards the two perpendicular components of the electrical vector by different amounts thus alternating the polarization state of the wave. The azimuth angle of the compensator α_C is measured relative to the direction of the π eigenpolarization.

The surface where a fraction of the light wave is transmitted and another is reflected due to the Fresnel reflection and transmission coefficients ρ_π, ρ_σ, τ_π and τ_σ as described in Appendix B.

The analyzer is a linear polarizer at a rotational azimuth angle α_A relative to the π direction of the linear eigenpolarization.

The detector measures the intensity of the light from the analyzer. The detector can be any device able to measure the intensity of a light wave.

Upon making ellipsometric measurements of a surface the rotational angles of the polarizer, the compensator and the analyzer and the degree of retardation in the compensator must be known in order to determine the ellipsometric parameters ψ and Δ. There exists a variety of ways to perform the task of determining the ellipsometric parameters. In the next section the principles behind two such methods are described.

4.2 Different Ellipsometer Configurations

In this section two general ellipsometer configurations are described; the null and the photometric ellipsometer.

4.2.1 Null Ellipsometer

The null ellipsometer was historically the first ellipsometer, to be constructed. An illustration of the general structure of the null ellipsometer and the polarization state of the light between the components is shown in Figure 4.2. The principle behind this ellipsometer type is to minimize the intensity of the light wave at the detector. This is done by adjusting the rotational azimuth angle of the polarizer P, the compensator C and the analyzer A. As illustrated in the figure the source emits unpolarized light, which is made linearly polarized by the polarizer. By adjusting the azimuth angle of the polarizer and compensator the light can be made linearly polarized after reflection at the surface boundary. By adjusting the azimuth angle of the analyzer in order to achieve a perpendicular orientation relative to the linearly polarized wave the light intensity at the detector is minimized or ”nulled”. The ellipsometric parameters can then be calculated. As the degree of retardation in the compensator

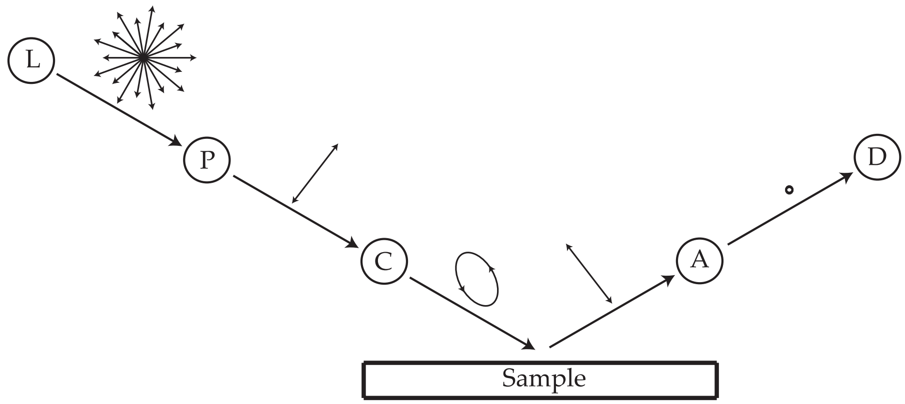


Figure 4.2: A null ellipsometer. The components of the ellipsometer are illustrated by encircled letters. The polarization state between the components is illustrated above. The black dot between the analyzer and the detector illustrates that the light wave intensity has been nulled.

is dependent on wavelength it is not possible to perform spectroscopic measurements in a large range of wavelengths with a null ellipsometer.

By use of the Jones matrix formalism the system matrix for a null ellipsometer can be found.[1] The input to this system matrix must be a Jones vector describing the light wave at the source $\mathbf{E}_{Lo}^{\pi\sigma}$. The superscript shows that the Jones vector is defined relative to the π and σ directions i.e. parallel and perpendicular to the plane of incidence and perpendicular to the direction of propagation. The subscript shows that it is the Jones vector at the light source output. The output Jones vector of the source is the same as the input Jones vector to the polarizer i.e. $\mathbf{E}_{Pi}^{\pi\sigma} = \mathbf{E}_{Lo}^{\pi\sigma}$. The Jones vector at the output of the polarizer is then given as

$$\mathbf{E}_{Po}^{\pi\sigma} = \mathsf{R}(-P)\mathsf{T}_P^{te}\mathsf{R}(P)\mathbf{E}_{Lo}^{\pi\sigma} \tag{4.1}$$

where $\mathsf{R}(P)$ is a Jones matrix that rotates coordinate system from $\pi\sigma$ to te, which is an abbreviation for transmission extinction referring to the fact that a polarizer has a transmission and an extinction axis. T_P^{te} is the Jones matrix for the polarizer. $\mathsf{R}(-P)$ rotates the Jones vector back to the $\pi\sigma$-coordinate system.

With the Jones vector at the output of the polarizer given, the Jones vector at the output of the compensator is expressed as

$$\mathbf{E}_{Co}^{\pi\sigma} = \mathsf{R}(-C)\mathsf{T}_C^{fs}\mathsf{R}(C)\mathbf{E}_{Po}^{\pi\sigma} \tag{4.2}$$

where T_C^{fs} is the Jones matrix of the compensator. Again the Jones vector is rotated to the coordinate system of the compensator, which is denoted fs for fast-slow, referring to the fact that a compensator has a fast and a slow axis. The Jones vector at the output side of the surface can be expressed as

$$\mathbf{E}_{So}^{\pi\sigma} = \mathsf{T}_S^{\pi\sigma}\mathbf{E}_{Co}^{\pi\sigma} \tag{4.3}$$

[1]See Appendix D for an explanation of the Jones matrix formalism.

where $\mathbf{T}_S^{\pi\sigma}$ is the Jones matrix of the surface. Finally the Jones vector at the output of the analyzer and hence at the detector is given as

$$\mathbf{E}_{Ao}^{te} = \mathbf{T}_A^{te}\mathbf{R}(A)\mathbf{E}_{So}^{\pi\sigma} \tag{4.4}$$

where $\mathbf{T}_A^{te}$ is the Jones matrix of the analyzer. There is no rotational matrix after the analyzer that transforms the Jones vector back to the π, σ system of coordinates. This is because the light detector, in the absence of errors is insensitive to polarization. Thus $\mathbf{E}_o = \mathbf{E}_{Ao}^{te}$

By combining (4.1), (4.2), (4.3) and (4.4), an expression for the Jones vector of the light wave at the detector as a function of the Jones vector of the light wave at the source can be derived

$$\mathbf{E}_o = \mathbf{T}_A^{te}\mathbf{R}(A)\mathbf{T}_s^{\pi\sigma}\mathbf{R}(-C)\mathbf{T}_C^{fs}\mathbf{R}(C-P)\mathbf{T}_P^{te}\mathbf{R}(P)\mathbf{E}_{Lo}^{\pi\sigma} \tag{4.5}$$

This equation describes a null ellipsometer where a compensator has been placed before the surface, but a compensator can also be placed after the surface. In that case the equation describing the system will be

$$\mathbf{E}_o = \mathbf{T}_A^{te}\mathbf{R}(A-C)\mathbf{T}_C^{fs}\mathbf{R}(C)\mathbf{T}_s^{\pi\sigma}\mathbf{R}(-P)\mathbf{T}_P^{te}\mathbf{R}(P)\mathbf{E}_{Lo}^{\pi\sigma} \tag{4.6}$$

The light wave intensity measured at the detector I_o is then given as the multiplication of $\mathbf{E}_o$ with its Hermitian adjoint $\mathbf{E}_o^\dagger$ [Röseler 1990, p. 60]. The Hermitian adjoint of a matrix is defined as the complex conjugate of the transpose of the matrix i.e.

$$I_o = \mathbf{E}^\dagger\mathbf{E} \tag{4.7}$$

In both cases the only unknown is the Jones matrix for the surface $\mathbf{T}_S^{\pi\sigma}$, which can be found if the output intensity is "nulled" and the rotational angles of the polarizer, compensator, analyzer, the relative phase retardation of the compensator and the angle of incidence are known.

4.2.2 Photometric Ellipsometer

In photometric ellipsometry one or more conditions are varied while the light intensity at the detector is measured. This is unlike null ellipsometry, as it is not the means of a photometric ellipsometer to have zero light intensity at the detector. Thus the output of photometric ellipsometry measurements are light intensity values at a number of prescribed conditions. The varied conditions could be the rotational azimuth angle of the polarizer, compensator or analyzer, the relative retardation of the compensator or the angle of incidence. In most cases the varied condition is the angle of the polarizer or analyzer, and thus only these two cases are considered in the following.

Unlike the null ellipsometer the photometric ellipsometer does not necessarily include a retarding element. This has the apparent advantage of making spectroscopic measurements possible as the polarizers generally are achromatic over a wider spectral range than retarders. Other advantages include that polarizers are relatively easy to construct compared to compensators and that they are easy to align within a system. On the other hand a disadvantage is that the system looses sensitivity when Δ is near 0 or 180°, which will be described further in the next section.

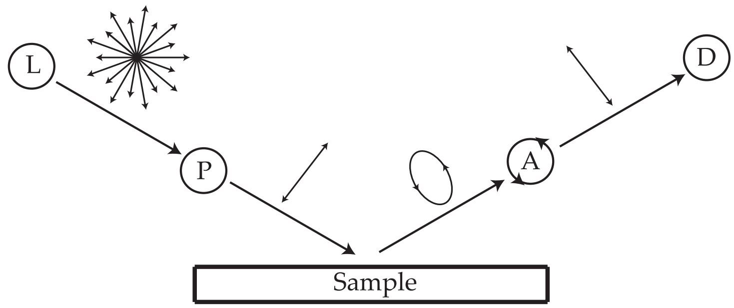


Figure 4.3: A photometric ellipsometer. The components of the ellipsometer are illustrated by encircled letters. The polarization state between the components is illustrated above. The arrows on the circle that illustrates the analyzer shows that it is rotating.

The general structure of a photometric rotating analyzer ellipsometer (RAE) is shown in Figure 4.3. Also shown in the figure is the polarization state between the different components of the ellipsometer. The light source emits unpolarized light, which is linearly polarized by the polarizer. After reflection at the surface boundary the polarization state of the light wave is changed from linearly polarized to elliptical polarized. The analyzer is rotated and the light intensity is measured at different rotational azimuth angles of the analyzer. The general principle behind a rotating analyzer photometric ellipsometer is thus to measure the intensity at different analyzer rotational angles, and from these measurements calculate the ellipsometric parameters ψ, Δ. It is also possible to vary the angle of the polarizer in which case the ellipsometer will be denoted a photometric rotating polarizer ellipsometer (RPE). The operation characteristics of the RAE and the RPE are basically the same, but some disadvantages / disadvantages exist for both configurations. The RPE requires the source to be totally unpolarized in order to perform accurate measurements. Correspondingly the RAE requires photodetectors that are insensitive to polarization in order to minimize errors. [Röseler 1990], [Jawoollam 2004]

Static and Dynamic Photometric Ellipsometers

As mentioned the light intensity is measured when either the angle of the polarizer or the analyzer is varied in a photometric ellipsometer in order to measure the ellipsometric parameters ψ and Δ. This variation can be done in one of two different ways. One is to measure the light intensity at predetermined fixed azimuthal positions. This method is denoted static photometric ellipsometry. The other is to periodically vary the azimuth angle of either or both the analyzer and polarizer with time. The detected signal is then Fourier-analyzed in order to determine ψ and Δ. In the next section a description of a photometric RAE is given by use of the Jones matrix formalism. [Azzam & Bashara 1977, pp. 255-260]

4.3 Determination of ψ and Δ with a Static Photometric RAE

The ellipsometer available in this project is a photometric RAE ellipsometer and thus this section concerns this type of ellipsometer only. This ellipsometer utilizes static analyzer angles in the determination of the ellipsometric parameters in the ultra violet (UV) and visible (VIS) region. As the tests performed in this project are done in the UV-VIS area the static method of determining ψ and Δ is treated. The determination of the ellipsometric parameters ψ and Δ with a photometric RAE is performed by measuring the intensity of the reflected light at three or more analyzer angles and making a calculation of the ellipsometric parameters from these light intensity values. The principles underlying these calculations are explained in this section. In the following the light waves are considered being monochromatic plane waves.

4.3.1 Description of an RAE by use of the Jones Matrix Formalism

Measurement of the ellipsometric parameters of a sample is illustrated in Figure 4.4. The

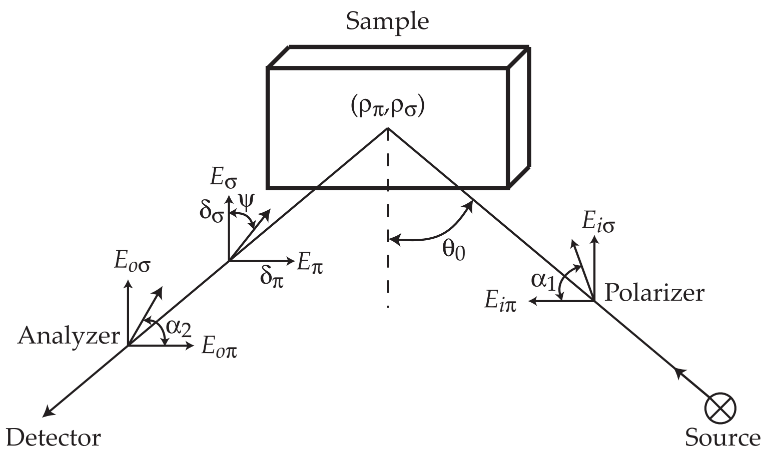


Figure 4.4: Illustration of ellipsometry performed with a photometric RAE without a compensator. [Röseler 1990, p. 73]

light from the source becomes linearly polarized at the fixed polarizer. The Jones vector of the light wave after the polarizer $\mathbf{E}_i^{\pi\sigma}$ is

$$\mathbf{E}_i^{\pi\sigma} = \begin{bmatrix} E_{i\pi} \\ E_{i\sigma} \end{bmatrix} = \begin{bmatrix} E_i \cos(\alpha_1) \\ E_i \sin(\alpha_1) \end{bmatrix} \tag{4.8}$$

where E_i is the magnitude of the Jones vector $\mathbf{E}_i^{\pi\sigma}$ and α_1 is the azimuth angle of the polarizer measured from the direction of the π eigenpolarization.

The light is reflected by the surface, which in Jones notation corresponds to multiplication by the Jones matrix of the surface

$$\mathbf{T}_s^{\pi\sigma} = \begin{bmatrix} \rho_\pi & 0 \\ 0 & \rho_\sigma \end{bmatrix} \tag{4.9}$$

Next the Jones vector of the light wave after the surface must be rotated to the coordinate system of the analyzer by the Jones transform matrix

$$\mathbf{R}(\alpha_2) = \begin{bmatrix} \cos(\alpha_2) & \sin(\alpha_2) \\ -\sin(\alpha_2) & \cos(\alpha_2) \end{bmatrix} \tag{4.10}$$

With the Jones vector given in the coordinates system of the analyzer the Jones matrix of the analyzer is given by

$$\mathbf{T}_A^{te} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \tag{4.11}$$

as the analyzer is considered ideal. [Röseler 1990, pp. 60-63], [Azzam & Bashara 1977, p. 76]

The Jones vector at the detector $\mathbf{E}_o^{te}$ can be expressed as

$$\mathbf{E}_o^{te} = \mathbf{T}_A^{te}\mathbf{R}(\alpha_2)\mathbf{T}_s^{\pi\sigma}\mathbf{E}_i^{\pi\sigma} \tag{4.12}$$

$$= \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \cos(\alpha_2) & \sin(\alpha_2) \\ -\sin(\alpha_2) & \cos(\alpha_2) \end{bmatrix} \begin{bmatrix} \rho_\pi & 0 \\ 0 & \rho_\sigma \end{bmatrix} \begin{bmatrix} E_i\cos(\alpha_1) \\ E_i\sin(\alpha_1) \end{bmatrix} \tag{4.13}$$

$$= \begin{bmatrix} \cos(\alpha_2)\rho_\pi\cos(\alpha_1)E_i + \sin(\alpha_2)\rho_\sigma\sin(\alpha_1)E_i \\ 0 \end{bmatrix} \tag{4.14}$$

$$= \begin{bmatrix} \cos(\alpha_2)E_\pi + \sin(\alpha_2)E_\sigma \\ 0 \end{bmatrix} \tag{4.15}$$

where $E_\pi = \rho_\pi\cos(\alpha_1)E_i$ and $E_\sigma = \rho_\sigma\sin(\alpha_1)E_i$.

4.3.2 Light Wave Intensity at the Detector

The light wave intensity at the detector I_o is given as

$$I_o = \mathbf{E}_o^\dagger\mathbf{E}_o \tag{4.16}$$

$$= \begin{bmatrix} \cos(\alpha_2)E_\pi^* + \sin(\alpha_2)E_\sigma^* & 0 \end{bmatrix} \begin{bmatrix} \cos(\alpha_2)E_\pi + \sin(\alpha_2)E_\sigma \\ 0 \end{bmatrix} \tag{4.17}$$

$$= \cos^2(\alpha_2)E_\pi E_\pi^* + \sin^2(\alpha_2)E_\sigma E_\sigma^* + \cos(\alpha_2)\sin(\alpha_2)\left(E_\pi E_\sigma^* + E_\sigma E_\pi^*\right) \tag{4.18}$$

where the *te* notation is omitted. This expression for the intensity can be rewritten by utilizing the following trigonometric identities [Råde & Westergren 1998, p.124]

$$\cos(\alpha_2)\sin(\alpha_2) = \frac{1}{2}\sin(2\alpha_2) \tag{4.19a}$$

$$\sin^2(\alpha_2) = \frac{1-\cos(2\alpha_2)}{2} \tag{4.19b}$$

$$\cos^2(\alpha_2) = \frac{1+\cos(2\alpha_2)}{2} \tag{4.19c}$$

The intensity is then given as

$$I_o = \frac{1}{2}\left(E_\pi E_\pi^* + E_\pi E_\pi^*\cos(2\alpha_2)\right) + \frac{1}{2}\left(E_\sigma E_\sigma^* - E_\sigma E_\sigma^*\cos(2\alpha_2)\right) + \frac{1}{2}\left(E_\pi E_\sigma^* + E_\sigma E_\pi^*\right)\sin(2\alpha_2) \tag{4.20}$$

$$= \frac{1}{2}\left[E_\pi E_\pi^* + E_\sigma E_\sigma^* + \left(E_\pi E_\pi^* - E_\sigma E_\sigma^*\right)\cos(2\alpha_2) + \left(E_\pi E_\sigma^* + E_\sigma E_\pi^*\right)\sin(2\alpha_2)\right] \tag{4.21}$$

$$= \frac{1}{2}\left[s_0 + s_1\cos(2\alpha_2) + s_2\sin(2\alpha_2)\right] \tag{4.22}$$

where the three Stokes parameters $s_0 = E_\pi E_\pi^* + E_\sigma E_\sigma^*$, $s_1 = E_\pi E_\pi^* - E_\sigma E_\sigma^*$ and $s_2 = E_\pi E_\sigma^* + E_\sigma E_\pi^*$ are introduced. [Röseler 1990, p. 74]

4.3.3 Determination of ψ and Δ with a Static Photometric RAE

From (4.22) expressions for the light wave intensity at different analyzer angles can be calculated. The light intensity at four specific values of α_2 in steps of 45° is

$$I_o(0^\circ) = \frac{1}{2}(s_0 + s_1) \tag{4.23a}$$

$$I_o(45^\circ) = \frac{1}{2}(s_0 + s_2) \tag{4.23b}$$

$$I_o(90^\circ) = \frac{1}{2}(s_0 - s_1) \tag{4.23c}$$

$$I_o(-45^\circ) = \frac{1}{2}(s_0 - s_2) \tag{4.23d}$$

The determination of the ellipsometric parameters ψ and Δ requires only three analyzer angle setting e.g. $\alpha_2 = 0^\circ$, $\alpha_2 = 45^\circ$ and $\alpha_2 = 90^\circ$. Additional measurements would be redundant, but due to practical imperfections in the ellipsometer they might increase the precision of the determined parameter values.

The Stokes parameters are connected to the measured light wave intensities at the detector due to (4.23). The Stokes parameters are furthermore connected to the ellipsometric parameters in Appendix E due to (E.26). Combining these equations yields

$$\cos(2\psi') = \frac{-s_1}{s_0} = \frac{\frac{1}{2}(s_0 - s_1) - \frac{1}{2}(s_0 + s_1)}{\frac{1}{2}(s_0 - s_1) + \frac{1}{2}(s_0 + s_1)} = \frac{I_o(90^\circ) - I_o(0^\circ)}{I_o(90^\circ) + I_o(0^\circ)} \tag{4.24}$$

and

$$\sin(2\psi')\cos(\Delta) = \frac{s_2}{s_0} = \frac{s_0 + s_2}{s_0} = \frac{2I_o(45^\circ)}{I_o(90^\circ) + I_o(0^\circ)} \tag{4.25}$$

where the new variable ψ' is given by the relation

$$\tan(\psi') = \frac{\tan(\psi)}{\tan(\alpha_1)} \tag{4.26}$$

In the case where the polarizer angle is 45° i.e. $\alpha_1 = 45^\circ$ the relation reduces to

$$\tan(\psi') = \tan(\psi) \tag{4.27}$$

and hence $\psi' = \psi$.

As can be seen from (4.24) and (4.25) the ellipsometric parameters can, as mentioned above, be calculated from only three measurements of the light wave intensity, however some limitations are present. Δ is determined in the region $0^\circ \leq \Delta \leq 180^\circ$ only. In the region of $\cos(\Delta) \approx 1$ the determined Δ can be very inaccurate because a small variation in $\cos(\Delta)$ causes a large variation in the determined Δ. These problems can be minimized by introducing a retarder in the system. [Röseler 1990, p. 76]

4.4 Description of the Sentech SE 850 Ellipsometer

The ellipsometer used for experiments in this project is the spectroscopic ellipsometer SE 850 from Sentech. This is a photometric RAE ellipsometer that utilizes both static and dynamic measurements. The SE 850 is computer controlled via the Sentech software ”Spectraray”. The ellipsometer has a range of wavelength from 350 nm to 1700 nm.

During this project it has not been possible to use the NIR part of the ellipsometer due to software failure. This means that the range of wavelength is limited to 350 nm - 850 nm in all measurements.

4.4.1 Functional Description

A block scheme showing the structure of the SE 850 is depicted in Figure 4.5. The ellip-

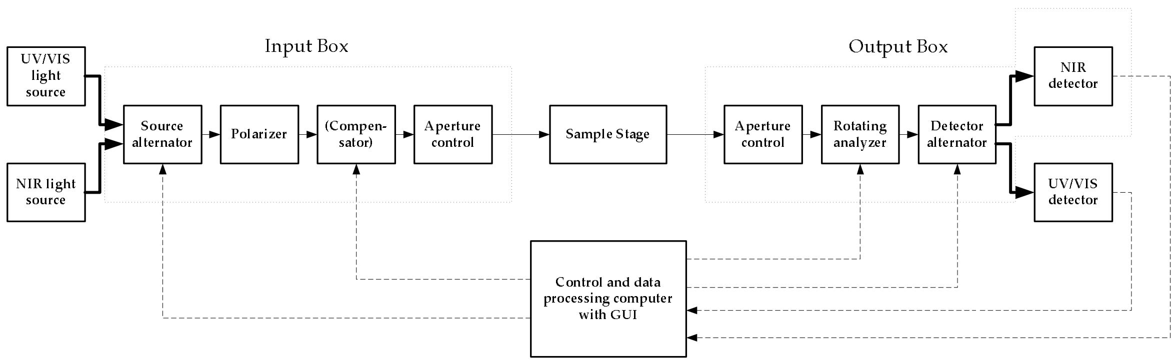


Figure 4.5: A block scheme of the SE 850. Control signals are illustrated with dashed lines, the light waves travelling through air are illustrated by fully drawn lines, and the light waves travelling through optical fibers are illustrated by thick fully drawn lines.

someter is centered around the control and data processing computer. This computer also has a graphical user interface (GUI) in order for the user to initiate the ellipsometric measurement and perform data processing of the measured data. The control signals from and to the computer are shown as dashed lines. These output signals are control signals for the choice of source and detector, control signal for the compensator if this is to be used in the measurement and a control signal for the rotating analyzer. The input signals are the measured intensities from the detectors. The fully drawn lines in the figure illustrate light waves travelling through air. The light wave is propagated through an optical fiber between the sources and the source alternator. The same is the case between the detector alternator and the detectors. The optical fibers are illustrated by thick fully drawn lines. Note that the compensator is enclosed by brackets as this component only is utilized in some special cases. Further specifications of the SE 850 are listed below.

4.4.2 Specifications

The specifications for the SE 850 are found at Sentech’s web page [Spectroscopic Ellipsometer SE 850 2004].

UV/VIS Light Source: The light source used for UltraViolet / Visible (UV / VIS) measurements is a 75 W xenon lamp. With this light source measurements in the spectrum from 350 nm to 850 nm can be performed.

NIR Light Source: A halogen lamb is used for measurements in the Near InfraRed (NIR) range between 850 nm to 1700 nm.

UV/VIS Detector: A photodiode array with 1024 elements is used to detect the light intensity in the UV / VIS range. This unit is placed in the control computer cabinet.

NIR Detector: A Fourier Transform InfraRed (FT-IR) photodetector is used in the NIR range. This unit is placed in the output box of the ellipsometer after the source alternator.

Polarizer: The polarizer is fixed at a rotational azimuth angle of 45°.

Analyzer: The azimuth angle of the analyzer is variable and is controlled by the spectraray software running on the computer.

Compensators: Computer controlled super achromatic retarder for UV / VIS spectral range. (Optional)

Goniometer: The angle of incidence is controlled by a manual goniometer which has a range from 30° to 90° with a step size of 5°.

Sample Stage: The sample stage is manually controlled. Possible adjustment parameters are the height and inclination of the sample stage. Furthermore it is possible to control the azimuth angle of the sample stage with a resolution of 1° and the translational position in one dimension of the sample in the plane of incidence with a resolution of 10 μm.

Apertures A manual aperture control is placed on the input and output side of the sample stage. With this component it is possible to adjust the spot size and hence the intensity of the light wave.

A picture of the SE 850 ellipsometer is shown in Figure 4.6. The box to the left is the input box with the source alternator, the polarizer, the compensator and the aperture control. The box to the right is the output box with the aperture control, the analyzer, detector alternator and the NIR detector. A picture of the two boxes without the cover can be seen in Figure 4.7.

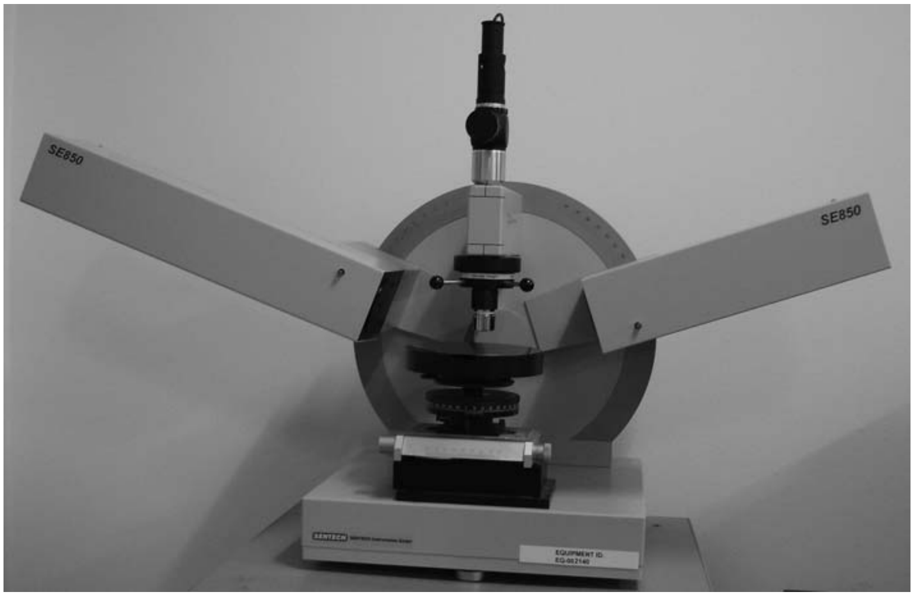
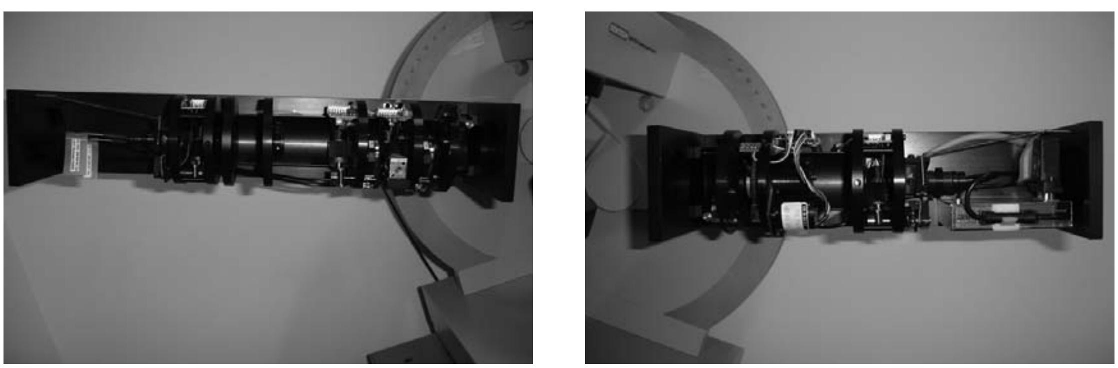


Figure 4.6: The Sentech SE 850 ellipsometer.



(a) The input box of the ellipsometer..

(b) The output box of the ellipsometer.

Figure 4.7: The input and output units of the ellipsometer without the covers.

Calculations of Physical Properties 5

This chapter describes the calculation of the complex refractive index and the film thickness of a thin film. Furthermore, the method of calculating the thickness of an optically thick film is described.

5.1 Index of Refraction

This section describes the relation between the ellipsometric parameters ψ and Δ measured with the ellipsometer and the complex index of refraction $\tilde{n}_1$. Figure 5.1 shows the basic setup in order to calculate the refractive index. The basic equation for an ellipsometer found

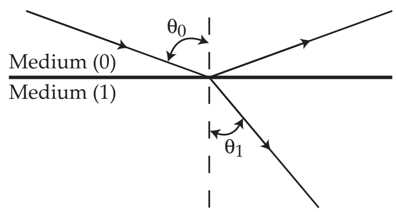


Figure 5.1: Reflection and transmission of an incident light wave at a surface boundary.

in (3.35) on page 19 contains the Fresnel reflection coefficients ρ_π and ρ_σ which are deduced in Appendix B. In this appendix, they are given by (B.30a) and (B.25) as

$$\rho_\pi = \frac{\tilde{n}_1\cos(\theta_0) - \tilde{n}_0\cos(\theta_1)}{\tilde{n}_1\cos(\theta_0) + \tilde{n}_0\cos(\theta_1)} \tag{5.1}$$

$$\rho_\sigma = \frac{\tilde{n}_0\cos(\theta_0) - \tilde{n}_1\cos(\theta_1)}{\tilde{n}_0\cos(\theta_0) + \tilde{n}_1\cos(\theta_1)} \tag{5.2}$$

where $\cos(\theta_1)$ can be found via Snell's law and the trigonometric identity as

$$\cos(\theta_1) = \sqrt{1 - \left(\frac{\tilde{n}_0}{\tilde{n}_1}\right)^2 \sin^2(\theta_0)} \tag{5.3}$$

Here, $\tilde{n}_1$ is the complex refractive index of medium 1, $\tilde{n}_0$ is the complex refractive index of the ambient, θ_0 is the angle of incidence and θ_1 is the unknown angle of transmission. Inserting (5.1), (5.2) and (5.3) into (3.35) and solving for $\tilde{n}_1$ yields

$$\tilde{n}_1 = \frac{\left[\sqrt{1 - 4\sin^2(\theta_0)\tan(\psi)\,e^{j\Delta} + 2\tan(\psi)\,e^{j\Delta} + \tan^2(\psi)\,e^{j\Delta}}\right]\tilde{n}_0\sin(\theta_0)}{\cos(\theta_0)\left[1 + \tan(\psi)\,e^{j\Delta}\right]} \tag{5.4}$$

The data from the ellipsometer are values of ψ and Δ as a function of wavelength. Using (5.4), these data can be used to calculate the complex index of refraction as a function of wavelength.

5.2 Film Thickness

When ellipsometric measurements are performed on a three phase optical system consisting of an ambient-film-substrate structure, it is possible to determine the thickness of the film, if the refractive indexes for the three media are known. This section concerns relating the film thickness to the ellipsometric parameters ψ and Δ. An ambient-film-substrate optical system is depicted in Figure 5.2 The incident light wave from the ellipsometer strikes the surface

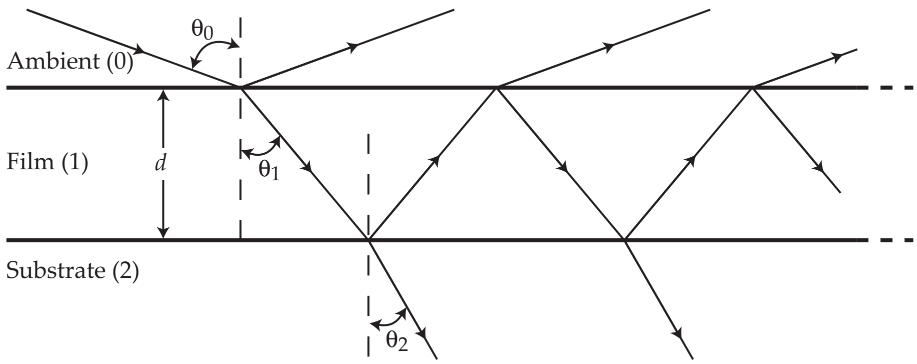


Figure 5.2: Illustration of an ambient-film-substrate optical system. The incident wave is partially reflected and partially transmitted.

boundary between ambient and the film at an angle of θ_0, which will also be the angle of the reflected wave due to Snell's law. Reflection and transmission of a polarized wave due to the surface boundaries in a three phase optical system is treated in Appendix C. In this appendix the total reflection coefficients of σ and π polarized light are found to be

$$P_\sigma = \frac{\rho_{01,\sigma} + \rho_{12,\sigma} e^{-j2\beta}}{1 + \rho_{01,\sigma}\rho_{12,\sigma} e^{-j2\beta}} \tag{5.5a}$$

$$P_\pi = \frac{\rho_{01,\pi} + \rho_{12,\pi} e^{-j2\beta}}{1 + \rho_{01,\pi}\rho_{12,\pi} e^{-j2\beta}} \tag{5.5b}$$

due to (C.29a) and (C.29b). P is the Greek letter capital ρ. The reflection coefficients in these equations are given in (C.30). An expression for β is given in (C.16).

5.2.1 Relation Between Ellipsometric Parameters and Film Thickness

(5.5a) and (5.5b) can be related to the ellipsometric parameters due to (3.35) where the reflection coefficients in a two-phase optical system ρ_π and ρ_σ are replaced by the reflection coefficients of a three-phase optical system P_π and P_σ

$$P = \frac{P_\pi}{P_\sigma} = \tan(\psi) e^{j\Delta} \tag{5.6}$$

where the parameter P is introduced as the complex reflection ratio [Azzam & Bashara 1977, p. 288]. By inserting the expressions for P_σ and P_π the following is given

$$P = P_\pi \cdot \frac{1}{P_\sigma} = \frac{\rho_{01,\pi} + \rho_{12,\pi} e^{-j2\beta}}{1 + \rho_{01,\pi}\rho_{12,\pi} e^{-j2\beta}} \cdot \frac{1 + \rho_{01,\sigma}\rho_{12,\sigma} e^{-j2\beta}}{\rho_{01,\sigma} + \rho_{12,\sigma} e^{-j2\beta}} \tag{5.7}$$

$$= \frac{\rho_{12,\pi}\rho_{01,\sigma}\rho_{12,\sigma} e^{-j4\beta} + \left(\rho_{01,\pi}\rho_{01,\sigma}\rho_{12,\sigma} + \rho_{12,\pi}\right) e^{-j2\beta} + \rho_{01,\pi}}{\rho_{01,\pi}\rho_{12,\pi}\rho_{12,\sigma} e^{-j4\beta} + \left(\rho_{01,\pi}\rho_{12,\pi}\rho_{01,\sigma} + \rho_{12,\sigma}\right) e^{-j2\beta} + \rho_{01,\sigma}} \tag{5.8}$$

This is an equation of 11 parameters, where the two ellipsometric parameters ψ and Δ are related to nine real parameters. These parameters are the real and imaginary parts of the complex refractive indexes, $\tilde{n}_0$, $\tilde{n}_1$, $\tilde{n}_2$, the angle of incidence θ_0, the free-space wavelength of the incident light wave λ and the film thickness d. If a set of ellipsometric parameters are measured at a given angle of incidence and a given wavelength the thickness of the film is the only unknown, assuming that the refractive indexes of the ambient, film and substrate are known. Thus by solving (5.8) for d, the film thickness of a sample can be determined.

5.2.2 Solving for the Film Thickness

(5.8) can be rewritten to

$$P = \frac{AX^2 + BX + C}{DX^2 + EX + F} \tag{5.9}$$

where $A = \rho_{12,\pi}\rho_{01,\sigma}\rho_{12,\sigma}$, $B = \rho_{01,\pi}\rho_{01,\sigma}\rho_{12,\sigma} + \rho_{12,\pi}$, $C = \rho_{01,\pi}$, $D = \rho_{01,\pi}\rho_{12,\pi}\rho_{12,\sigma}$, $E = \rho_{01,\pi}\rho_{12,\pi}\rho_{01,\sigma} + \rho_{12,\sigma}$, $F = \rho_{01,\sigma}$ and $X = e^{-j2\beta}$. Rearrangement of this equation yields

$$(PD - A)X^2 + (PE - B)X + (PF - C) = 0 \tag{5.10}$$

which is a complex quadratic equation with the solution

$$X = \frac{-(PE - B) \pm \sqrt{(PE - B)^2 - 4(PD - A)(PF - C)}}{2(PD - A)} \tag{5.11}$$

If the refractive index for the film is known, two analytical solutions to this equation exist, namely X_1 and X_2.

If the refractive index for the film is not known, but is assumed real i.e. $\tilde{n}_1 = n_1$, solutions to (5.11) can be found by iteration. In this iteration procedure n_1 is varied until the condition $|X| = 1$ is satisfied. As $X = e^{-j2\beta}$, where β is given by (C.16) on page 87 it is given that $|X|$ must equal 1. With the determined value of n_1 a value for X is also given.

With X determined from either of the methods, it is possible to calculate the film thickness due to

$$X = e^{-j2\beta} \tag{5.12}$$

$$\ln(X) = -j4\pi \frac{d}{\lambda} \tilde{n}_1 \cos(\theta_1) \tag{5.13}$$

$$d = \frac{j \ln(X) \lambda}{4\pi \tilde{n}_1 \cos(\theta_1)} \tag{5.14}$$

where X is either of the previously calculated solutions to (5.11). Obviously only one solution for the film thickness is valid, which should be real and positive. In the presence of errors the calculated thickness may be complex. In this case the solution with the smaller imaginary part should be chosen.

5.3 Film Thickness of a Thick Thin Film

In cases where the film is transparent i.e. the refractive index is purely real, multiple solutions for the film thickness exist. This can be seen from (5.12) which can be rewritten to

$$X = e^{-j4\pi\frac{d}{\lambda}\tilde{n}_1\cos(\theta_1)} = e^{-j2\pi\left(\frac{d}{D}\right)} \tag{5.15}$$

where

$$D = \frac{\lambda}{2\tilde{n}_1\cos(\theta_1)} \tag{5.16}$$

. From this equation it can be seen that X is a periodic function of d with a period of D, thus D is denoted the film thickness period. The film thickness period is a function of the angle of incidence, the wavelength of the light in free-space and the refractive indexes of the ambient and the film. The complete solution for the film thickness is then given as

$$d = d_0 + mD \tag{5.17}$$

where d_0 is the solution found in (5.14), which is called the standard solution and m is either 0 or a natural number i.e. $m = \{0, 1, 2, ..\}$. Without knowledge of the range of the thickness in advance it can thus prove difficult to explicitly determine the film thickness if the film is non-absorbing. The next section treats this subject. [Azzam & Bashara 1977, pp. 283-317]

5.3.1 Solving for the Film Thickness of a Thick Thin Film

When the film thickness d exceeds the film thickness period D, interference in the reflected light will appear, as the different components[1] of the reflected wave will be in phase at some wavelengths and in counter phase at other wavelengths. This will result in ψ and Δ angles that vary between positive and negative interference with a period that is dependent on wavelength. An example of this is given in Figure 5.3 where Δ is plotted as a function of wavelength. It is emphasized that the graph serves as an illustration only, and that it is not an actual experimental result. From a Δ-spectrum as this, it is possible to calculate the film thickness, as the distance between the local maxima are determined by the angle of incidence θ_0, the refractive index of the ambient $\tilde{n}_0$, the film $\tilde{n}_1$, the substrate $\tilde{n}_2$, the wavelength of the light λ and the film thickness d. Usually the only unknown is the film thickness which can then be calculated. This is done by determining the wavelengths of two adjacent peaks. At these two wavelengths the standard solution d_0 and the thickness period D can be calculated as described above. Two expressions for the film thickness can be set up due to (5.17). One at the first maximum at $\lambda = \lambda_0$

$$d = d_{00} + m_0 D_0 \tag{5.18}$$

and one at the next at $\lambda = \lambda_1$.

$$d = d_{01} + m_1 D_1 \tag{5.19}$$

[1] See Figure 5.2

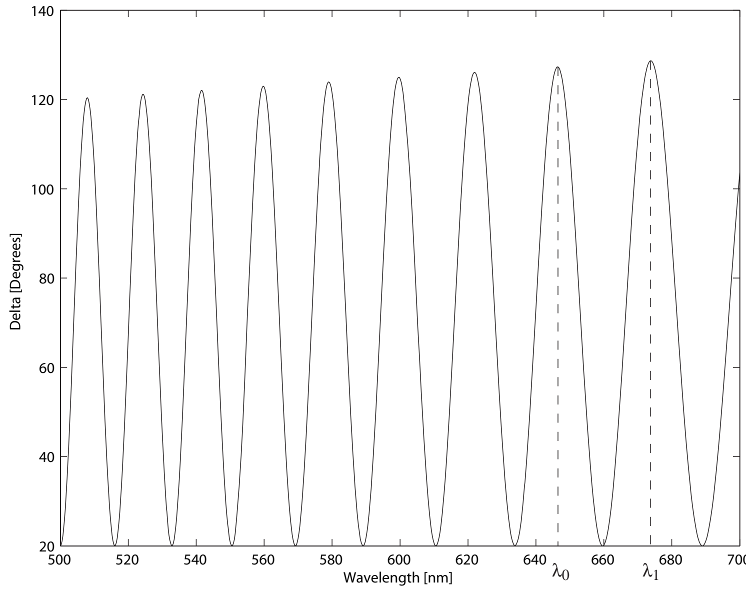


Figure 5.3: Illustration of interference as the film thickness exceeds the film thickness period. It can be seen that the distance between to adjacent peaks increases as the wavelength increases. Two adjacent peaks has been marked as λ_0 and λ_1.

As the thickness of the film is not dependent of wavelength, d must be the same in both equations. Subtraction of (5.18) from (5.19) yields

$$0 = d_{01} - d_{00} + m_1 D_1 - m_0 D_0 \tag{5.20}$$

The factors m_0 and m_1 are then the only unknowns. If the measured Δ spectrum has sufficient resolution to enable determination of all peaks, i.e. it is certain that there are no peaks between λ_0 and λ_1 it can be reasoned that

$$m_0 = m_1 + 1 \tag{5.21}$$

With a relation between m_0 and m_1 (5.20) can be rewritten to

$$0 = d_{01} - d_{00} + m_1 D_1 - (m_1 + 1) D_0 \tag{5.22}$$

$$m_1 = \frac{D_0 + d_{00} - d_{01}}{D_1 - D_0} \tag{5.23}$$

The only unknown parameter in (5.23) is m_1 and thus the value for this can be calculated. In the absence of errors m_1 is a natural number. Inserting the expression for m_1 into (5.19) yields

$$d = d_{01} + \frac{D_0 + d_{00} - d_{01}}{D_1 - D_0} D_1 \tag{5.24}$$

from which the film thickness can be directly calculated.