Outline of the ellipsometry of thin layers using the Picometer Ellipsometer

Ellipsometry determines the complex ratio r of the amplitude reflectivities for p and s polarised electromagnetic waves:

$$r = r_p / r_s = r_r + i r_i = \tan\Psi\, e^{i\Delta} = \rho\, e^{i\Delta}$$

We assume here that the reflection takes place at an interface characterised just by the amplitude reflection coefficients r_s and r_p. This covers the situations of reflection from isotropic layers on isotropic substrates, and uniaxial layers with optic axis normal to the surface on isotropic substrates.

When the substrate is a transparent dielectric, then in principle r is real for all angles of incidence, varying between 1 at normal incidence $\theta = 0°$, to –1 at grazing incidence $\theta = 90°$. At the Brewster angle θ_B the value of r passes through zero. In practice most bare substrates have small values of r_i at θ_B, associated with departures from the ideal dielectric constant step function at the interface. Typical values are usually in the range 1 to 5 x 10^{-3} . Absorbing substrates have complex refractive indices, and these generate larger ellipticities at the Brewster angle. Metals are the extreme case, with $r_i \sim 1$ at θ_B.

When a thin layer is formed on a substrate then all the changes made to both r_p and r_s are to first order functions of the one variable η, given by

$$\eta = \int \mathrm{d}z\,(\varepsilon - \varepsilon_1)(\varepsilon - \varepsilon_2)/\varepsilon$$

where ε_1, ε_2, and ε are the dielectric constants of the incident, reflecting and layer media, respectively. If any of the media are absorbing, then η becomes a complex function. In the case of uniaxial surface anisotropy the expression for η becomes

$$\eta = \int \mathrm{d}z\left\{\varepsilon_x + \varepsilon_1\varepsilon_2/\varepsilon_z - (\varepsilon_1 + \varepsilon_2)\right\}$$

with ε_x and ε_z being the dielectric constant components of the layer in the x (normal to the plane of incidence) and z (normal to the surface) directions.

Note that in these expressions the first order change results from the integrated surface profile function, and does not require the assumption of a well-formed layer. If ε is near say ε_2 then alternative forms for η are

$$\eta = (\varepsilon_2 - \varepsilon_1)\Gamma_\varepsilon/\varepsilon_2 \text{ and } \eta = \Gamma_a + \eta(\varepsilon_z).$$

In the first function Γ_ε is the *dielectric constant excess*, $\Gamma_\varepsilon = \int \mathrm{d}z(\varepsilon - \varepsilon_2)$, while in the second function Γ_a is the *anisotropy excess* $\Gamma_a = \int \mathrm{d}z(\varepsilon_x - \varepsilon_z)$, and $\eta(\varepsilon_z)$ is the ε_z *excess*.

Model calculations using the unifom layer equations show that in practice first order linearity as a function of η extends as a function of layer thickness up to several hundred Ångstroms. It should then also be appreciated that within this range the data does not contain more information than obtained in this function η. In other words, it is not possible to separately determine an effective layer thickness and value for its dielectric constant, as it is possible to do for thicker layers beyond the first order approximation.

When the substrate and layer are transparent, then the simplest measurement is to determine η by a measurement of r_i at the Brewster angle. Then

$$r_r = 0$$

$$r_i = (\pi/\lambda)\left\{(\varepsilon_1 + \varepsilon_2)^{1/2}/(\varepsilon_1 - \varepsilon_2)\right\}\eta$$

In practice weakly absorbing materials such as silicon act effectively as transparent dielectrics, having only a small value of r_i at θ_B. In addition, thin oxide layers on the surface of silicon add to the background value for r_i at the Brewster angle. Changes in r_i due to a layer are still given by the function above.

When the substrate is a highly reflecting metal then $r_i \sim 1$ at θ_B. Thin layers cause r_r to be linear in layer thickness up to about 100 Å. Again the complete layer equation can be used to take into account nonlinearities.

The Birefringence Modulator

To measure r, the polarisation a probe beam of light is analysed after it is reflected by the sample. For this, the polarisation is modulated either by a rotating polariser or, as in the Picometer Ellipsometer, by a photoelastic Birefringence Modulator. An isotropic glass slab (which can be fused silica for operation in the UV) of thickness d (typically 1 cm) is set into longitudinal oscillation at its resonance frequency ω where the wavelength of vibration is $2L$, with L the length of the slab. The periodic uniaxial strain $\delta(\omega)$ which is produced in the center of the slab gives a periodic change in the refractive index for light polarised parallel to the

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oscillation direction, and this leads to a periodic variation $\Delta n(\omega)$ in the refractive index difference for light polarised parallel and perpendicular to the oscillation direction given by

$$\Delta n(\delta,\omega) = \alpha\delta(\omega)$$

with α the piezo-optic constant. This strain-induced birefringence results in a periodic change of the optical phase shift along the direction of oscillation, given by

$$\Phi(\omega) = 2\pi\Delta nd/\lambda = \Phi_0 \sin(\varpi t)$$

where λ is the wavelength of the light.

Optical Arrangement

Jasperson and Schnatterley first used the Birefringence Modulator ellipsometer configuration in association with their studies of optical properties of solids. Subsequently Beaglehole found that configuration A (below) was ideal for the study of liquid surfaces, and in that form the Birefringence Modulator ellipsometer is now finding extensive use, due to its high sensitivity, stability and ease of use. The BME has three components, Polariser P, Birefringence modulator BM placed before the sample, and Analyser.

Configuration A:

The incident Polariser is oriented at 45° to provide equal s and p amplitudes. The BM is oriented with the oscillation axis in the p direction. The Analyser is oriented parallel or perpendicular to the Polariser. The intensity varies as

$$I = I_0\rho s^2\left\{1+\rho^2 \pm 2\rho\cos(\Delta-\Phi)\right\}$$

The plus and minus signs $\pm$ refer to the two directions of the Analyser, and $\Phi = \Phi_0 \sin(\omega t)$ is the strain-induced birefringence.

Configuration B:

The BM is oriented parallel to the Polariser

The intensity varies as

$$I = I_0\rho s^2\left\{1+\rho^2 \pm \left(1-\rho^2\right)\cos(\Phi)\right\}$$

The signals detected by amplifiers at frequency ω and 2ω normalised by the zero frequency signal are

Configuration A:

$$\omega/dc = \pm 4J_1(\Phi_0)r_i \Big/ \left\{1+\rho^2 \pm 2J_0(\Phi_0)\rho\cos\Delta\right\}$$

$$2\omega/dc = \pm 4J_2(\Phi_0)r_r \Big/ \left\{1+\rho^2 \pm 2J_0(\Phi_0)\rho\cos\Delta\right\}$$

Configuration B:

$$2\omega/dc = \pm 2J_2(\Phi_0)\left(1-\rho^2\right) \Big/ \left\{1+\rho^2 \pm J_0(\Phi_0)\left(1-\rho^2\right)\right\}$$

These expressions look complicated, but simplify in practice.

(i) $J_0(\phi_0)$, $J_1(\phi_0)$ and $J_2(\phi_0)$ are the standard Bessel functions. If ϕ_0 is adjusted to about 2.4 radians then J_0 is zero, and J_1 and J_2 are not far from their maximal values.

(ii) Configuration A: Near the Brewster angle for transparent substrates ρ is small; for metal substates $\rho \sim 1$, but $\rho\cos\Delta$ is small.

Optical Calibration

The ellipsometer needs to be calibrated to eliminate the unkown gain factors of its electronic subsystems. In direct transmission, $\rho = 1$ and $\Delta = 0$. Then the $2\omega/dc$ signal ratio equals $J_2(\phi_0)$. With a quarter wave plate inserted in the optical beam with its fast axis in the p direction, $\Delta = 90°$ and the ω/dc signal ratio equals $J_1(\phi_0)$. The gain factors and any stray birefringence can be determined from measurements at these standard conditions.

Electronics

The ω and the 2ω signals should be extracted from the detector using lock-in amplifiers, while the dc signal is directly available at the detector output. Each of these varies in proportion to the incident intensity level, and is subject to light source fluctuations as well as sample changes. The former are removed if the ratio of these is taken continuously, for instance with a ratio amplifier or computer. Alternatively, a voltage-controlled amplifer can be put in the signal channel, and its gain varied to maintain a constant dc signal level. If the detector is a photomultiplier, a very convenient method is to use a feedback loop that adjusts the photomultiplier high voltage to keep the dc output current level constant.

References

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