Ellipsometry

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Definition

Collective name for a number of techniques dealing with the measurement and interpretation of the change in the polarization state of a polarized beam of radiation which is reflected from a surface.

From this change, optical properties of the reflecting surface can be derived.

Theory and Application

Basic Theory for Reflection and Transmission at an Interface and the Basic Ellipsometry Equation

In Fig. 1 the beam trajectories are sketched for a wave incident on a plane interface between two media having a real refractive index n_1 and n_2 , respectively. The incoming beam with amplitude E_i is reflected by the interface, giving a reflected beam with amplitude E_2 and a transmitted beam with amplitude E_3 .

The condition that the phase of the three waves must be the same at the interface gives $\Theta_1 = \Theta_2$ and $\sin(\Theta_1)/\sin(\Theta_3) = n_1/n_2$ which is Snell's law. The ratio between the incident amplitude E_i and

the reflected amplitude E_2 will be different between light that is polarized parallel to the interface (p-direction) and the direction perpendicular to this (s-direction, as the arrows in Fig. 1). In general it can be written that

$$r(\lambda, \theta) = \frac{r_p(\lambda, \theta)}{r_s(\lambda, \theta)} = \tan(\psi(\lambda, \theta)) \cdot \exp(i\Delta(\lambda, \theta)) \quad (1)$$

where r_p and r_s are the amplitude reflectances for light polarized in the p- and s-directions, respectively. This equation defines the ellipsometric angles Ψ and Δ that can be determined in an ellipsometric measurement as shown below. Equation 1 states that the ratio between the reflectances, and with that the ellipsometric angles Ψ and Δ , will depend on the angle of incidence ϑ and the wavelength λ for a given interface, whether it consists of a single homogeneous material or is a complicated system consisting of several absorbing and nonabsorbing thin films.

Considering Eq. 1, ellipsometry consists of:

1. Measurement of the angles Ψ and Δ
An instrument that enables the determination of these quantities is called an ellipsometer.
2. Give a physical interpretation to the measured angles Ψ and Δ
Using the Fresnel coefficients of stratified surfaces, the theoretical angles Ψ and Δ can be

Ellipsometry,**Fig. 1** Reflection and refraction at a plane interface **Ellipsometry, Fig. 2** Schematic of an ellipsometer according to the PSCA arrangement

calculated of a surface, whether it consists of a single homogeneous material, a birefringent material, or a combination of absorbing and transparent coatings on a surface.

Measurement of Ψ and Δ : The Ellipsometer**Static Null Ellipsometer**

An example of an ellipsometer arrangement is given in Fig. 2. It is one of the most elaborate arrangements but it well illustrates the key points of ellipsometry.

Figure 2 depicts an ellipsometer in the PCSA (polarizer-compensator-sample-analyzer) arrangement. The polarizer, compensator, and analyzer can be rotated around the axis that is defined by the light beam. The polarizer and analyzer are in fact linear polarizers; the compensator is a $1/4\text{-}\lambda$ plate that is commonly oriented at 45° from the p- and s-direction. The polarizer can be rotated to make a linear polarized beam in any polarizing direction. Together with the compensator, this means that polarized light can be made, that is, either linear polarized in the p- or s-direction or circular or elliptically polarized in any other direction. It is always possible to adjust the ellipticity of this light in such a way that after reflection a linearly polarized beam remains. This light can be extinguished by another polarizer that is called the analyzer.

With every position of the compensator at $+$ or -45° , there are two positions of the polarizer (P) and analyzer (A) where extinction occurs. These four solutions are called the four zones, for which Δ and Ψ are derived according to Table 1:

Table 1 illustrates in the first place that the relationship between the ellipsometer angles and the polarizer position is rather straightforward. In the second place there are four solutions.

The effects of alignment errors in the polarizer, analyzer, and compensator angles, and the retardation of compensator, can be eliminated by taking the average solutions $\Delta = \sum \Delta_i / 4$ and $\psi = \sum \psi_i / 4$, respectively. It is a big advantage of null ellipsometry that this method exists to eliminate most of the systematic alignment errors in this way. The only remaining systematic errors are the rotary scale errors of the P and A position and the error in Θ .

Ellipsometry, Table 1 Zone relations for a PCSA null ellipsometer. P is the polarizer angle, C is the compensator angle, and A is the analyzer angle

Zone	Delta	Psi
$C = -\pi/4$	$\Delta_1 = 2P_1 + \pi/2$	$\Psi_1 = A_1$
$C = -\pi/4$	$\Delta_2 = -2P_2 - \pi/2$	$\Psi_2 = A_2$
$C = \pi/4$	$\Delta_3 = 2P_3 - \pi/2$	$\Psi_3 = -A_3$
$C = \pi/4$	$\Delta_4 = -2P_4 + \pi/2$	$\Psi_4 = -A_4$

The measurement itself consists of rotating the polarizer and analyzer and finding the settings of the polarizer P and analyzer A where light extinction takes place; in practice, this is the point where the light intensity has a minimum. This position of P and A is insensitive to intensity fluctuations of the light source and is also insensitive to absolute intensity measurements. By watching the intensity at the detector location, this measurement can even be done visually.

Dynamic Ellipsometers

As the null ellipsometer is rather tedious to operate, dynamic ellipsometers have been developed. An example is that the analyzer is rotating continuously in the PCSA configuration. A Fourier analysis of the intensity signal gives the ellipsometer angles Δ and Ψ if the position of the compensator C and polarizer P are known. Such a signal can be used to monitor a surface. The automatic error compensation of the four-zone null technique must be replaced by a calibration technique for the offsets.

Measurement of a Single Set or Multiple Sets of Ellipsometric Angles Δ and Ψ

Determination of Two Parameters

An obvious attractive feature of ellipsometry is that two parameters are obtained in a single measurement. If there is only one perfectly homogeneous surface with a complex refractive index, the real and complex part of the refractive index can be calculated from the two ellipsometric angles. The situation becomes more complicated if the assumed system becomes more complicated: every thin film has a thickness and a complex refractive index, which means three additional parameters.

This means that if useful information is to be obtained from a film-substrate system, there are five parameters: the complex refractive index (n and k) of film (two parameters) and substrate (two parameters) and a film thickness (one parameter). Usually some parameters are known or can be assumed, such as the refractive index of the substrate material and $k = 0$ for a transparent

film. In that case, the film refractive index and thickness can be obtained from a single ellipsometric measurement. If one needs to determine more parameters, the number of free parameters can be increased by varying the angle and/or the wavelength.

Multiple Angle of Incidence (MAI) Ellipsometry

With MAI ellipsometry measurements at a same specimen at a same location on a specimen are taken, but the angle Θ is varied. This gives a new Ψ and Δ value at every angle Θ . This means that more parameters can be fitted in a model that contains one or more thin films on a substrate. However, in the model some parameters can be correlated and the dependence on Θ can be limited. Haitjema and Woerlee (1989) used this method and showed that tin oxide coatings can be anisotropic and that a surface layer must be assumed in a model to achieve consistent result, unless the surface is polished.

Spectroscopic Ellipsometry

With spectroscopic ellipsometry, measurements at a same location on a specimen are taken at several, or at continuously scanned, wavelengths. This increases the number of measured parameters; however, many parameters are also wavelength dependent, so in that not much is gained. However, clearly one parameter does not change: the thickness of coatings on the surface.

Calculation of Substrate and Thin-Film Parameters

In general there are no straightforward equations that relate the measured ellipsometric angles to thin-film thickness and/or optical constants. The few cases for which an analytic solution exists are given by Azzam and Bashara (1977). However, for the general case, optical constants must be obtained by fitting a model to the obtained ellipsometric angles. The ellipsometric angles of a thin-film/substrate system can be calculated using the Fresnel coefficient and using a thin-film model. This is described in classical

textbooks (Azzam and Bashara 1977; Jackson 1998; Heavens 1991). For more complicated multiple-film systems, a matrix method is developed. Fresnel coefficients of an anisotropic material are given by Haitjema and Woerlee (1989).

Bare Substrate

For a bare substrate, only two parameters are to fit: the real and complex part of the complex refractive index $\mathbf{n} = n - ik$ of the substrate. For this case in air ($n_{\text{air}} = 1$), there is an analytical solution:

$$n = \tan(\theta) \cdot \sqrt{1 - \frac{4r}{1+r} \cdot \sin^2(\theta)} \quad (2)$$

where r is the complex number as calculated in Eq. 1.

Single Thin Film

The single-film model is relatively straightforward, especially for the case of a transparent film on a transparent substrate with a known refractive index. In that case the film thickness and refractive index can be obtained by measuring the ellipsometric angles at a single angle of incidence. For a few cases, there are analytical solutions that directly relate film thickness and refractive index to the ellipsometric angles.

Anisotropic and Multiple Films

The determination of anisotropy in a film is shown by Haitjema and Woerlee (1989). In general, multiple films give high parameter correlations when all parameters of every film are to be determined. Often, optical properties are quite well known, e.g., a SiO_2 coating on Si, so in that case ellipsometry is mainly used for film thickness determinations.

Applications in Chemistry and Biology

Further applications are in physical/chemical/biological phenomena at surfaces. Because of its extreme sensitivity, an ellipsometer gives an immediate response if “something” happens at a surface: a thin film grows, a clean surface

oxidates, a chemical reaction appears, blood coagulates, (Vroman 1964) etc.

Advantages of Ellipsometry

Accuracy

The ellipsometric angles can be determined quite accurately and rather independently on absolute intensity. Several reversal and calibration methods are available so the ellipsometric angles can be obtained accurately and bias-free.

Sensitivity

An ellipsometer can be highly sensitive. The sensitivity for a film thickness can be of the order of $1^\circ/\text{nm}$ for the sensitivity of Δ for a film thickness or a change in film thickness. As ellipsometric angles can be measured with about 0.01° uncertainty for a good-quality ellipsometer, the deposition of monatomic layers can be detected.

Contactless

Obviously, ellipsometry is a noncontact measurement method. By applying windows, measurements can be carried out with the specimen in process or in a vacuum.

Disadvantages of Ellipsometry

Sensitivity

The sensitivity can be a disadvantage when measurements of less ideal specimens are needed. A thin-film measurement can easily be disturbed by a small roughness of the top of a coating. A measurement of a substrate is easily disturbed by a small roughness or oxide/water layer of a few atoms. If these effects are not taken into account in the calculation, quite erroneous values can easily be obtained.

Model Dependence

If the model consists of two coatings with two thicknesses, a calculation will give two refractive indices and two thicknesses. If the model consists of one anisotropic film, a calculation will give values for anisotropy. As the method is indirect

and model dependent, there is no warning against erroneous or nonsensical results, e.g., an ellipsometric measurement can give a high value for the extinction coefficient of a substrate while it is obviously transparent, meaning that the extinction coefficient must be effectively zero and should be fixed so in the model used.

Ellipsometry and Traceability

For this item there are different approaches. The straightforward approach is that a measurement is just a measurement of angles, so the traceability is in the traceability of the angles, combined with the wavelength/frequency of the light source used.

A different approach is considering the ellipsometer as a system that measures a specific thin film. As a reference material, a thin film is supplied with a calibrated thickness and the user is supposed to measure that same thickness on his ellipsometer.

Because the results are very dependent on the assumed model of the measured surface, traceability and uncertainty of the measured angles Ψ and Δ are far easier to guarantee than, for example, a film thickness or a refractive index.

Cross-References

- [Accuracy](#)
- [Traceability](#)

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