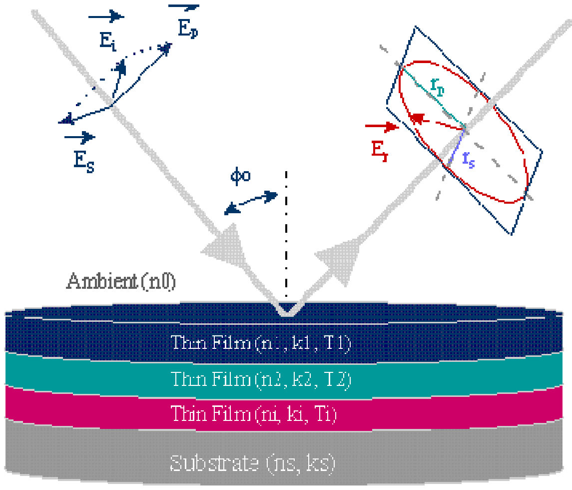
Spectroscopic Ellipsometry

Introduction

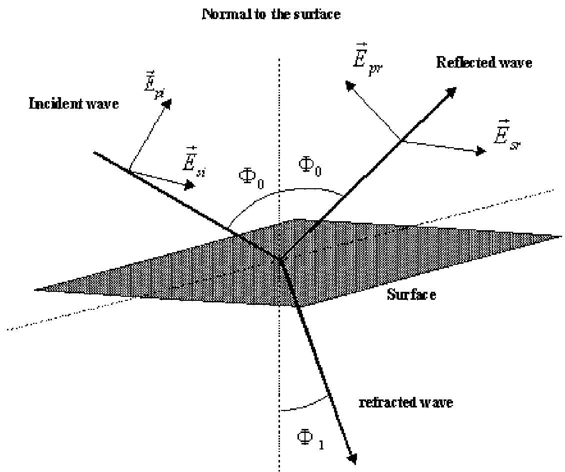
The ellipsometry is an optical technique devoted to the analysis of surfaces. It is based on the measurement of the variation of the polarization state of the light after reflection on a plane surface. The ellipsometry technique has been discovered one hundred years ago but it is only since the early 80's, thanks to the development of electronic and computers that the technique expands largely in numerous fields.
The strong advantages of ellipsometry are its non destructive character, its high sensitivity due to the measurement of the phase of the reflected light, its large measurement range (from fractions of single layers to micrometers), and the possibilities to control in real time complex processes.
We must distinguish between single wavelength ellipsometry which can measure only two parameters and spectroscopic ellipsometry which can analyze complex structures such as multilayers, interface roughness, inhomogeneous layers, anisotropic layers and much more.
We are interested here only by Spectroscopic Ellipsometry.



THEORY OF ELLIPSOMETRY

After reflection on a sample surface, a linearly polarized light beam is generally elliptically polarized. The reflected light has phase changes that are different for electric field components polarized parallel (p) and perpendicular (s) to the plane of incidence. Ellipsometry measure this state of polarization or more precisely the complex ratio rho written as:

$$\rho = \frac{r_p}{r_s} = \tan\psi * \exp(i\Delta)$$



where Psi and Delta are the amplitude ratio and phase shift, respectively, of the p and s components and are the ellipsometric parameters (often given as tan Psi, cos Delta) measured as described in the Signal treatment and calibration section. The reflectance coefficients are directly related to the optical constants of the surface by assuming the ambient is air (Fresnel relations):

$$r_p = \frac{n\cos\phi_i - \cos\phi_t}{n\cos\phi_i + \cos\phi_t} \qquad r_s = \frac{\cos\phi_i - n\cos\phi_t}{\cos\phi_i + n\cos\phi_t}$$

where n is the complex refractive index n = N – iK of the surface.
The angle of refraction may be obtained using Snell-Descartes's Law:

$$\sin\phi_i = n\sin\phi_t$$

Thus if the sample is an ideal bulk, the real and imaginary parts of the complex refractive index may be calculated from the measured tan Psi and cos Delta parameters with the knowledge of the incidence angle. The optical index and thickness of a transparent layer on known substrate can also be deduced in the same way. This kind of analysis is characteristic of a single wavelength ellipsometric measurement.

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For the analysis of more complex (and realistic samples), the solution is offered by the spectroscopic ellipsometry technique. The idea is to measure the two ellipsometric parameters in a large range of wavelength and to assume that the optical indices of the materials are known. Using an optical model is then possible to extract the different physical parameters of the sample.

MEASUREMENT TECHNIQUES

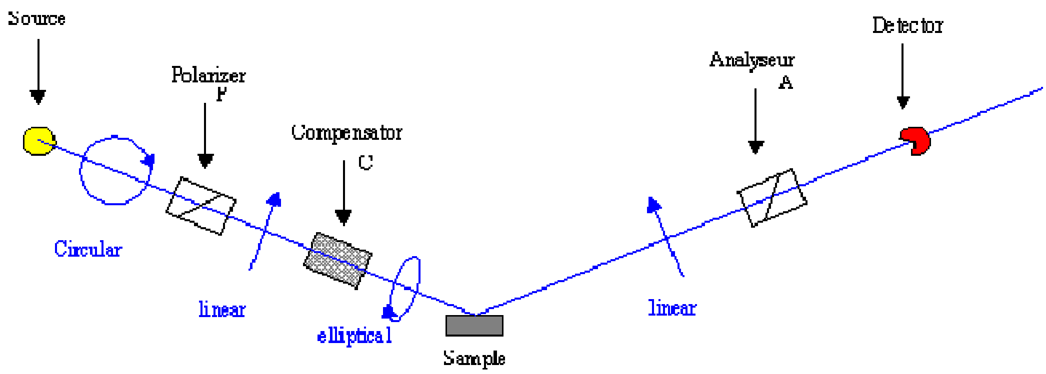
Different measurement techniques of the polarization after reflection exist. Their all use the same optical components: a source, a polarizer, an analyzer and a detector. At these basic elements different other components like modulators or compensators can be added.

Extinction Method

The method uses the extinction of the signal to make an angular measurement. The optical setup is constituted by a monochromatic source (laser or lamp + spectrograph), a polarizer, a compensator (a quarter wavelength plate for example), an analyzer and a photomultiplier tube. The polarization is linear after the polarizer. It is elliptical after the compensator which is orientated to obtain a linear polarization after reflection on the sample. The analyzer is then orientated to extinguish the beam. The orientation of the polarizer **P**, of the compensator **C** and of the analyzer **A** allow to obtain the ellipsometric parameters of the sample from:

$$\tan\psi \exp(j\Delta) = -\tan A * \frac{\tan C - \tan(P-C)}{1 + j\tan C \tan(P-C)}$$

This method is long even if it is automatic and its precision depends directly on the noise of the detector since it is working at the minimum of the signal in any case. It is finally difficult to apply for spectroscopic measurements.



Modulation by a rotating element

Rotating element methods are generally easy to automate and can be used on a large spectral range. The light beam can be modulated by the rotation of the polarizer, of the analyzer or of a compensator.

Rotating polarizer technique

A source with well known polarization state is needed. After reflection on the sample, the analyzer is fixed. So, it is not necessary to have a detector insensitive to the polarization and the spectrometer can be located between the analyzer and the detector. The parasitic light is suppressed with this kind of configuration.

Rotating analyzer technique

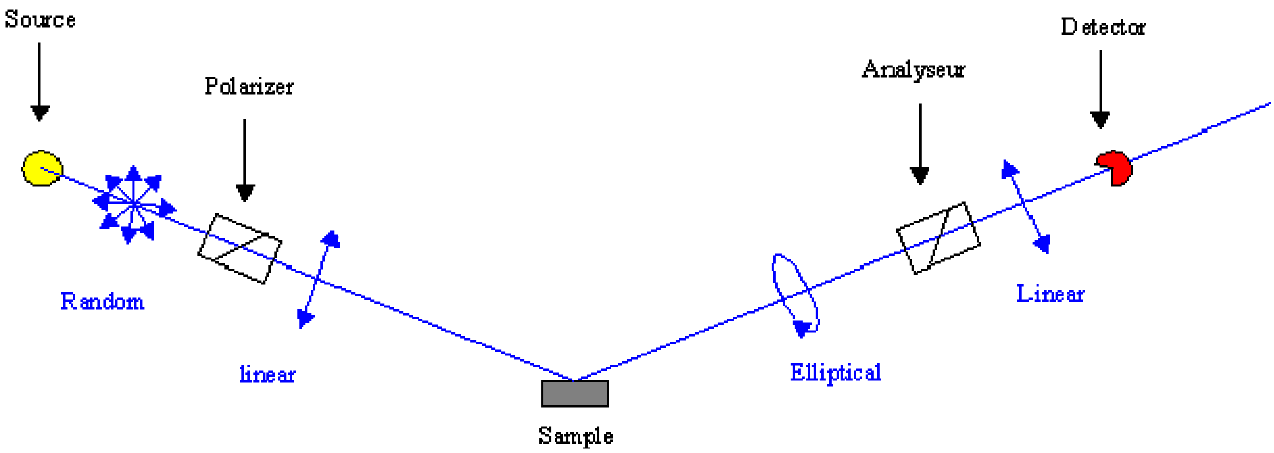
In this case, the detector must be insensitive to the polarization. So the spectrometer must be located between the source and the polarizer. The system is then more sensitive to the parasitic light.

Rotating compensator technique

Polarization problems at the source and detector levels can be suppressed with this kind of ellipsometer but the spectral calibration of the compensator is difficult and always source of systematic errors on the measurements.

Phase modulation

In this case, the optical setup is the same than previously but includes a modulator after the polarizer. The main advantages are the poor sensitivity to the polarization of the source and detector, speed of modulation and the easier adjustment. The main disadvantage is the necessity to calibrate the modulator versus the wavelength and temperature and to adjust the modulation at each wavelength for optimum sensitivity. The fast speed of modulation is then counter balanced by the need to adapt at each wavelength the modulation, setting then the measurement time by the mechanical speed of the spectrometer (the slowest component). This makes in any case this set up not compatible with CCD technology.



SOPRA choice

At SOPRA the rotating polarizer configuration has been selected for its intrinsic advantages (simplicity and suppression of parasitic light). The standard setup has been improved using an optical fiber to introduce the light in the spectrometer (patented system by SOPRA). In addition to an easier setup of the system (the spectrometer can be far from the analyzer arm), the light beam is more stable at the entrance of the spectrometer. For the R&D instruments the polarization of the source is taken into account by calibration.

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Theory of the rotating polarizer technique

The field amplitude is splitted into the S and P components perpendicular and parallel to the plane of incidence respectively. The effect of each element is represented by a complex matrix:

- Polarizer or analyzer:

$$Pol = Ana = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

- Sample:

$$E = \begin{pmatrix} r_p & 0 \\ 0 & r_s \end{pmatrix}$$

- Theta angle rotation:

$$R(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

- Lamp:

$$L = \begin{pmatrix} E_0 \\ E_0 \end{pmatrix}$$

On the detector the field amplitude is the following:

$$E_d = Ana * R(A) * E * R(-P) * Pol * L$$

Finally the intensity **I** seen by the detector can be expressed by:

$$I = I_0\left(\alpha * \cos 2P + \beta * \sin 2P + 1\right)$$

with:

$$\alpha = \frac{\tan^2\psi - \tan^2 A}{\tan^2\psi + \tan^2 A} \qquad \beta = 2 * \cos\Delta * \frac{\tan\psi * \tan A}{\tan^2\psi + \tan^2 A} \qquad I_0 = \frac{|r_s|^2 |E_0|^2}{2} * \frac{\cos^2 A}{\tan^2\psi + \tan^2 A}$$

The coefficients alpha and beta do not depend on the intensity of the lamp so that there is no need of reference measurement for the intensity. The ellipsometric parameters can be expressed versus alpha, beta and A

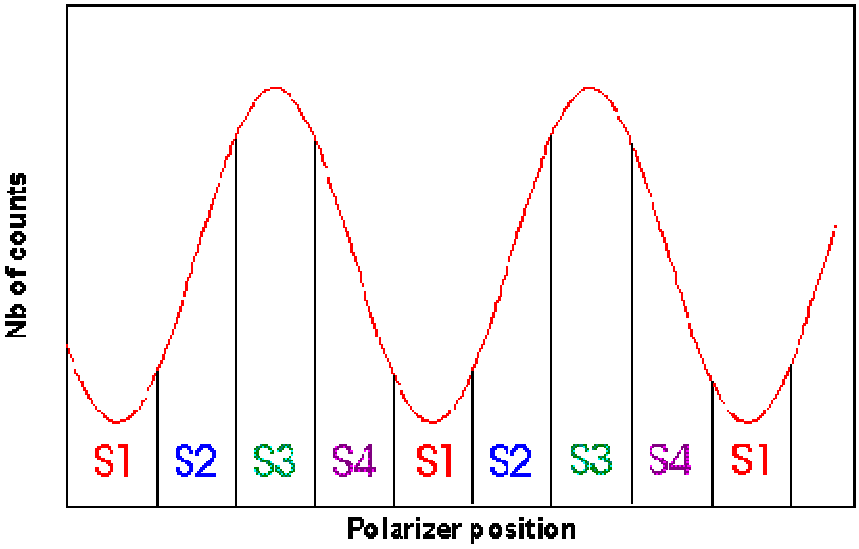
$$\tan\psi = \sqrt{\frac{1+\alpha}{1-\alpha}} \tan A \qquad \cos\Delta = \frac{\beta}{\sqrt{1-\alpha^2}}$$

SIGNAL TREATMENT

To analyze the signal and extract the two components at the double frequency **2P** of rotation of the polarizer, we use the Hadamard method. The signal is integrated every quarter of period. Each sum can be calculated following:

$$S_1 = \int_0^{\pi/4} I(P)dP = \frac{I_0}{2}(\alpha + \beta + \pi/2) \qquad S_3 = \int_{\pi/2}^{3\pi/4} I(P)dP = \frac{I_0}{2}(-\alpha - \beta - \pi/2)$$

$$S_2 = \int_{\pi/4}^{\pi/2} I(P)dP = \frac{I_0}{2}(-\alpha + \beta + \pi/2) \qquad S_4 = \int_{3\pi/2}^{\pi} I(P)dP = \frac{I_0}{2}(\alpha - \beta + \pi/2)$$



The parameters of the signal can then be expressed versus the sums following:

$$\alpha = \frac{1}{2I_0}(S_1 - S_2 - S_3 + S_4) \qquad \beta = \frac{1}{2I_0}(S_1 + S_2 - S_3 - S_4) \qquad I_0 = \frac{1}{\pi}(S_1 + S_2 + S_3 + S_4)$$

In practice the signal integration is realized by counting pulses generated by a photomultiplier tube used in photon counting mode (or another detector). This method allows to suppress the **4P** components and **P** (summing the sums of the first half turn of polarizer with the second half turn).

On the SOPRA's instrument the possibility is given to use 8 counters by half turn of polarizer instead of 4. In this case the **4P** components can be deduced and used to correct the non linearity of the detector.

CALIBRATION AND MEASUREMENT

As reported in the Signal treatment method, a precise measurement of the position of the incidence plane is necessary to deduce precisely the position of the analyzer **A**. In the case of the rotating polarizer instrument, this procedure is easy using for example the technique of the residual minimum.

The light beam polarization is linear after the polarizer. After reflection on the sample surface, the polarization of the reflected beam is only linear in two cases: when the axis of the polarizer is in the incidence plane and when this axis is perpendicular to the plane of incidence. It is sufficient then to put the analyzer perpendicular to these orientations to reduce to zero the intensity of the signal during the rotation of the polarizer.

The signal minimum can be expressed following:

$$I_{min} = I_0\left(1 - \sqrt{\alpha^2 + \beta^2}\right)$$

The residual parameter **R** is defined by:

$$R = 1 - \alpha^2 - \beta^2$$

Its intensity is zero when the analyzer is aligned with the incidence plane. In practice different measurements are made at different analyzer positions around zero. The position of the incidence plane is determined by the minimum of the residual parameter.

During the measurement it is better to maximize the signal/noise ratio and then to decrease the sinusoidal contribution compared to the constant contribution of the signal adjusting the analyzer position **A**..

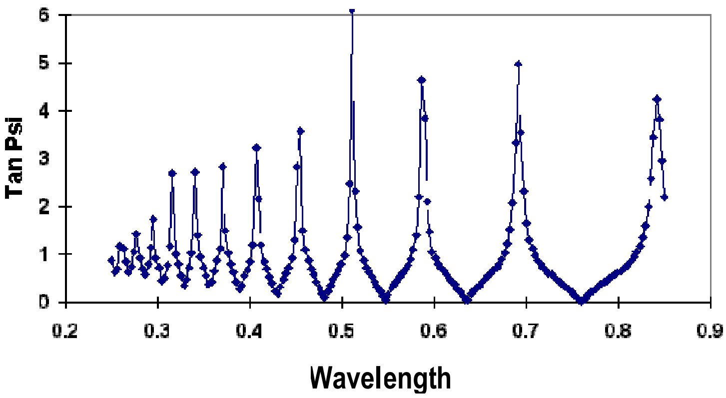
The derivative of the sinusoidal contribution versus **A** is given by:

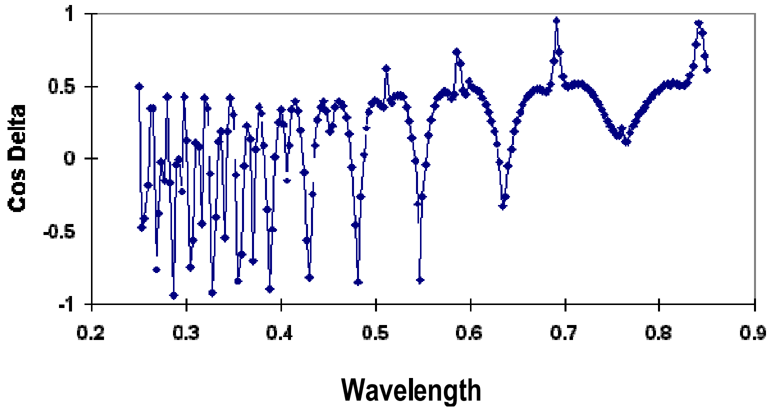
$$\frac{\partial(\alpha^2 + \beta^2)}{\partial A} = (\tan^2 A - \tan^2 \psi)(4 - 2\cos^2 \Delta)$$

This derivative is zero for:

$$\tan^2 A = \tan^2 \psi$$

It will be then better to work with the analyzer position around the Psi value (tracking method).





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ANALYSIS

Ellipsometry is not a direct deductive method except in one simple case: the case of a bulk material. It is generally necessary to build a priori multilayers models to extract physical informations after numerical adjustment.

Case of a substrate

In the ideal case of a substrate without native oxide and surface roughness the ellipsometric parameters depend only on the angle of incidence and on the indices of the substrate.
The following expression can be obtained:

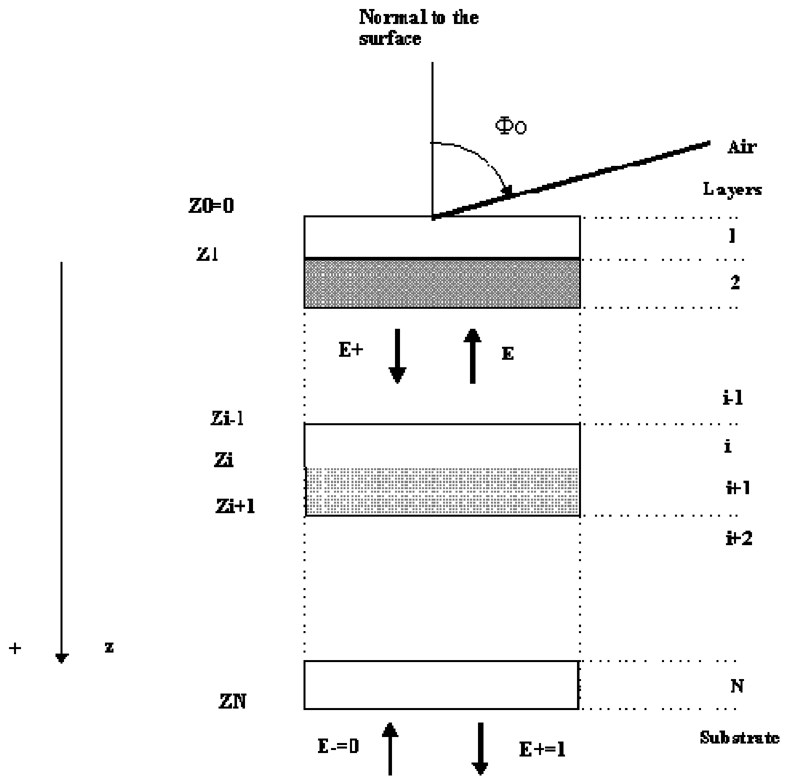
$$\frac{n_1 + jk_1}{n_0} = \sin\Phi_0 \sqrt{1 + \left(\frac{1-\rho}{1+\rho}\right)^2 \tan^2 \Phi_0}$$

where:

- $n_1 + jk_1$ is the optical index of the substrate.
- n_0 is the optical index of the media in which we make measurement (usually void = 1).
- Φ_0 is the angle of incidence

General case of a multilayers structure

One method to calculate the reflectance of a complex multilayers structure is reported below:



We define the field amplitude E+ and E- of the wave propagating in the positive and in the negative direction respectively.

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At the depth z, the field is represented by the vector:

$$\begin{bmatrix} E^+ \\ E^- \end{bmatrix}$$

The field continuity at the interface between the layer i and the layer i+1 is represented by:

$$\begin{bmatrix} E^+(z_i^-) \\ E^-(z_i^-) \end{bmatrix} = I_i \begin{bmatrix} E^+(z_i^+) \\ E^-(z_i^+) \end{bmatrix} = \frac{1}{t_{i,i+1}} \begin{bmatrix} 1 & r_{i,i+1} \\ r_{i,i+1} & 1 \end{bmatrix} \begin{bmatrix} E^+(z_i^+) \\ E^-(z_i^+) \end{bmatrix}$$

where:

E(zi-) is the value of the electric field in the layer i at the interface with the layer i+1.
E(zi+) is the value of the electric field in the layer i+1 at the interface with the layer i.
ri,i+1 and ti,i+1 and the reflection and transmission coefficients at the interface between layer i and i+1.
Propagation across one layer is represented by a transfer matrix Li following:

$$\begin{bmatrix} E^+(z_{i-1}^+) \\ E^-(z_{i-1}^+) \end{bmatrix} = L_i \begin{bmatrix} E^+(z_i^+) \\ E^-(z_i^+) \end{bmatrix} = \begin{bmatrix} \exp j\beta_i & 0 \\ 0 & \exp - j\beta_i \end{bmatrix} \begin{bmatrix} E^+(z_i^+) \\ E^-(z_i^+) \end{bmatrix}$$

where:

$$\beta_i = \frac{2\pi}{\lambda} d_i (n_i + jk_i) \cos\Phi_i$$

The angle phi is deduced from the Snell-Descartes relation. At the surface the expression of the field amplitudes is finally expressed by an iterative formula:

$$\begin{bmatrix} E^+(z_0^+) \\ E^-(z_0^+) \end{bmatrix} = I_0 L_1 I_1 \ldots I_{N-1} L_N \begin{bmatrix} E^+(z_N^+) \\ E^-(z_N^+) \end{bmatrix}$$

At the interface between substrate and layer N, we assume that E+=1 and E-=0. Finally the reflection coefficients are obtained making the amplitude ratio of the incident and reflected waves.

$$r_p = \frac{E_p^-(z_0^-)}{E_p^+(z_0^-)} \qquad r_s = \frac{E_s^-(z_0^-)}{E_s^+(z_0^-)}$$