6.1.2. Experimental Determination of Optical Functions

Reflection

In oblique incidence techniques, the reflectance of the s- and p-polarized components of the incident light, $\mathcal{R}_s$ and $\mathcal{R}_p$ (perpendicular and parallel to the plane of incidence) obey the Fresnel formulae

$$\mathcal{R}_s = |r_s|^2 = \left|\frac{\cos\phi - (\tilde{n}^2 - \sin^2\phi)^{1/2}}{\cos\phi + (\tilde{n}^2 - \sin^2\phi)^{1/2}}\right|^2 \qquad (6.12a)$$

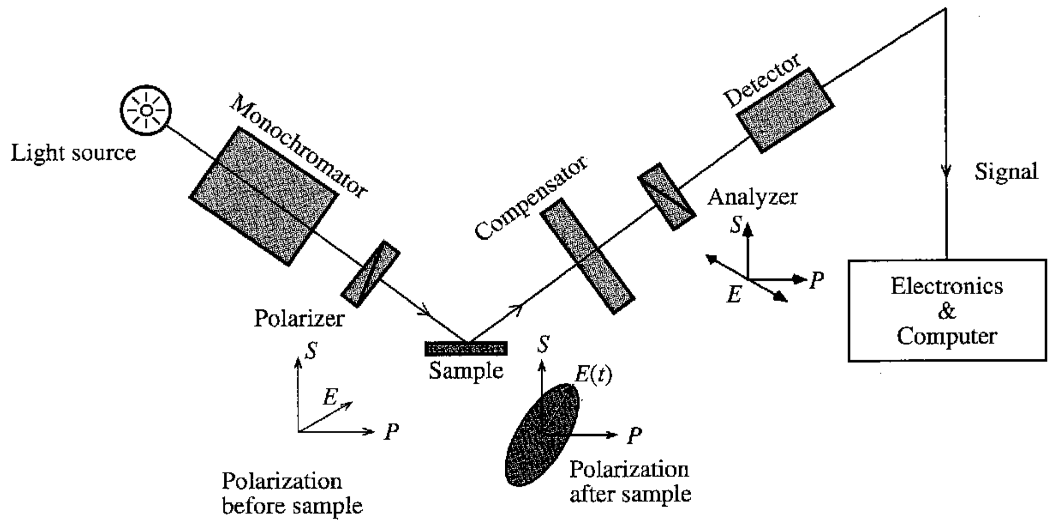
and

$$\mathcal{R}_p = |r_p|^2 = \left|\frac{\tilde{n}^2\cos\phi - (\tilde{n}^2 - \sin^2\phi)^{1/2}}{\tilde{n}^2\cos\phi + (\tilde{n}^2 - \sin^2\phi)^{1/2}}\right|^2 \qquad (6.12b)$$

where r_s and r_p are the corresponding complex reflectivities.

Ellipsometry

is an oblique angle of incidence technique, where the ratio of the *complex reflectivities* $\sigma = r_s / r_p$ is measured.



It can be shown that the complex dielectric function is

$$\varepsilon = \sin^2\phi + \sin^2\phi \sin^2\phi \, ((1 - \sigma) / (1 + \sigma))^2, \qquad (6.13)$$

expressed in terms of the incident angle ϕ and σ.

Ellipsometry over a wide range of photon frequencies is called as *spectroscopic ellipsometry.*

6.1.3. Kramers–Kronig Relations

Equivalent information is of the optical properties of material is represented by

Determining one of these functions allows one to evaluate the others.

If *linear optical response* can be assumed, it can be shown that the response function $\varepsilon = \varepsilon_r(\omega) + i\varepsilon_i(\omega)$ (or χ) satisfies the Kramers–Kronig relations

$$\varepsilon_r(\omega) = 1 + \frac{2}{\pi}\,\mathcal{P}\int_0^\infty \frac{\omega'\,\varepsilon_i(\omega')}{\omega'^2 - \omega^2}\,d\omega' \qquad (6.14)$$

and

$$\varepsilon_i(\omega) = -\frac{2\omega}{\pi}\,\mathcal{P}\int_0^\infty \frac{\varepsilon_r(\omega') - 1}{\omega'^2 - \omega^2}\,d\omega' \qquad (6.15)$$

where $\mathcal{P}$ indicates the (Cauchy) principal value of the integral:

$$\mathcal{P}\int_{-\infty}^{\infty} f(x)\,dx = \lim_{\delta \to \infty} \left\{ \int_{-\infty}^{x_0 - \delta} f(x)\,dx + \int_{x_0 - \delta}^{\infty} f(x)\,dx \right\}$$

Proof of the KKR relations is based on the principle of causality.

In order the KKR relations to be applicable $\varepsilon_r(\omega) - 1$ and $\varepsilon_i(\omega)$ should be analytic and rapidly vanishing. As this is true for the complex refractive index $\tilde{n}$, the KKR relations can be derived for $\tilde{n}$, resulting in (6.14) and (6.15) with $\varepsilon_r(\omega)$ and $\varepsilon_i(\omega)$ replaced by $n(\omega)$ and $\kappa(\omega)$, respectively.

To obtain optical response functions from the normal incidence reflection measurements consider the *complex reflectivity*

$$\tilde{r} = (\tilde{n} - 1) / (\tilde{n} + 1) = \rho\, e^{i\theta}. \qquad (6.16)$$

The reflection coefficient or reflectance is

$$\mathcal{R} = |\tilde{r}|^2 = \rho^2,$$

but to obtain $\tilde{n}$ or ε we need θ, too. Therefore, consider a function

Thus,

$$\mathcal{P}\int_{-\infty}^{\infty} \frac{(1 + \omega'\,\omega)\,\ln[\rho(\omega')]}{(1 + \omega'^2)\,(\omega' - \omega)}\,d\omega' \;=\; -2\pi\,\theta(\omega)\ , \qquad (6.19)$$

or further,

$$\theta(\omega) \;=\; -\frac{2\omega}{\pi}\,\mathcal{P}\int_{0}^{\infty} \frac{\ln[\rho(\omega')]}{\omega'^2 - \omega^2}\,d\omega'\ , \qquad (6.20)$$

which allows evaluation of $\theta(\omega)$ from measurements of $\rho(\omega)$.

If needed, for low ω one can approximate $\mathcal{R} = \rho^2$ with a constant and for high ω with the electron gas dielectric function

$$\varepsilon \;=\; 1 - (\omega_p/\omega)^2, \qquad (6.21)$$

where the free electron plasma frequency is

$$\omega_p \;=\; (Ne^2 / \varepsilon_0 m_e)^{1/2}$$

for the electron density N and mass m_e. Here, only the valence electrons should be counted for N.

6.2. The Dielectric Function

6.2.1. Experimental Results

Reflectance spectra $\mathcal{R}(\hbar\omega)$, components of complex dielectric function, $\varepsilon_r(\hbar\omega)$ and $\varepsilon_i(\hbar\omega)$, and the imaginary part of the *energy loss function* $\varepsilon^{-1}(\hbar\omega)$ of Si, Ge and GaAs.

The main structures arise from transitions between valence and conduction bands, that we start to consider next.