Equations in Spectroscopic Ellipsometry

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Ellipsometry measures the two values $(\psi, \triangle)$. These represent the amplitude ratio ψ and phase difference $\triangle$ between light waves known as p- and s-polarized light waves. In spectroscopic ellipsometry, $(\psi, \triangle)$ spectra are measured by changing the wavelength of light. In general, the spectroscopic ellipsometry measurement is carried out in the ultraviolet/visible region, but measurement in the infrared region has also been performed widely. There are two general restrictions on the ellipsometry measurement; specifically: (1) surface roughness of samples has to be rather small, and (2) the measurement must be performed at oblique incidence.

1 Maxwell equations and boundary conditions

$$\begin{aligned}
&\nabla \times \boldsymbol{H} = \boldsymbol{J} + \frac{\partial \boldsymbol{D}}{\partial t} \\
&\nabla \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t} \\
&\nabla \cdot \boldsymbol{D} = \rho \\
&\nabla \cdot \boldsymbol{B} = 0
\end{aligned} \tag{1}$$

Differential equations in SI. ρ is charge density. There are

$$\begin{aligned}
&\boldsymbol{D} = \epsilon \boldsymbol{D} \\
&\boldsymbol{B} = \mu \boldsymbol{H} \\
&\boldsymbol{J} = \sigma \boldsymbol{E}
\end{aligned} \tag{2}$$

Boundary conditions are

$$\begin{aligned}
&\boldsymbol{e_n} \times (\boldsymbol{E_t} - \boldsymbol{E_i}) = 0 \\
&\boldsymbol{e_n} \times (\boldsymbol{H_t} - \boldsymbol{H_i}) = \boldsymbol{\alpha} \\
&\boldsymbol{e_n} \cdot (\boldsymbol{D_t} - \boldsymbol{D_i}) = \sigma \\
&\boldsymbol{e_n} \cdot (\boldsymbol{B_t} - \boldsymbol{B_i}) = 0
\end{aligned} \tag{3}$$

2 Refraction of light

When light is reflected or transmitted by samples at oblique incidence, the light is classified into p- and s-polarized light waves depending on the oscillatory direction of its electric field and each light wave shows quite different behavior. In p-polarization, the electric fields of incident and reflected light waves oscillate within the same plane. This particular plane is called the plane of incidence. The boundary conditions for electromagnetic waves require that E and B components parallel to an interface are continuous at the interface. In other words, the parallel components on the incident side must be equal to that on the transmission side.

In Fig.1, there are

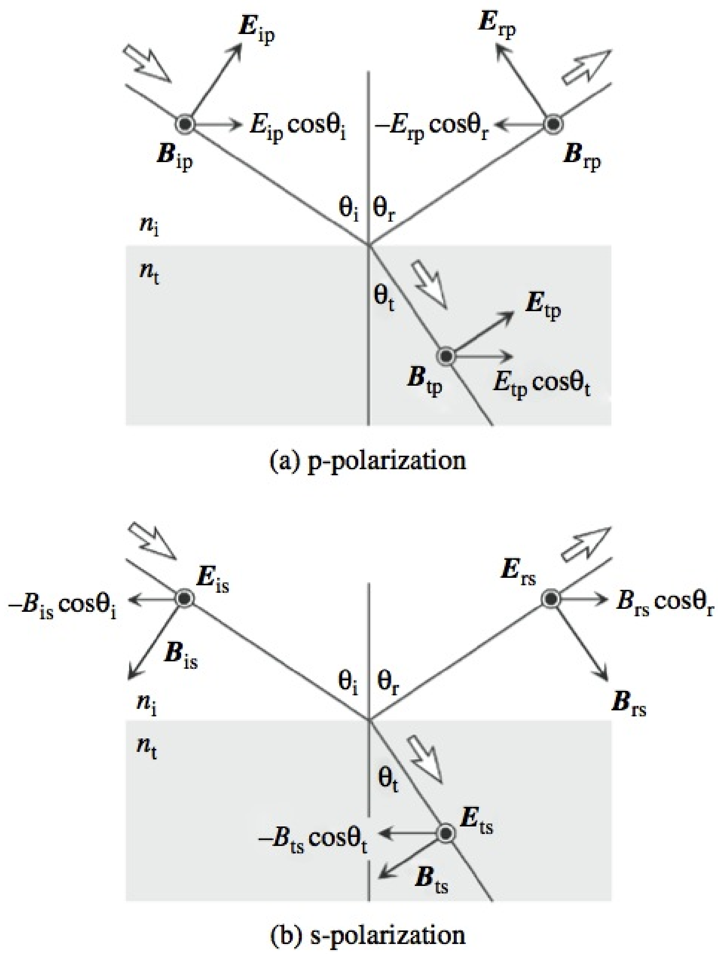

Figure 1: Electric field $\boldsymbol{E}$ and magnetic induction $\boldsymbol{B}$ for (a) p-polarization and (b) s-polarization.

$$\begin{aligned} &\theta_i = \theta_r \\ &n_i sin\theta_i = n_t sin\theta_t \\ &E = \frac{c}{n} B \end{aligned} \tag{4}$$

For case of p-polarized light, the boundary conditions are

$$\begin{aligned} &E_{ip} cos\theta_i - E_{rp} cos\theta_r = E_{tp} cos\theta_t \\ &B_{ip} + B_{rp} = B_{tp} \end{aligned} \tag{5}$$

we obtain the amplitude reflection coefficient and transmission coefficient for p-polarized light

$$\begin{aligned} r_p &= \frac{E_{rp}}{E_{ip}} = \frac{n_t cos\theta_i - n_i cos\theta_t}{n_t cos\theta_i + n_i cos\theta_t} \\ t_p &= \frac{E_{tp}}{E_{ip}} = \frac{2 n_i cos\theta_i}{n_t cos\theta_i + n_i cos\theta_t} \end{aligned} \tag{6}$$

On the other hand, the boundary conditions for s-polarized light are given by

$$\begin{aligned} &B_{is} cos\theta_i - B_{rs} cos\theta_r = B_{ts} cos\theta_t \\ &E_{is} + E_{rs} = E_{ts} \end{aligned} \tag{7}$$

we obtain the amplitude reflection coefficient and transmission coefficient for s-polarized light

$$\begin{aligned} r_s &= \frac{E_{rs}}{E_{is}} = \frac{n_i cos\theta_i - n_t cos\theta_t}{n_i cos\theta_i + n_t cos\theta_t} \\ t_s &= \frac{E_{ts}}{E_{is}} = \frac{2n_i cos\theta_i}{n_i cos\theta_i + n_t cos\theta_t} \end{aligned} \tag{8}$$

amplitude coefficients are expressed by

$$\begin{aligned} r_p &= |r_p|exp(i\delta_{rp}) \qquad r_s = |r_s|exp(i\delta_{rs}) \\ t_p &= |t_p|exp(i\delta_{rp}) \qquad t_s = |t_s|exp(i\delta_{rs}) \end{aligned} \tag{9}$$

The reflectance R obtained in conventional measurements is defined by the ratio of reflected light intensity Ir to incident light intensity I_i, $R = I_r/I_i$. The reflectances for p- and s-polarized waves are expressed by

$$R_p = \frac{I_{rp}}{I_{ip}} = |\frac{E_{rp}}{E_{ip}}|^2 = |r_p|^2, \quad R_s = \frac{I_{rs}}{I_{is}} = |\frac{E_{rs}}{E_{is}}|^2 = |r_s|^2 \tag{10}$$

3 Krammers-Kronig relation

The refraction index $N_{complex}$ can be expressed as $N_{complex}(\omega) = \sqrt{\mu(\omega)\epsilon(\omega)}$, for non-magnetic materials, we can take $\mu = 1$. Thus, there is

$$N_{complex}(\omega) = \sqrt{\epsilon(\omega)} = n + ik \tag{11}$$

the relation between complex dielectic and complex refraction index can be expressed as

$$\begin{aligned} \epsilon_{complex} &= \epsilon_1 + \epsilon_2 = (n + ik)^2 \\ \epsilon_1 &= n^2 - k^2 \\ \epsilon_2 &= 2nk \end{aligned} \tag{12}$$

If choose $\theta_i = \theta_t = 0$ in Eq.(7) or (8), the expression of reflection coefficient becomes

$$r = \sqrt{R}exp(i\phi) = \frac{1 - N_{complex}}{1 + N_{complex}} = \frac{1 - n - ik}{1 + n + ik} \tag{13}$$

From here, the refractive index n abd extinction coefficient k can be extract from reflectivity

$$\begin{aligned} n &= \frac{1 - R}{1 + R - 2\sqrt{Rcos\phi}} \\ k &= \frac{2Rsin\phi}{1 + R - 2\sqrt{Rcos\phi}} \end{aligned} \tag{14}$$

Kramers-Kronig relation Let $\chi(\omega) = \chi_1(\omega) + i\chi_2(\omega)$ be a complex function of the complex variable ω, where $\chi_1(\omega)$ and $\chi_2(\omega)$ are real. Suppose this function is analytic in the closed upper half-plane of ω and vanishes like $1/|\omega|$ or faster as $|\omega| \to \infty$. Slightly weaker conditions are also possible. The KramersKronig relations are given by application of Cauchy's residue theorem.

$$\begin{aligned} \chi_1(\omega) &= \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} \frac{\chi_2(\omega')}{\omega' - \omega} d\omega' \\ \chi_2(\omega) &= -\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} \frac{\chi_1(\omega')}{\omega' - \omega} d\omega' \end{aligned} \tag{15}$$

where $\mathcal{P}$ denotes the Cauchy principal value. So the real and imaginary parts of such a function are not independent, and the full function can be reconstructed given just one of its parts.

While, $\chi_1(\omega)$ is even and $\chi_2(\omega)$ is odd. If we now multiply the integrand by $(\omega+\omega_0)/(\omega+\omega_0)$ and make use of the even- and oddness of the integrands, we get:

$$\begin{aligned}\chi_1(\omega) &= \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty}\frac{\chi_2(\omega^{'})(\omega^{'}+\omega)}{(\omega^{'})^2-\omega^2}d\omega^{'} = \frac{2}{\pi}\mathcal{P}\int_{0}^{\infty}\frac{\chi_2(\omega^{'})\omega^{'}}{(\omega^{'})^2-\omega^2}d\omega^{'} \\ \chi_2(\omega) &= -\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty}\frac{\chi_1(\omega^{'})(\omega^{'}+\omega)}{(\omega^{'})^2-\omega^2}d\omega^{'} = -\frac{2}{\pi}\mathcal{P}\int_{0}^{\infty}\frac{\chi_2(\omega^{'})\omega}{(\omega^{'})^2-\omega^2}d\omega^{'}\end{aligned} \tag{16}$$

In this case, we have

$$r(\omega) = \sqrt{R(\omega)}exp(i\phi(\omega)) \tag{17}$$

let $lnr(\omega) = \chi(\omega)$, $\frac{1}{2}lnR(\omega) = \chi_1(\omega)$, $\phi(\omega) = \chi_2(\omega)$, we can get

$$\phi(\omega) = -\frac{\omega}{\pi}\mathcal{P}\int_{-\infty}^{\infty}\frac{lnR(\omega^{'})}{(\omega^{'})^2-\omega^2}d\omega^{'} + \phi(0) \tag{18}$$

Like R and ϕ, ϵ_1 and ϵ_2 are also related through the Kramers-Kronig relation according to

$$\begin{aligned}\epsilon_1(\omega) - 1 &= \frac{2}{\pi}\mathcal{P}\int_{0}^{\infty}\frac{\epsilon_2(\omega^{'})\omega^{'}}{(\omega^{'})^2-\omega^2}d\omega^{'} \\ \epsilon_2(\omega) &= -\frac{2\omega}{\pi}\mathcal{P}\int_{0}^{\infty}\frac{\epsilon_2(\omega^{'})}{(\omega^{'})^2-\omega^2}d\omega^{'} + \frac{4\pi\sigma_{DC}}{\omega}\end{aligned} \tag{19}$$

4 Analysis of multilayered materials

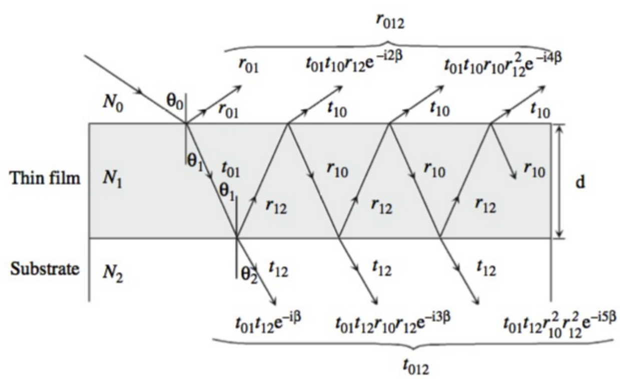

Figure 2: Optical model for an ambient/thin film/substrate structure.

If the material is composed of several layers, things become more complicate. Took a two-layer material as an example. the phase variation caused by the difference in the optical pass length is given by $exp(i2\delta)$. Where $\delta = \frac{2\pi d_i}{\lambda}n_i cos\theta_i$

The amplitude reflection coefficient for the ambient/thin film/substrate structure is expressed from the sum of all the reflected waves:

$$
\begin{aligned}
r_{012} &= r_{01} + t_{01}t_{10}r_{12}exp(i2\delta) + t_{01}t_{10}r_{10}r_{12}^2exp(i4\delta)... \\
&= r_{01} + \frac{t_{01}t_{10}r_{12}exp(i2\delta)}{1 - r_{10}r_{12}exp(i2\delta)} \\
&= r_{01} + \frac{(1 - r_{01}^2))r_{12}exp(i2\delta)}{1 + r_{01}r_{12}exp(i2\delta)} \\
&= \frac{r_{01} + r_{12}exp(i2\delta)}{1 + r_{01}r_{12}exp(i2\delta)}
\end{aligned} \tag{20}
$$

We can do the same thing when there are more layers.

5 Measured values in ellipsometry

The $(\psi, \triangle)$ measured from ellipsometry are defined from the ratio of the amplitude reflection coefficients for p- and s-polarizations:

$$
\rho = tan\psi exp(i\triangle) = \frac{r_p}{r_s} \tag{21}
$$

$$
\psi = arctan(\frac{|r_p|}{|r_s|}) = arctan[(\frac{R_p}{R_s})^{\frac{1}{2}}] \tag{22}
$$

$$
\triangle = arg(\rho) = \begin{cases} arctan(Im(\rho)/Re(\rho)), \ \ when \ Re(\rho) > 0, \\ arctan(Im(\rho)/Re(\rho)) + \pi, \ \ when \ Re(\rho) < 0, \ Im(\rho) > 0 \\ arctan(Im(\rho)/Re(\rho)) - \pi, \ \ when \ Re(\rho) < 0, \ Im(\rho) < 0 \end{cases} \tag{23}
$$