example of this is shown in table 4.3 where the uncertainty of Δ becomes larger at a large angle of incidence. The optimum choice of angles for measurement is a compromise between the need for increased sensitivity of the DEHM values, the absence of cross correlation, and the uncertainty of Δ caused by inaccuracy of measurement of the angle of incidence.

The above computational considerations of MAI measurements have been successfully applied [175] to resolve numerous questions concerning this technique in earlier investigations particularly those of McCrackin and Colson [167], Burge and Bennet [156], Oldham [172], and Johnson and Bashara [179].

4.6. Reflection and transmission by isotropic stratified planar structures

The method of addition of multiple reflections becomes impractical when considering the reflection and transmission of polarized light at oblique incidence by a multilayer film between semi-infinite ambient and substrate media. A more elegant approach that employs 2×2 matrices will now be discussed, and is based on the fact that the equations that govern the propagation of light are linear and that the continuity of the tangential fields across an interface between two isotropic media can be regarded as a 2×2-linear-matrix transformation.[24]

Consider a stratified structure that consists of a stack of $1, 2, 3, \ldots, j, \ldots m$ parallel layers (strata) sandwiched between two semi-infinite ambient (0) and substrate $(m+1)$ media, fig. 4.38. Let all media be linear homogeneous and isotropic, and let the complex index of refraction of the jth layer be N_j and its thickness d_j. N_0 and N_{m+1} represent the complex indices of refraction of the ambient and substrate media, respectively. An incident monochromatic plane wave in medium 0 (the ambient) generates a resultant reflected plane wave in the same medium and a resultant transmitted plane wave in medium $m+1$ (the substrate). The total field inside the jth layer, which is excited by the incident plane wave, consists of two plane waves: a forward-travelling plane wave denoted by (+), and a backward-travelling plane wave denoted by (−). The wave-vectors of all plane waves lie in the same plane (the plane of incidence), and the wave-vectors of the two plane waves in the jth layer make equal angles with the z-axis which is perpendicular to the plane boundaries directed toward the substrate. When the incident wave in the ambient is linearly polarized with its electric vector

[24]Work on the use of 2×2-matrix methods to study the reflection and transmission of light by multilayered structures was pioneered by Abelès. (For an account of Abelès work see, for example, ref. 23, pp. 51ff.) The present development is similar to that used by Hayfield and White [146].

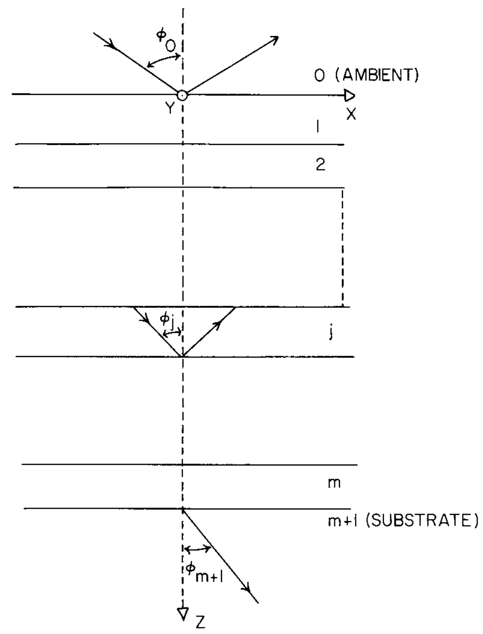

Fig. 4.38. Reflection and transmission of a plane wave by a multi-film structure (films $1, 2, \ldots m$) sandwiched between semi-infinite ambient (0) and substrate $(m+1)$ media. ϕ_0 is the angle of incidence; ϕ_j and ϕ_{m+1} are the angles of refraction in the j^{th} film and substrate, respectively.

vibrating parallel (p) or perpendicular (s) to the plane of incidence, all plane waves excited by that incident wave in the various layers of the stratified structure will be similarly polarized, parallel or perpendicular to the plane of incidence, respectively. In the following, it will be assumed that all waves are either p- or s-polarized.

Let $E^+(z)$ and $E^-(z)$ denote the complex amplitudes of the forward- and backward-travelling plane waves at an arbitrary plane z. The total field at z can be described by a 2×1-column vector

$$\boldsymbol{E}(z) = \begin{bmatrix} E^+(z) \\ E^-(z) \end{bmatrix}. \tag{4.145}$$

If we consider the fields at two different planes z' and z'' parallel to the layer boundaries then, by virtue of system linearity, $\boldsymbol{E}(z'')$ and $\boldsymbol{E}(z')$ must be related by a 2×2-matrix transformation

$$\begin{bmatrix} E^+(z') \\ E^-(z') \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \begin{bmatrix} E^+(z'') \\ E^-(z'') \end{bmatrix}. \tag{4.146}$$

More concisely, eq. (4.146) can be written as

$$\boldsymbol{E}(z') = \boldsymbol{SE}(z''), \tag{4.147}$$

where

$$\boldsymbol{S} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix}. \tag{4.148}$$

Note that $\boldsymbol{S}$ must characterize that part of the stratified structure confined between the two parallel planes at z' and z''.

By choosing z' and z'' to lie immediately on opposite sides of the $(j-1)j$ interface, located at z_j between layers $j-1$ and j, eq. (4.147) becomes

$$\boldsymbol{E}(z_j - 0) = \boldsymbol{I}_{(j-1)j}\boldsymbol{E}(z_j + 0), \tag{4.149}$$

where $\boldsymbol{I}_{(j-1)j}$ is a 2×2 matrix characteristic of the $(j-1)j$ *interface* alone. On the other hand, if z' and z'' are chosen inside the jth layer at its boundaries, eq. (4.147) becomes

$$\boldsymbol{E}(z_j + 0) = \boldsymbol{L}_j\boldsymbol{E}(z_j + d_j - 0), \tag{4.150}$$

where $\boldsymbol{L}_j$ is a 2×2 matrix characteristic of the jth *layer* alone whose thickness is d_j. Only the reflected wave in the ambient medium and the transmitted wave in the substrate are accessible for measurement, so that it is necessary to relate their fields to those of the incident wave. By taking the planes z' and z'' to lie in the ambient and substrate media, immediately adjacent to the 01 and $m(m+1)$ interfaces respectively, eq. (4.147) will read

$$\boldsymbol{E}(z_1 - 0) = \boldsymbol{SE}(z_{m+1} + 0). \tag{4.151}$$

Equation (4.151) defines a *scattering matrix* $\boldsymbol{S}$ which represents the overall reflection and transmission properties of the stratified structure. $\boldsymbol{S}$ can be expressed as a product of the interface and layer matrices $\boldsymbol{I}$ and $\boldsymbol{L}$ that describe the effects of the individual interfaces and layers of the entire stratified structure, taken in proper order, as follows:

$$\boldsymbol{S} = \boldsymbol{I}_{01}\boldsymbol{L}_1\boldsymbol{I}_{12}\boldsymbol{L}_2 \ldots \boldsymbol{I}_{(j-1)j}\boldsymbol{L}_j \ldots \boldsymbol{L}_m\boldsymbol{I}_{m(m+1)} \tag{4.152}$$

Equation (4.152) may be proved readily by repeated application of eq. (4.147) to the successive interfaces and layers of the stratified structure, starting with the ambient-first film (01) interface and ending by the last film-substrate interface $[m(m+1)]$.

From eq. (4.152) it is evident that to determine the stratified structure scattering matrix $\boldsymbol{S}$, the individual interface and layer matrices $\boldsymbol{I}$ and $\boldsymbol{L}$ have to be calculated.

The matrix $\boldsymbol{I}$ of an interface between two media a and b relates the fields on both its sides as

$$\begin{bmatrix} E_a^+ \\ E_a^- \end{bmatrix} = \begin{bmatrix} I_{11} & I_{12} \\ I_{21} & I_{22} \end{bmatrix} \begin{bmatrix} E_b^+ \\ E_b^- \end{bmatrix}. \tag{4.153}$$

Consider the special cases when one plane wave is incident on the ab interface. In terms of the complex amplitude E_a^+ of an incident plane wave in medium a, the complex amplitudes of the transmitted and reflected plane waves in media b and a, respectively (fig. 4.39–*left*), are given by

$$E_b^+ = t_{ab}E_a^+, \tag{4.154a}$$

$$E_a^- = r_{ab}E_a^+, \tag{4.154b}$$

and $E_b^- = 0$, where r_{ab} and t_{ab} are the Fresnel reflection and transmission coefficients of the ab interface. However, in accordance with eq. (4.153) we have

$$\begin{bmatrix} E_a^+ \\ E_a^- \end{bmatrix} = \begin{bmatrix} I_{11} & I_{12} \\ I_{21} & I_{22} \end{bmatrix} \begin{bmatrix} E_b^+ \\ 0 \end{bmatrix},$$

whose expansion gives

$$E_a^+ = I_{11}E_b^+, \tag{4.155a}$$

$$E_a^- = I_{21}E_b^+. \tag{4.155b}$$

Comparison between eqs. (4.154) and (4.155) leads to

$$I_{11} = 1/t_{ab}, \tag{4.156}$$

$$I_{21} = r_{ab}/t_{ab}. \tag{4.157}$$

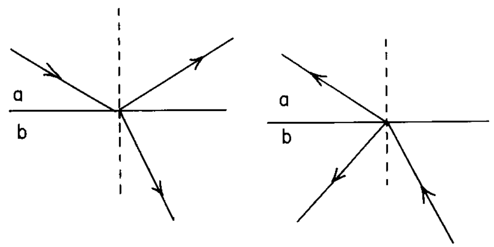

Fig. 4.39. *Left*: reflection and transmission (or refraction) of a plane wave at a two-media (ab) interface. *Right*: the direction of propagation of the transmitted (refracted) wave is assumed to have been reversed.

Now consider a plane wave incident on the ba interface from medium b, fig. 4.39–*right*, at an angle of incidence equal to the angle of refraction in medium b in the above case described in fig. 4.39–*left*. In this case, the fields immediately adjacent to the ba interface are related by

$$E_b^+ = r_{ba} E_b^-, \tag{4.158a}$$

$$E_a^- = t_{ba} E_b^-, \tag{4.158b}$$

and $E_a^+ = 0$, where r_{ba} and t_{ba} are the Fresnel reflection coefficients of the ba interface, respectively. On the other hand, eq. (4.153) tells us that, in this case,

$$\begin{bmatrix} 0 \\ E_a^- \end{bmatrix} = \begin{bmatrix} I_{11} & I_{12} \\ I_{21} & I_{22} \end{bmatrix} \begin{bmatrix} E_b^+ \\ E_b^- \end{bmatrix},$$

$$0 = I_{11} E_b^+ + I_{12} E_b^-, \tag{4.159a}$$

$$E_a^- = I_{21} E_b^+ + I_{22} E_b^-. \tag{4.159b}$$

Substitution of I_{11} and I_{21} from eqs. (4.156) and (4.157) into eqs. (4.159) transforms the latter equations into

$$E_b^+ = -I_{12} t_{ab} E_b^-, \tag{4.160a}$$

$$E_a^- = \left[\frac{r_{ab} r_{ba}}{t_{ab}} + I_{22}\right] E_b^-. \tag{4.160b}$$

Identification of the results shown by eqs. (4.158) and (4.160) leads to

$$I_{12} = -r_{ba}/t_{ab} \tag{4.161}$$

$$I_{22} = (t_{ab} t_{ba} - r_{ab} r_{ba})/t_{ab}. \tag{4.162}$$

Finally, use of the relationships between the interface Fresnel coefficients for both directions of propagation, namely $r_{ba} = -r_{ab}$ and $t_{ba} = (1 - r_{ab}^2)/t_{ab}$ [eqs. (4.29) and (4.30)], produces a final interface matrix of the form

$$\begin{aligned} \boldsymbol{I}_{ab} &= \begin{bmatrix} 1/t_{ab} & r_{ab}/t_{ab} \\ r_{ab}/t_{ab} & 1/t_{ab} \end{bmatrix} \\ &= (1/t_{ab}) \begin{bmatrix} 1 & r_{ab} \\ r_{ab} & 1 \end{bmatrix}. \end{aligned} \tag{4.163}$$

The interface Fresnel reflection and transmission coefficients that appear in eq. (4.163) must be evaluated using the complex indices of refraction of the two media that define the interface and the *local* angle of incidence. The latter can be found by the repeated application of Snell's law

$$N_0 \sin \phi_0 = N_1 \sin \phi_1 = \ldots = N_j \sin \phi_j = \ldots = N_{m+1} \sin \phi_{m+1}. \tag{4.164}$$

Now that we have determined the interface matrix $\boldsymbol{I}$, we turn our attention to the effect of propagation through a homogenous layer of index of refraction N and thickness d on the relationship between the fields inside that layer at both ends. This can be simply described by

$$\begin{bmatrix} E_0^+ \\ E_0^- \end{bmatrix} = \begin{bmatrix} e^{j\beta} & 0 \\ 0 & e^{-j\beta} \end{bmatrix} \begin{bmatrix} E_d^+ \\ E_d^- \end{bmatrix}, \tag{4.165}$$

where the subscripts 0 and d identify the beginning and end of the layer (along the direction of the forward-travelling wave) and the phase shift (layer phase thickness) β is given by

$$\beta = \frac{2\pi d N}{\lambda} \cos \phi, \tag{4.166}$$

with ϕ representing the angle between the direction of propagation in the layer and the perpendicular to its boundaries (the z-axis). The layer matrix $\boldsymbol{L}$ can therefore be written as

$$\boldsymbol{L} = \begin{bmatrix} e^{j\beta} & 0 \\ 0 & e^{-j\beta} \end{bmatrix}. \tag{4.167}$$

From the interface and layer matrices $\boldsymbol{I}$ and $\boldsymbol{L}$ of eqs. (4.163) and (4.167) the overall scattering matrix $\boldsymbol{S}$ of the stratified structure can be found by straightforward matrix multiplication as indicated by eq. (4.152). Equation (4.151) can be expanded as

$$\begin{bmatrix} E_a^+ \\ E_a^- \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \begin{bmatrix} E_s^+ \\ 0 \end{bmatrix}, \tag{4.168}$$

where, for simplicity, the subscripts a and s refer to the ambient and substrate media respectively, and $E_s^- = 0$. Further expansion of eq. (4.168) yields the overall reflection and transmission coefficients of the stratified structures as

$$R = \frac{E_a^-}{E_a^+} = \frac{S_{21}}{S_{11}}, \tag{4.169}$$

$$T = \frac{E_s^+}{E_a^+} = \frac{1}{S_{21}}, \tag{4.170}$$

respectively. From eq. (4.169) and (4.170) it is clear that only the elements of the first column of scattering matrix $\boldsymbol{S}$ determine the overall reflection and transmission coefficients of the stratified structure.

For the purpose of ellipsometry, the stratified-structure scattering matrix $\boldsymbol{S}$ (or its elements S_{11} and S_{21}) have to be calculated for both linear polarizations parallel (p) and perpendicular (s) to the plane of incidence. Such calculations are readily programmable for execution on a digital computer. Let $\boldsymbol{S}_p$ and $\boldsymbol{S}_s$ represent the scattering matrices for the p and s polarizations. The p and s reflection and transmission coefficients become

$$R_p = \frac{S_{21p}}{S_{11p}}, \tag{4.171}$$

$$R_s = \frac{S_{21s}}{S_{11s}}, \tag{4.172}$$

$$T_p = \frac{1}{S_{21p}}, \tag{4.173}$$

$$T_s = \frac{1}{S_{21s}}. \tag{4.174}$$

The quantities that are measurable by the ellipsometer are the ratio of the complex reflection coefficients for the p and s polarizations

$$\rho_r = R_p/R_s = \frac{S_{21p}}{S_{11p}} \times \frac{S_{11s}}{S_{21s}}, \tag{4.175}$$

and the ratio of the complex transmission coefficients for the same polarizations

$$\rho_t = T_p/T_s = \frac{S_{21s}}{S_{21p}}. \tag{4.176}$$

Note that $\boldsymbol{S}_p$ and $\boldsymbol{S}_s$ are different because each of the interface matrices $\boldsymbol{I}$ that appear in eq. (4.152) is different for the p and s polarizations. The layer matrices $\boldsymbol{L}$ appearing in eq. (4.152) are the same for these two polarizations.

As an example of the application of the above procedure, consider the case of a single film (1) sandwiched between semi-infinite ambient (0) and substrate (2) media, fig. 4.14. From eq. (4.152) the scattering matrix $\boldsymbol{S}$ in this case is given by

$$\boldsymbol{S} = \boldsymbol{I}_{01}\boldsymbol{L}_1\boldsymbol{I}_{12}, \tag{4.177}$$

which upon substitution from eqs. (4.163) and (4.167) becomes

$$\boldsymbol{S} = \left(\frac{1}{t_{01}t_{12}}\right)\begin{bmatrix} 1 & r_{01} \\ r_{01} & 1 \end{bmatrix}\begin{bmatrix} e^{j\beta} & 0 \\ 0 & e^{-j\beta} \end{bmatrix}\begin{bmatrix} 1 & r_{12} \\ r_{12} & 1 \end{bmatrix}, \tag{4.178}$$

or

$$\boldsymbol{S} = \left(\frac{e^{j\beta}}{t_{01}t_{12}}\right)\begin{bmatrix} (1 + r_{01}r_{12}\,e^{-j2\beta}) & (r_{12} + r_{01}\,e^{-j2\beta}) \\ (r_{01} + r_{12}\,e^{-j2\beta}) & (r_{01}r_{02} + e^{-j2\beta}) \end{bmatrix}, \tag{4.179}$$

when matrix multiplication is carried out. From eq. (4.179) we have

$$S_{11} = \left(\frac{e^{j\beta}}{t_{01}t_{12}}\right)(1 + r_{01}r_{12}\,e^{-j2\beta}), \tag{4.180a}$$

$$S_{21} = \left(\frac{e^{j\beta}}{t_{01}t_{12}}\right)(r_{01} + r_{12}\,e^{-j2\beta}). \tag{4.180b}$$

Substitution of these values of S_{11} and S_{21} into eqs. (4.169) and (4.170) yields

$$R = \frac{r_{01} + r_{12}\,e^{-j2\beta}}{1 + r_{01}r_{02}\,e^{-j2\beta}},$$

$$T = \frac{t_{01}t_{12}\,e^{-j\beta}}{r_{01} + r_{12}\,e^{-j2\beta}},$$

which are the same expressions as previously found in §4.3 [eqs. (4.34) and (4.36)] by use of the method of adding multiply-reflected and transmitted partial waves.

For another example, consider the case of two films (1 and 2) between semi-infinite ambient (0) and substrate (3) media. The method of adding multiply-reflected and transmitted waves becomes quite awkward in this case, although such calculation has been made [180]. In contrast, by use of eq. (4.152) the scattering matrix for this system can be easily obtained as

$$\boldsymbol{S} = \boldsymbol{I}_{01}\boldsymbol{L}_1\boldsymbol{I}_{12}\boldsymbol{L}_2\boldsymbol{I}_{23}. \tag{4.181}$$

Upon substitution from eqs. (4.163) and (4.167) eq. (4.181) becomes

$$\boldsymbol{S} = \left(\frac{1}{t_{01}t_{12}t_{23}}\right)\begin{bmatrix} 1 & r_{01} \\ r_{01} & 1 \end{bmatrix}\begin{bmatrix} e^{j\beta_1} & 0 \\ 0 & e^{-j\beta_1} \end{bmatrix}\begin{bmatrix} 1 & r_{12} \\ r_{12} & 1 \end{bmatrix}\begin{bmatrix} e^{j\beta_2} & 0 \\ 0 & e^{-j\beta_2} \end{bmatrix}\begin{bmatrix} 1 & r_{23} \\ r_{23} & 1 \end{bmatrix}, \tag{4.182}$$

or

$$\boldsymbol{S} = \left(\frac{e^{j(\beta_1+\beta_2)}}{t_{01}t_{12}t_{23}}\right)\begin{bmatrix} \begin{matrix}[(1 + r_{01}r_{12}\,e^{-j2\beta_1}) \\ \quad + (r_{12} + r_{01}\,e^{-j2\beta_1})r_{23}\,e^{-j2\beta_2}]\end{matrix} & \begin{matrix}[(1 + r_{01}r_{12}\,e^{-j2\beta_1})r_{23} \\ \quad + (r_{12} + r_{01}\,e^{-j2\beta_1})\,e^{-j2\beta_2}]\end{matrix} \\ \begin{matrix}[(r_{01} + r_{12}\,e^{-j2\beta_1}) \\ \quad + (r_{01}r_{12} + e^{-j2\beta_1})r_{23}\,e^{-j2\beta_2}]\end{matrix} & \begin{matrix}[(r_{01} + r_{12}\,e^{-j2\beta_1})r_{23} \\ \quad + (r_{01}r_{12} + e^{-j2\beta_1})\,e^{-j2\beta_2}]\end{matrix} \end{bmatrix} \tag{4.183}$$

after matrix multiplications have been carried out explicitly. From eq. (4.183) we have

$$S_{11} = \left(\frac{e^{j(\beta_1+\beta_2)}}{t_{01}t_{12}t_{23}}\right)[(1 + r_{01}r_{12}\,e^{-j2\beta_1}) + (r_{12} + r_{01}\,e^{-j2\beta_1})r_{23}\,e^{-j2\beta_2}], \tag{4.184a}$$

$$S_{21} = \left(\frac{e^{j(\beta_1+\beta_2)}}{t_{01}t_{12}t_{23}}\right)[(r_{01} + r_{12}\,e^{-j2\beta_1}) + (r_{01}r_{12} + e^{-j2\beta_1})r_{23}\,e^{-j2\beta_2}]. \tag{4.184b}$$

Substitution of eqs. (4.184a) and (4.184b) into eqs. (4.169) and (4.170) yields

$$R = \frac{(r_{01} + r_{12}\,e^{-j2\beta_1}) + (r_{01}r_{12} + e^{-j2\beta_1})r_{23}\,e^{-j2\beta_2}}{(1 + r_{01}r_{12}\,e^{-j2\beta_1}) + (r_{12} + r_{01}\,e^{-j2\beta_1})r_{23}\,e^{-j2\beta_2}}, \tag{4.185}$$

and

$$T = \frac{t_{01}t_{12}t_{23}\,e^{-j(\beta_1+\beta_2)}}{(r_{01} + r_{12}\,e^{-j2\beta_1}) + (r_{01}r_{12} + e^{-j2\beta_1})r_{23}\,e^{-j2\beta_2}}. \tag{4.186}$$

Equations (4.185) and (4.186) apply to the p and s polarizations by simple attachment of a subscript p or s to R, T and the individual interface Fresnel reflection (r_{01}, r_{12}, r_{23}) and transmission (t_{01}, t_{12}, t_{23}) coefficients. The ratios of overall reflection and transmission coefficients that can be measured ellipsometrically are given by eqs. (4.175) and (4.176).

Although the 2×2-matrix method can be easily extended to derive explicit expressions for R and T in cases that involve three or more films, such explicit expressions are of little practical value because all calculations can be handled by a computer without them.

Throughout this section, we assumed that the optical properties are uniform within each layer of the stratified structure, and that they change abruptly at the sharp interfaces between layers. When the optical properties change continuously (and not in a discontinuous step-like fashion) within an inhomogeneous layer, the method of this section can still be applied. This requires, however, that we divide the inhomogeneous layer into an adequately large number of sublayers, each of which is approximately homogeneous. In fact, this is the most general approach for a problem of this kind, because closed-form solutions are only possible for a few simple cases as, for example, when the refractive index of the layer changes linearly or exponentially along the direction of stratification [181].

4.7. Reflection and transmission by anisotropic stratified planar structures

A 4×4-matrix method has recently been developed by Billard [182], Teitler and Henvis [183], and Berreman and Scheffer [184] to study the reflection and transmission of obliquely incident polarized light by stratified anisotropic planar structures. The method is a generalization of the Abelès 2×2-matrix method [185] applicable to stratified isotropic media and previously discussed in §4.6. The following presentation of the 4×4-matrix method is based on the general exposition given by Berreman [186]. Notice, however, that we use Maxwell's equations in rationalized units, that we adhere to the $e^{j\omega t}$ time dependence, and that we use different notation in some places.

With the $e^{j\omega t}$ time dependence assumed, the two Maxwell's "curl" equations take the form

$$-\boldsymbol{curl}\,\boldsymbol{E} = j\omega\boldsymbol{B}, \qquad \boldsymbol{curl}\,\boldsymbol{H} = j\omega\boldsymbol{D} \tag{4.187}$$

where $\boldsymbol{E}$, $\boldsymbol{H}$, $\boldsymbol{D}$, and $\boldsymbol{B}$ are the electromagnetic-field vectors, as usual. In Cartesian coordinates, eqs. (4.187) can be combined in matrix form as

$$\begin{bmatrix} 0 & 0 & 0 & 0 & -\partial/\partial z & \partial/\partial y \\ 0 & 0 & 0 & \partial/\partial z & 0 & -\partial/\partial x \\ 0 & 0 & 0 & -\partial/\partial y & \partial/\partial x & 0 \\ 0 & \partial/\partial z & -\partial/\partial y & 0 & 0 & 0 \\ -\partial/\partial z & 0 & \partial/\partial x & 0 & 0 & 0 \\ \partial/\partial y & -\partial/\partial x & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} E_x \\ E_y \\ E_z \\ H_x \\ H_y \\ H_z \end{bmatrix} = j\omega \begin{bmatrix} D_x \\ D_y \\ D_z \\ B_x \\ B_y \\ B_z \end{bmatrix}, \tag{4.188}$$

or shortly,

$$\boldsymbol{O}\boldsymbol{G} = j\omega\boldsymbol{C}. \tag{4.189}$$

In eq. (4.189), $\boldsymbol{O}$ is a 6×6 symmetric matrix operator which can be partitioned into four 3×3 submatrices to take the form

$$\boldsymbol{O} = \begin{bmatrix} \boldsymbol{0} & \boldsymbol{curl} \\ -\boldsymbol{curl} & \boldsymbol{0} \end{bmatrix}. \tag{4.190}$$

$\boldsymbol{0}$ denotes the 3×3 zero matrix, and $\boldsymbol{curl}$ is the curl operator

$$\boldsymbol{curl} = \begin{bmatrix} 0 & -\partial/\partial z & \partial/\partial y \\ \partial/\partial z & 0 & -\partial/\partial x \\ -\partial/\partial y & \partial/\partial x & 0 \end{bmatrix}. \tag{4.191}$$

$\boldsymbol{G}$ is a 6×1 column vector whose elements are the Cartesian components of $\boldsymbol{E}$ followed by those of $\boldsymbol{H}$, and $\boldsymbol{C}$ is a 6×1 column vector whose elements are the Cartesian components of $\boldsymbol{D}$ followed by those of $\boldsymbol{B}$.

In the absence of nonlinear optical effects and spatial dispersion, the constitutive relation between $\boldsymbol{C}$ and $\boldsymbol{G}$ can be generally put as

$$\boldsymbol{C} = \boldsymbol{M}\boldsymbol{G}, \tag{4.192}$$

where the 6×6 matrix $\boldsymbol{M}$ carries all the information about the anisotropic optical properties of the medium that supports the electromagnetic fields. $\boldsymbol{M}$, to be called the optical matrix, can be conveniently partitioned as follows

$$M = \begin{bmatrix} \boldsymbol{\epsilon} & \boldsymbol{\rho} \\ \boldsymbol{\rho}' & \boldsymbol{\mu} \end{bmatrix}, \tag{4.193}$$

where $\boldsymbol{\epsilon} = (M_{ij})$ and $\boldsymbol{\mu} = (M_{i+3,j+3})$, $i, j = 1, 2, 3$ are the (dielectric) permittivity and (magnetic) permiability tensors, respectively, and $\boldsymbol{\rho} = (M_{i,j+3})$ and $\boldsymbol{\rho}'(M_{i+3,j})$, $i, j = 1, 2, 3$ are optical-rotation tensors.[25]

Substitution of eq. (4.192) into eq. (4.189) yields

$$\boldsymbol{OG} = \mathrm{j}\omega \boldsymbol{MG}.$$

Next, if in the above equation we replace $\boldsymbol{G}$ by

$$\boldsymbol{G} = \mathrm{e}^{\mathrm{j}\omega t}\boldsymbol{\Gamma}, \tag{4.194}$$

where $\boldsymbol{\Gamma}$ is the spatial part of $\boldsymbol{G}$, it becomes

$$\boldsymbol{O\Gamma} = \mathrm{j}\omega \boldsymbol{M\Gamma}, \tag{4.195}$$

which is the spatial wave equation for frequency ω.

The particular problem under consideration involves the reflection and transmission of a monochromatic plane wave obliquely incident from an isotropic ambient medium ($z < 0$) onto an anisotropic planar structure ($z > 0$) stratified along the z-axis. The x-axis of the reference xyz Cartesian coordinate system is assumed to coincide with the line of intersection of the plane of incidence (the plane of the incident wave-vector and the z-axis) and the $z = 0$ interface (see fig. 4.38). From the symmetry of the problem, there is no variation in the y direction of any field component, so that

$$\partial/\partial y = 0. \tag{4.196a}$$

For the tangential fields to match across the boundary $z = 0$, at all of its points at all time, all the waves that are excited by the incident plane wave must have the same spatial dependence in the x-direction as the incident wave. Therefore, if ξ denotes the x component of the wave-vector of the incident wave, all fields should vary in the x-direction as $\mathrm{e}^{-\mathrm{j}\xi x}$, hence

$$\partial/\partial x = -\mathrm{j}\xi. \tag{4.196b}$$

In terms of the refractive index N_0 of the ambient medium and the angle of incidence ϕ_0, ξ is given by

$$\xi = \frac{\omega}{c} N_0 \sin\phi_0, \tag{4.197}$$

[25] The bold face letter $\boldsymbol{\rho}$ which denotes the optical-rotation tensor should not be confused with ρ which denotes the ellipsometric ratio of reflection or transmission coefficients.

where c is the free-space wave velocity. Use of eqs. (4.196) simplifies the curl operator of eq. (4.191)

$$\boldsymbol{curl} = \begin{bmatrix} 0 & -\partial/\partial z & 0 \\ \partial/\partial z & 0 & \mathrm{j}\xi \\ 0 & -\mathrm{j}\xi & 0 \end{bmatrix}. \tag{4.198}$$

The possibility of using a 4×4-matrix method to study the reflection and transmission of polarized light by anisotropic planar structures is a consequence of the special form assumed by the curl operator in eq. (4.198). In particular, if eq. (4.198) is substituted into eq. (4.190), the resulting operator $\boldsymbol{O}$ generates two linear homogeneous algebraic equations and four linear homogeneous first-order differential equations in the six components of $\boldsymbol{\Gamma}$ when eq. (4.195) is expanded. The two linear homogeneous algebraic equations can be solved for the field components $E_z(\Gamma_3)$ and $H_z(\Gamma_6)$ along the z-axis in terms of the other four field components $E_x(\Gamma_1)$, $E_y(\Gamma_2)$, $H_x(\Gamma_4)$, $H_y(\Gamma_5)$, along the x- and y-axes. The values E_z and H_z thus obtained are subsequently substituted into the remaining four differential equations to produce four linear homogeneous first-order differential equations in the four field variables E_x, E_y, H_x, and H_y. These can be cast in 4×4 matrix form as follows

$$\frac{\partial}{\partial z}\begin{bmatrix} E_x \\ H_y \\ E_y \\ -H_x \end{bmatrix} = -\mathrm{j}\omega \begin{bmatrix} \Delta_{11} & \Delta_{12} & \Delta_{13} & \Delta_{14} \\ \Delta_{21} & \Delta_{22} & \Delta_{23} & \Delta_{24} \\ \Delta_{31} & \Delta_{32} & \Delta_{33} & \Delta_{34} \\ \Delta_{41} & \Delta_{42} & \Delta_{43} & \Delta_{44} \end{bmatrix} \begin{bmatrix} E_x \\ H_y \\ E_y \\ -H_x \end{bmatrix}, \tag{4.199}$$

or

$$\frac{\partial}{\partial z}\boldsymbol{\psi} = -\mathrm{j}\omega \boldsymbol{\Delta\psi}. \tag{4.200}$$

Equation (4.200) is the wave equation for the 4×1 generalized field vector

$$\boldsymbol{\psi} = \begin{bmatrix} E_x \\ H_y \\ E_y \\ -H_x \end{bmatrix}, \tag{4.201}$$

with $\boldsymbol{\Delta}$ defining a 4×4 differential propagation matrix of the medium.[26] The elements of $\boldsymbol{\Delta}$ are functions of the elements of the 6×6 optical matrix $\boldsymbol{M}$ [eq. (4.193)] obtained by carrying out the operations indicated above. The relations between the elements of $\boldsymbol{\Delta}$ and the elements of $\boldsymbol{M}$ are

$$\begin{aligned}
\Delta_{11} &= M_{51}+(M_{53}+\eta)A_1+M_{56}A_5,\\
\Delta_{12} &= M_{55}+(M_{53}+\eta)A_4+M_{56}A_8,\\
\Delta_{13} &= M_{52}+(M_{53}+\eta)A_2+M_{56}A_6,\\
-\Delta_{14} &= M_{54}+(M_{53}+\eta)A_3+M_{56}A_7,\\
\Delta_{21} &= M_{11}+M_{13}A_1+M_{16}A_5,\\
\Delta_{22} &= M_{15}+M_{13}A_4+M_{16}A_8,\\
\Delta_{23} &= M_{12}+M_{13}A_2+M_{16}A_6,\\
-\Delta_{24} &= M_{14}+M_{13}A_3+M_{16}A_7,\\
-\Delta_{31} &= M_{41}+M_{43}A_1+M_{46}A_5,\\
-\Delta_{32} &= M_{45}+M_{43}A_4+M_{46}A_8,\\
-\Delta_{33} &= M_{42}+M_{43}A_2+M_{46}A_6,\\
\Delta_{34} &= M_{44}+M_{43}A_3+M_{46}A_7,\\
\Delta_{41} &= M_{21}+M_{23}A_1+(M_{26}-\eta)A_5,\\
\Delta_{42} &= M_{25}+M_{23}A_4+(M_{26}-\eta)A_8,\\
\Delta_{43} &= M_{22}+M_{23}A_2+(M_{26}-\eta)A_6,\\
-\Delta_{44} &= M_{24}+M_{23}A_3+(M_{26}-\eta)A_7,
\end{aligned} \tag{4.202}$$

where

$$\begin{aligned}
A_1 &= (M_{61}M_{36}-M_{31}M_{66})/D,\\
A_2 &= [(M_{62}-\eta)M_{36}-M_{32}M_{66}]/D,\\
A_3 &= (M_{64}M_{36}-M_{34}M_{66})/D,\\
A_4 &= [M_{65}M_{36}-(M_{35}+\eta)M_{66}]/D,\\
A_5 &= (M_{63}M_{31}-M_{33}M_{61})/D,\\
A_6 &= [M_{63}M_{32}-(M_{62}-\eta)M_{33}]/D,\\
A_7 &= (M_{63}M_{34}-M_{33}M_{64})/D,\\
A_8 &= [(M_{35}+\eta)M_{63}-M_{33}M_{65}]/D,
\end{aligned} \tag{4.203}$$

[26] The differential wave equation for the Jones vector $\boldsymbol{E}$ discussed in §2.10 [eq. (2.164)] may be considered as a special case of the more general wave equation for the generalized field vector $\boldsymbol{\psi}$. Instead of the differential propagation Jones matrix $\boldsymbol{N}$ in the 2×2-matrix formalism, we now have the differential propagation matrix $-\mathrm{j}\omega\boldsymbol{\Delta}$ in the 4×4-matrix formalism. Obviously, the bold face symbols $\boldsymbol{\psi}$ and $\boldsymbol{\Delta}$ which denote the wave vector and differential propagation matrix respectively, should not be confused with the ordinary ellipsometric parameters ψ and Δ.

$$D = M_{33}M_{66}-M_{36}M_{63}, \tag{4.204a}$$

$$\eta = \xi/\omega = N_0 \sin\phi_0/c. \tag{4.204b}$$

Recall that the 6×6 optical matrix $\boldsymbol{M}$ is structured from the permittivity $\boldsymbol{\epsilon}$, permiability $\boldsymbol{\mu}$ and optical-rotation $\boldsymbol{\rho}$, $\boldsymbol{\rho}'$ tensors, according to eq. (4.193). From $\boldsymbol{\epsilon}$, $\boldsymbol{\mu}$, $\boldsymbol{\rho}$ and $\boldsymbol{\rho}'$, as well as η, the differential propagation matrix $\boldsymbol{\Delta}$ can be calculated using eqs. (4.202)–(4.204). With $\boldsymbol{\Delta}$ known, the law of propagation (wave equation) for the generalized field vector $\boldsymbol{\psi}$ (or, equivalently, its elements, the components of $\boldsymbol{E}$ and $\boldsymbol{H}$ parallel to the x- and y-axes) is specified by eq. (4.200). Berreman calculated $\boldsymbol{\Delta}$ for a number of special cases: (i) an orthorhombic crystal with its principal axes parallel to the x, y, and z coordinates axes, (ii) an isotropic optically active medium [187], (iii) an isotropic medium subjected to a magnetic field along the z-axis and exhibiting Faraday effect [188], and (iv) single-domain, cholesteric or twisted-nematic, liquid-crystal cell with parallel surfaces [186]. These results are summarized in table 4.5.

In the general case of a stratified anisotropic structure, $\boldsymbol{M}$ is some arbitrary function of z and the wave equation (4.200) does not, in general, have an analytical solution. In the special case when $\boldsymbol{M}$ is constant independent of z (over some continuous interval of z), eq. (4.200) is directly integrable to yield

$$\boldsymbol{\psi}(z+h) = \boldsymbol{L}(h)\boldsymbol{\psi}(z), \tag{4.205}$$

where

$$\begin{aligned}
\boldsymbol{L}(h) &= \mathrm{e}^{-\mathrm{j}\omega h\boldsymbol{\Delta}}\\
&= \left[\boldsymbol{I}-\mathrm{j}\omega h\boldsymbol{\Delta}-\frac{(\omega h)^2}{2!}\boldsymbol{\Delta}^2+\mathrm{j}\frac{(\omega h)^3}{3!}\boldsymbol{\Delta}^3+\dots\right].
\end{aligned} \tag{4.206}$$

Equation (4.205) represents a linear matrix relationship between the generalized field vectors $\boldsymbol{\psi}$ [eq. (4.201)] at two different parallel planes, separated by a distance h, in a homogeneous anisotropic medium whose fields are excited by an incident plane wave. The layer matrix $\boldsymbol{L}(h)$ is determined by the differential propagation matrix $\boldsymbol{\Delta}$ in accordance with eq. (4.206). In the latter equation, $\boldsymbol{I}$ represents the 4×4 identity matrix, and the summation of the exponential series can be carried out analytically in some simple cases (when $\boldsymbol{\Delta}^n$ has a closed-form expression), or numerically.

An alternative expression for the layer matrix $\boldsymbol{L}(h)$ can be determined from the fact that when $\boldsymbol{\Delta}$ is constant independent of z, eq. (4.200) has four particular plane-wave solutions of the form

$$\boldsymbol{\psi}(z) = \boldsymbol{\psi}_\ell(0)\,\mathrm{e}^{-\mathrm{j}q_\ell z}, \qquad \ell = 1,2,3,4. \tag{4.207}$$

In eq. (4.207), $\boldsymbol{\psi}(0)$ is the value of the generalized field vector of the plane

Table 4.5. The differential propagation matrix $\boldsymbol{\Delta}$ for certain anisotropic media*

Orthorombic Crystal (Principal axes parallel to the xyz coordinate axes)	Isotropic Optical Activity	Faraday Rotation (Magnetic field parallel to z-axis)	Cholesteric Liquid Crystal (Helical axis along the z-axis)
$\boldsymbol{\Delta} = \begin{bmatrix} 0 & a^2 & 0 & 0 \\ b^2 & 0 & 0 & 0 \\ 0 & 0 & 0 & u^2 \\ 0 & 0 & v^2 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 1-(\eta^2/\epsilon) & -\mathrm{j}g\eta^2/\epsilon & 0 \\ \epsilon & 0 & 0 & -\mathrm{j}g \\ 0 & 0 & 0 & 1 \\ 0 & +\mathrm{j}g & \epsilon-\eta^2 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 1-(\eta^2/\epsilon) & 0 & 0 \\ \epsilon & 0 & \mathrm{j}\gamma & 0 \\ 0 & 0 & 0 & 1 \\ -\mathrm{j}\gamma & 0 & \epsilon-\eta^2 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 1-(\eta^2/\epsilon') & 0 & 0 \\ (\epsilon+\delta\cos 2\beta z) & 0 & \delta\sin 2\beta z & 0 \\ 0 & 0 & 0 & 1 \\ \delta\sin 2\beta z & 0 & (\epsilon-\eta^2-\delta\cos 2\beta z) & 0 \end{bmatrix}$
$a^2 = \mu_{22} - (\eta^2/\epsilon_{33})$ $b^2 = \epsilon_{11}$ $u^2 = \mu_{11}$ $v^2 = \epsilon_{22} - (\eta^2/\mu_{33})$ $\boldsymbol{\epsilon}$ and $\boldsymbol{\mu}$, the dielectric and permeability tensors, are diagonal	ϵ = isotropic dielectric constant g = isotropic optical-activity parameter	γ = Faraday-rotation parameter proportional to the magnetic field	$\epsilon+\delta = \epsilon_{11}$, $\epsilon-\delta = \epsilon_{22}$, $\epsilon' = \epsilon_{33}$ are the principal values of the dielectric tensor of the molecular planes. $\beta = 2\pi/p$, where p is the pitch of the helical structure

*Compiled from ref. 158. η is given by eq. (4.204b).

wave at $z=0$, and q_ℓ equals the component of the propagation vector of the plane wave parallel to the z-axis. Substitution of eq. (4.207) into eq. (4.200), gives the matrix-eigenvalue equation

$$[\omega\boldsymbol{\Delta} - q\boldsymbol{I}]\boldsymbol{\psi}(0) = \boldsymbol{0}, \tag{4.208}$$

whose eigenvalues q_ℓ are the roots of the quartic polynomial equation

$$\det[\omega\boldsymbol{\Delta} - q\boldsymbol{I}] = 0, \tag{4.209}$$

where det stands for the "determinant of". Insertion of each eigenvalue q_ℓ ($\ell = 1,2,3,4$) into eq. (4.208), leads to four homogeneous linear equations that can be solved for the elements of the corresponding eigenvector $\boldsymbol{\psi}_{k\ell}(0)$ (where $k = 1,2,3,4$). In terms of the 4×4 matrix $\boldsymbol{\Psi} = [\psi_{k\ell}(0)]$, which is constructed from the four eigenvectors of eq. (4.208) as columns, it can be readily shown that the layer matrix $\boldsymbol{L}(h)$ [relating the fields inside an anisotropic slab of thickness h at its two boundaries, eq. (4.205)] is given by

$$\boldsymbol{L}(h) = \boldsymbol{\Psi}\boldsymbol{K}(h)\boldsymbol{\Psi}^{-1}, \tag{4.210}$$

where $\boldsymbol{K}$ is a diagonal matrix with elements determined by the eigenvalues q_ℓ

$$K_{\ell\ell} = \mathrm{e}^{-\mathrm{j}q_\ell h}, \qquad \ell = 1,2,3,4. \tag{4.211}$$

Examples of the application of this procedure are given in ref. 186.

In an inhomogeneous anisotropic medium, where $\boldsymbol{M}$ is a continuous function of z, eq. (4.205) can be applied if we divide the medium into layers that are sufficiently thin to make $\boldsymbol{M}$ independent of z within each layer. By recursive application of eq. (4.205) to the successive layers, the fields at two planes distance d apart are related by

$$\boldsymbol{\psi}(z+d) = \mathscr{L}(z,d)\boldsymbol{\psi}(z), \tag{4.212}$$

where

$$\mathscr{L}(z,d) = \boldsymbol{L}(z+d-h_m, h_m)\ldots\boldsymbol{L}(z+h_1+h_2, h_3)\boldsymbol{L}(z+h_1, h_2)\boldsymbol{L}(z, h_1),$$
$$d = \sum_{i=1}^{m} h_i. \tag{4.213}$$

For generality, the layer thicknesses $h_1, h_2, \ldots h_m$, are assumed different. [Notice that $\boldsymbol{L}(z,h)$ characterizes a thin homogeneous layer located between z and $z+h$.] Alternative expressions from which the inhomogeneous layer matrix can be numerically computed with increased accuracy and more rapid convergence than that provided by eq. (4.213) have been discussed by Berreman in a more recent publication [189].

4.7.1. *Reflection and transmission by a finite anisotropic layer between semi-infinite isotropic ambient and substrate media*

Consider the case shown in fig. 4.40 of a stratified layer or slab of an optically anisotropic medium sandwiched between two isotropic ambient and substrate media of refractive indices N_0 and N_2, respectively [183, 186]. Let $z = 0$ and $z = d$ coincide with the interfaces between the layer and the ambient and substrate media, respectively. A plane wave incident from the ambient onto the layer at an angle of incidence ϕ_0 generates a resultant reflected wave in the same medium, at angle of reflection from the z-axis ϕ_0, and a transmitted wave in the substrate medium at an angle of refraction from the z-axis ϕ_2. The relationship between ϕ_0 and ϕ_2 is given by Snell's law

$$N_2 \sin \phi_2 = N_0 \sin \phi_0. \tag{4.214}$$

According to eq. (4.212) a 4×4 matrix $\mathscr{L}$

$$\mathscr{L} = (\ell_{ij}), \qquad i, j = 1, 2, 3, 4, \tag{4.215}$$

relates the generalized field vectors [defined by eq. (4.201)] $\boldsymbol{\psi}(d)$ and $\boldsymbol{\psi}(0)$ inside the layer at its two boundary surfaces according to

$$\boldsymbol{\psi}(d) = \mathscr{L}\boldsymbol{\psi}(0). \tag{4.216}$$

Starting from the permittivity $\boldsymbol{\epsilon}$, permiability $\boldsymbol{\mu}$ and optical-rotation $\boldsymbol{\rho}$, $\boldsymbol{\rho}'$ tensors of the medium, the 6×6 optical matrix $\boldsymbol{M}$ is constructed according to eq. (4.193). Next, the 4×4 differential propagation matrix $\boldsymbol{\Delta}$ is calculated

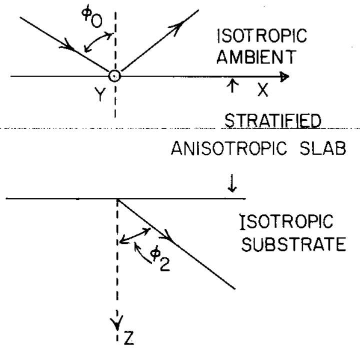

Fig. 4.40. Reflection and transmission of a plane wave by a stratified anisotropic slab sandwiched between semi-infinite isotropic ambient and substrate media. ϕ_0 is the angle of incidence in the ambient and ϕ_2 is the angle of refraction in the substrate. The mutually orthogonal axes x and y are in the ambient/slab interface parallel and perpendicular to the plane of incidence, respectively; the z axis is in the direction of stratification.

from the 6×6 optical matrix $\boldsymbol{M}$ using eqs. (4.202)–(4.204). Finally, the 4×4 layer matrix $\mathscr{L}$ is computed from $\boldsymbol{\Delta}$ using eq. (4.210) [or (4.206)] and eq. (4.213) (if the layer is inhomogeneous).

The total field in the ambient medium at $z = 0$ is made up of incident and reflected components, so that the condition of matching the generalized field vector $\boldsymbol{\psi}$ across the $z = 0$ interface can be put in the form

$$\boldsymbol{\psi}(0^+) = \boldsymbol{\psi}_i(0^-) + \boldsymbol{\psi}_r(0^-), \tag{4.217}$$

where the $-$ and $+$ superscripts distinguish the ambient and layer sides, respectively, of the $z = 0$ interface. The total field in the substrate is due to a single transmitted plane wave, and matching the generalized field vector $\boldsymbol{\psi}$ across the $z = d$ interface leads to

$$\boldsymbol{\psi}(d - 0) = \boldsymbol{\psi}_t(d + 0), \tag{4.218}$$

where $d - 0$ and $d + 0$ identify the layer and substrate sides, respectively, of the $z = d$ interface.

Let (E_{ip}, E_{is}), (E_{rp}, E_{rs}), and (E_{tp}, E_{ts}) represent the components of the electric field vectors of the incident, reflected, and transmitted waves, respectively, parallel (p) and perpendicular (s) to the plane of incidence. In a nonmagnetic ($\mu = 1$) optically isotropic medium, the magnetic field components are simply related to their associated orthogonal electric field components through the index of refraction N

$$H_p/E_s = H_s/E_p = N. \tag{4.219}$$

Thus, using eqs. (4.201) and (4.219), the three generalized field vectors $\boldsymbol{\psi}_i$, $\boldsymbol{\psi}_r$, and $\boldsymbol{\psi}_t$ of the incident, reflected, and transmitted waves, respectively, can be calculated from the p and s electric field components alone, without explicit reference to the magnetic field components

$$\boldsymbol{\psi}_i = \begin{bmatrix} E_{ip}\cos\phi_0 \\ N_0 E_{ip} \\ E_{is} \\ N_0 E_{is}\cos\phi_0 \end{bmatrix}, \qquad \boldsymbol{\psi}_r = \begin{bmatrix} -E_{rp}\cos\phi_0 \\ N_0 E_{rp} \\ E_{rs} \\ -N_0 E_{rs}\cos\phi_0 \end{bmatrix}, \tag{4.220}$$

and

$$\boldsymbol{\psi}_t = \begin{bmatrix} E_{tp}\cos\phi_2 \\ N_2 E_{tp} \\ E_{ts} \\ N_2 E_{ts}\cos\phi_2 \end{bmatrix}. \tag{4.221}$$

Notice that eqs. (4.220) and (4.221) are based on the convention that the p and s directions are as shown in fig. 4.1 and that $\boldsymbol{E} \times \boldsymbol{H}$ is in the direction of propagation.

Substitution of eqs. (4.220) and (4.221) into the boundary condition eqs. (4.217) and (4.218), respectively, gives the internal generalized field vectors $\boldsymbol{\psi}(0)$ and $\boldsymbol{\psi}(d)$ inside the anisotropic layer at its $z=0$ and $z=d$ boundaries, in terms of the external fields $\boldsymbol{\psi}_i$, $\boldsymbol{\psi}_r$, and $\boldsymbol{\psi}_t$. The internal fields inside the layer at $z=0$ and $z=d$ are subsequently interrelated by the layer matrix $\mathscr{L}$ according to eq. (4.216). The resulting equation reads

$$\begin{bmatrix} E_{tp}\cos\phi_2 \\ N_2E_{tp} \\ E_{ts} \\ N_2E_{ts}\cos\phi_2 \end{bmatrix} = \begin{bmatrix} \ell_{11} & \ell_{12} & \ell_{13} & \ell_{14} \\ \ell_{21} & \ell_{22} & \ell_{23} & \ell_{24} \\ \ell_{31} & \ell_{32} & \ell_{33} & \ell_{34} \\ \ell_{41} & \ell_{42} & \ell_{43} & \ell_{44} \end{bmatrix} \begin{bmatrix} (E_{ip}-E_{rp})\cos\phi_0 \\ N_0(E_{ip}+E_{rp}) \\ (E_{is}+E_{rs}) \\ N_0(E_{is}-E_{rs})\cos\phi_0 \end{bmatrix}. \tag{4.222}$$

Equation (4.222) can further be expanded into four separate linear algebraic equations in the six field components (E_{ip}, E_{is}), (E_{rp}, E_{rs}), and (E_{tp}, E_{ts}). E_{tp} can be readily eliminated from the first and second of these four equations, while E_{ts} can be eliminated from the third and fourth equations. This yields two linear algebraic equations connecting the incident and reflected fields alone

$$\begin{aligned} a_{ip}E_{ip} + a_{is}E_{is} + a_{rp}E_{rp} + a_{rs}E_{rs} &= 0, \\ b_{ip}E_{ip} + b_{is}E_{is} + b_{rp}E_{rp} + b_{rs}E_{rs} &= 0, \end{aligned} \tag{4.223}$$

where

$$\begin{aligned} \begin{matrix} a_{ip} \\ a_{rp} \end{matrix} &= \pm\cos\phi_0(\ell_{11}N_2 - \ell_{21}\cos\phi_2) + N_0(\ell_{12}N_2 - \ell_{22}\cos\phi_2), \\ \begin{matrix} a_{is} \\ a_{rs} \end{matrix} &= \pm N_0\cos\phi_0(\ell_{14}N_2 - \ell_{24}\cos\phi_2) + (\ell_{13}N_2 - \ell_{23}\cos\phi_2) \\ \begin{matrix} b_{ip} \\ b_{rp} \end{matrix} &= \pm\cos\phi_0(\ell_{31}N_2\cos\phi_2 - \ell_{41}) + N_0(\ell_{32}N_2\cos\phi_2 - \ell_{42}), \\ \begin{matrix} b_{is} \\ b_{rs} \end{matrix} &= \pm N_0\cos\phi_0(\ell_{34}N_2\cos\phi_2 - \ell_{44}) + (\ell_{33}N_2\cos\phi_2 - \ell_{43}). \end{aligned} \tag{4.224}$$

In the above equations, the upper and lower symbols on the left correspond, respectively, to the upper (+) and lower (−) signs on the right.

Equations (4.223) can be recast in the form

$$\begin{bmatrix} E_{rp} \\ E_{rs} \end{bmatrix} = \begin{bmatrix} R_{pp} & R_{ps} \\ R_{sp} & R_{ss} \end{bmatrix} \begin{bmatrix} E_{ip} \\ E_{is} \end{bmatrix}, \tag{4.225}$$

or

$$\boldsymbol{E}_r = \boldsymbol{R}\boldsymbol{E}_i. \tag{4.226}$$

$\boldsymbol{R}$ is the 2×2 complex-amplitude reflection matrix

$$\boldsymbol{R} = \begin{bmatrix} R_{pp} & R_{ps} \\ R_{sp} & R_{ss} \end{bmatrix}, \tag{4.227}$$

and is given by

$$\boldsymbol{R} = (a_{rs}b_{rp} - a_{rp}b_{rs})^{-1} \begin{bmatrix} (a_{ip}b_{rs} - a_{rs}b_{ip}) & (a_{is}b_{rs} - a_{rs}b_{is}) \\ (a_{rp}b_{ip} - a_{ip}b_{rp}) & (a_{rp}b_{is} - b_{rp}a_{is}) \end{bmatrix}. \tag{4.228}$$

By substituting, $E_{rp} = R_{pp}E_{ip} + R_{ps}E_{is}$ and $E_{rs} = R_{sp}E_{ip} + R_{ss}E_{is}$ [eq. (4.225)], into the second and third equations that are obtained from the expansion of eq. (4.222), the reflected field components are eliminated giving two linear equations that relate the transmitted fields (E_{tp}, E_{ts}) to the incident fields (E_{ip}, E_{is}) only. The two equations thus obtained can be readily put in the form

$$\begin{bmatrix} E_{tp} \\ E_{ts} \end{bmatrix} = \begin{bmatrix} T_{pp} & T_{ps} \\ T_{sp} & T_{ss} \end{bmatrix} \begin{bmatrix} E_{ip} \\ E_{is} \end{bmatrix}, \tag{4.229}$$

or

$$\boldsymbol{E}_t = \boldsymbol{T}\boldsymbol{E}_i. \tag{4.230}$$

where

$$\boldsymbol{T} = \begin{bmatrix} T_{pp} & T_{ps} \\ T_{sp} & T_{ss} \end{bmatrix}, \tag{4.231}$$

is the 2×2 complex-amplitude transmission matrix with elements

$$\begin{aligned} T_{pp} &= [(\ell_{21}\cos\phi_0 + \ell_{22}N_0) \\ &\quad + R_{pp}(-\ell_{21}\cos\phi_0 + \ell_{22}N_0) + R_{sp}(\ell_{23} - \ell_{24}N_0\cos\phi_0)]/N_2, \\ T_{ps} &= [(\ell_{23} + \ell_{24}N_0\cos\phi_0) \\ &\quad + R_{ps}(-\ell_{21}\cos\phi_0 + \ell_{22}N_0) + R_{ss}(\ell_{23} - \ell_{24}N_0\cos\phi_0)]/N_2, \end{aligned} \tag{4.232}$$

(4.232 *cont.*)

$$T_{sp} = (\ell_{31}\cos\phi_0 + \ell_{32}N_0) + R_{pp}(-\ell_{31}\cos\phi_0 + \ell_{32}N_0) + R_{sp}(\ell_{33} - \ell_{34}N_0\cos\phi_0),$$
$$T_{ss} = (\ell_{33} + \ell_{34}N_0\cos\phi_0) + R_{ps}(-\ell_{31}\cos\phi_0 + \ell_{32}N_0) + R_{ss}(\ell_{33} - \ell_{34}N_0\cos\phi_0).$$

The determination of the reflection $\boldsymbol{R}$ and transmission $\boldsymbol{T}$ matrices completes the solution of the problem. This is because $\boldsymbol{R}$ and $\boldsymbol{T}$ represent the external measurable entities that are accessible to the ellipsometer. A summary of the steps that are required to calculate $\boldsymbol{R}$ and $\boldsymbol{T}$ from given values of the permittivity $\boldsymbol{\epsilon}$, permeability $\boldsymbol{\mu}$ and optical rotation $\boldsymbol{\rho}$, $\boldsymbol{\rho}'$ tensors (and given geometry) is schematically shown in fig. 4.41.

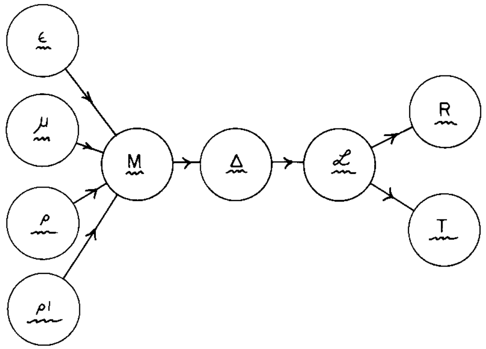

Fig. 4.41. Schematic flow chart of the steps required for the calculation of the reflection and transmission matrices $\boldsymbol{R}$ and $\boldsymbol{T}$ from the dielectric $\boldsymbol{\epsilon}$, magnetic permeability $\boldsymbol{\mu}$ and optical activity (rotation) $\boldsymbol{\rho}$, $\boldsymbol{\rho}'$ tensors.

4.7.2. *Reflection and transmission by a semi-infinite anisotropic substrate in an isotropic ambient*

We restrict our attention to the special, but important, case when the semi-infinite anisotropic medium is homogeneous, so that the optical matrix $\boldsymbol{M}$ is constant independent of z. No general solution exists when $\boldsymbol{M}$ is an arbitrary function of z [186].

When the optical matrix $\boldsymbol{M}$ of the substrate is constant, the differential propagation matrix $\boldsymbol{\Delta}$ is also constant. Under this condition, we have seen that the wave equation for the generalized field vector $\boldsymbol{\psi}$ [eq. (4.200)] has four plane-wave solutions [eq. (4.207)]. Of these four plane-wave solutions, only two could be excited in the semi-infinite substrate by the incident plane wave. These are the two plane waves that propagate (and have wave-vector components) in the positive z-direction. Let q_1 and q_2 denote the only two eigenvalues that have a positive real part of all the four eigenvalues (roots) of the quartic polynomial eq. (4.209). Also, let $C_1\boldsymbol{\psi}_1(0)$ and $C_2\boldsymbol{\psi}_2(0)$ be their associated eigenvectors [obtained from eq. (4.208)], which are known up to the constant amplitude factors C_1 and C_2. C_1 and C_2 will be determined from matching the tangential electric and magnetic field components in the ambient and in the substrate at their common interface $z = 0$. In terms of the generalized field vectors, the boundary conditions assume the form

$$\boldsymbol{\psi}_i(0^-) + \boldsymbol{\psi}_r(0^-) = C_1\boldsymbol{\psi}_1(0^+) + C_2\boldsymbol{\psi}_2(0^+), \tag{4.233}$$

where the $-$ and $+$ superscripts indicate the ambient and substrate sides of the $z = 0$ interface and the subscripts i and r indicate the incident- and reflected-wave components of the total field in the ambient, as before.

If we substitute into eq. (4.233) the values of $\boldsymbol{\psi}_i(0^-)$ and $\boldsymbol{\psi}_r(0^+)$ given by eq. (4.220), and subsequently expand both sides, we obtain

$$\begin{aligned}(E_{ip} - E_{rp})\cos\phi_0 &= C_1\psi_{11} + C_2\psi_{12},\\ N_0(E_{ip} + E_{rp}) &= C_1\psi_{21} + C_2\psi_{22},\\ (E_{is} + E_{rs}) &= C_1\psi_{31} + C_2\psi_{32},\\ N_0(E_{is} - E_{rs})\cos\phi_0 &= C_1\psi_{41} + C_2\psi_{42}.\end{aligned} \tag{4.234}$$

In eqs. (4.234), ψ_{k1} and ψ_{k2} ($k = 1, 2, 3, 4$) are the components of the two column eigenvectors $\boldsymbol{\psi}_1(0^+)$ and $\boldsymbol{\psi}_2(0^+)$, respectively. Let us introduce a vector $\boldsymbol{C}$

$$\boldsymbol{C} = \begin{bmatrix} C_1 \\ C_2 \end{bmatrix}, \tag{4.235}$$

whose components determine the amplitudes of the two refracted (transmitted) waves in the substrate. In terms of $\boldsymbol{C}$, $\boldsymbol{E}_i$, and $\boldsymbol{E}_r$ (where $\boldsymbol{E}_i$ and $\boldsymbol{E}_r$ are the 2×1 column vectors defined by eqs. (4.225), (4.226)), the first and fourth, and the second and third of eqs. (4.234) can be combined in two 2×2 matrix equations that can be solved for $\boldsymbol{C}$ as follows

$$\begin{aligned}\boldsymbol{C} &= \boldsymbol{S}_1(\boldsymbol{E}_i - \boldsymbol{E}_r),\\ \boldsymbol{C} &= \boldsymbol{S}_2(\boldsymbol{E}_i + \boldsymbol{E}_r),\end{aligned} \tag{4.236}$$

where

$$\boldsymbol{S}_1 = \cos\phi_0 \begin{bmatrix} \psi_{11} & \psi_{12} \\ \psi_{41}/N_0 & \psi_{42}/N_0 \end{bmatrix}^{-1}, \qquad \boldsymbol{S}_2 = \begin{bmatrix} \psi_{21}/N_0 & \psi_{22}/N_0 \\ \psi_{31} & \psi_{32} \end{bmatrix}^{-1}. \tag{4.237}$$

Elimination of $\boldsymbol{C}$ between eqs. (4.236) leads to

$$\boldsymbol{E}_r = \boldsymbol{R}\boldsymbol{E}_i,$$

where

$$R = (S_1 + S_2)^{-1}(S_2 - S_1), \tag{4.238}$$

is the required 2×2 reflection matrix.

A transmission or refraction matrix T can be defined which relates the amplitudes of the two refracted waves in the substrate to the amplitude of the incident wave as follows

$$C = TE_i, \tag{4.239}$$

From eqs. (4.236), it follows immediately that the transmission matrix T is given by

$$T = S_1(I - R) = S_2(I + R), \tag{4.240}$$

where I is the 2×2 identity matrix. Determination of the reflection (R) and transmission (T) matrices completes the solution of the problem.

4.7.3. *Explicit expressions for the reflection matrix in simple special cases*

The 4×4-matrix method given above represents a general unified approach to the computation of the reflection R and transmission T matrices of any anisotropic substrate or film-substrate system of interest in ellipsometry. There are a number of frequently encountered simple special cases of anisotropic systems for which explicit expressions of the reflection matrix have already been derived. A summary of these special cases is given below.

4.7.3.1. *Isotropic ambient and uniaxially anisotropic substrate*

We assume that light is obliquely incident at angle ϕ_0 from an isotropic ambient (medium 0) of refractive index N_0 onto a uniaxial anisotropic substrate (medium 1) with ordinary and extraordinary (complex) refractive indices N_{1o} and N_{1e}, respectively. First, consider the case when the optic axis is *perpendicular* to the ambient-substrate interface. In this orientation, the interface reflection matrix r is diagonal, so that

$$r_{ps} = r_{sp} = 0, \tag{4.241}$$

while the diagonal reflection coefficients r_{pp} and r_{ss} are given by [71]

$$r_{pp} = \frac{N_{1o}N_{1e}\cos\phi_0 - N_0(N_{1e}^2 - N_0^2\sin^2\phi_0)^{\frac{1}{2}}}{N_{1o}N_{1e}\cos\phi_0 + N_0(N_{1e}^2 - N_0^2\sin^2\phi_0)^{\frac{1}{2}}}, \tag{4.242}$$

$$r_{ss} = \frac{N_0\cos\phi_0 - (N_{1o}^2 - N_0^2\sin^2\phi_0)^{\frac{1}{2}}}{N_0\cos\phi_0 + (N_{1o}^2 - N_0^2\sin^2\phi_0)^{\frac{1}{2}}}. \tag{4.243}$$

In the limiting case when $N_{1o} = N_{1e} = N_1$, eqs. (4.242) and (4.243) reduce to the expressions for the reflection coefficients at the interface between two isotropic media [eqs. (4.4) and (4.5), after applying Snell's law, eq. (4.3)].

When the optic axis is *parallel* to the interface, and is oriented at an angle α from the plane of incidence, the elements of the reflection matrix (which is nondiagonal) are given by [190]

$$\begin{aligned} r_{pp} &= (F_1G_4 + F_2G_3)/(F_1 + F_2),\\ r_{ps} &= F_1F_2(G_2 - G_1)/(F_1 + F_2),\\ r_{sp} &= (G_4 - G_3)/(F_1 + F_2),\\ r_{ss} &= (F_1G_1 + F_2G_2)/(F_1 + F_2); \end{aligned} \tag{4.244}$$

where

$$\begin{aligned} F_1 &= J/(N_0\sin^2\phi_0 + J\cos\phi_0)\tan\alpha,\\ F_2 &= N_{1o}\tan\alpha(I + N_0N_{1o}\cos\phi_0)/(IN_{1o}\cos\phi_0 + N_0J^2),\\ G_1 &= (N_0\cos\phi_0 - J)/(N_0\cos\phi_0 + J),\\ G_2 &= (N_0N_{1o}\cos\phi_0 - I)/(N_0N_{1o}\cos\phi_0 + I),\\ G_3 &= (N_{1o}^2\cos\phi_0 - N_0J)/(N_{1o}^2\cos\phi_0 + N_0J),\\ G_4 &= (IN_{1o}\cos\phi_0 - N_0J^2)/(IN_{1o}\cos\phi_0 + N_0J^2); \end{aligned} \tag{4.245}$$

and

$$\begin{aligned} I^2 &= N_{1o}^2N_{1e}^2 - N_0^2\sin^2\phi_0(N_{1o}^2\sin^2\alpha + N_{1e}^2\cos^2\alpha),\\ J^2 &= N_{1o}^2 - N_0^2\sin^2\phi_0. \end{aligned} \tag{4.246}$$

In eqs. (4.245) and (4.246), ϕ_0 is the angle of incidence, N_0 is the refractive index of the isotropic ambient, and N_{1o}, N_{1e} are the ordinary and extraordinary (complex) refractive indices of the uniaxially anisotropic substrate, as before. When the optic axis is parallel to the interface, *in* or *normal* to the plane of incidence, the values $\alpha = 0$ or $\alpha = \frac{1}{2}\pi$, respectively, can be substituted into eqs. (4.245) and (4.246), leading to a diagonal reflection matrix [eqs. (4.244)] for these two symmetrical orientations.

4.7.3.2. *Isotropic ambient and biaxially anisotropic substrate*

We restrict ourselves to the case when the biaxially anisotropic substrate belongs to the orthorhombic system with its principal axes of absorption and refraction coincident. Furthermore, two of the three principal axes (x and y) are assumed to lie parallel to the ambient-substrate interface, while the third (z) is perpendicular to it. Light is obliquely incident from the isotropic ambient onto the biaxial substrate at an angle of incidence ϕ_0, with its direction of propagation in the xz plane.[27] Let N_0 be the index of refraction of the ambient, and N_{1x}, N_{1y}, and N_{1z} be the principal indices of

[27] This coordinate system is similar to that shown in fig. 4.40.

refraction of the substrate along its principal axes x, y, and z. In this symmetrical orientation, the reflection matrix r is diagonal ($r_{ps} = r_{sp} = 0$), and the diagonal r_{pp} and r_{ss} reflection coefficients are given by [191]

$$r_{pp} = \frac{N_{1x}N_{1z}\cos\phi_0 - N_0(N_{1z}^2 - N_0^2\sin^2\phi_0)^{\frac{1}{2}}}{N_{1x}N_{1z}\cos\phi_0 + N_0(N_{1z}^2 - N_0^2\sin^2\phi_0)^{\frac{1}{2}}}, \tag{4.247}$$

$$r_{ss} = \frac{N_0\cos\phi_0 - (N_{1y}^2 - N_0^2\sin^2\phi_0)^{\frac{1}{2}}}{N_0\cos\phi_0 + (N_{1y}^2 - N_0^2\sin^2\phi_0)^{\frac{1}{2}}}. \tag{4.248}$$

Upon substituting $N_{1x} = N_{1y} = N_{1o}$, $N_{1z} = N_{1e}$, eqs. (4.247) and (4.248) become identical with eqs. (4.242) and (4.243), respectively, appropriate to the case of a uniaxial substrate whose optic axis is perpendicular to its interface with the ambient.

Alternatively, if the substitutions $N_{1x} = N_{1e}$, $N_{1y} = N_{1z} = N_{1o}$, *or* $N_{1x} = N_{1z} = N_{1o}$, $N_{1y} = N_{1e}$ are made in eqs. (4.247), (4.248), we obtain the reflection coefficients for a uniaxial substrate whose optic axis lies parallel to the interface, in *or* perpendicular to the plane of incidence, respectively.

4.7.3.3. *Uniaxially anisotropic film on an isotropic substrate in an isotropic ambient* [192]

A special case of interest is that in which the optic axis of the uniaxial film is perpendicular to its boundaries with the ambient and substrate. This condition is encountered, for example, when Langmuir-Blodgett layers [193, 194] (which are monomolecular layers of well-oriented molecules) are deposited on isotropic substrates, or when thin vacuum-deposited films have island-like structure.

Because of symmetry, when the incident wave in the ambient is either p or s polarized, the excited waves in the uniaxial film and in the isotropic substrate will possess the same polarization, *i.e.*, p or s, respectively. (Hence the reflection matrix is diagonal.) The method of §4.3, in which multiply reflected and refracted waves in an isotropic film are superimposed to determine the resultant waves in the ambient and substrate, continues to hold in the present case of a uniaxial anisotropic film. However, the refracted wave in the film is affected by a different index of refraction, dependent on its polarization being p or s. Therefore, we may conclude that eqs. (4.37)–(4.40) apply to the present case, provided that the "phase thickness" β of the uniaxial film is assigned the proper value for each of the p and s polarizations. Rewriting eqs. (4.37) and (4.38), we obtain the diagonal reflection coefficients for the three-phase (ambient-film-substrate) system as

$$R_{pp} = \frac{r_{01pp} + r_{12pp}\,e^{-j2\beta_p}}{1 + r_{01pp}r_{12pp}\,e^{-j2\beta_p}}, \tag{4.249}$$

$$R_{ss} = \frac{r_{01ss} + r_{12ss}\,e^{-j2\beta_s}}{1 + r_{01ss}r_{12ss}\,e^{-j2\beta_s}}. \tag{4.250}$$

In eqs. (4.249) and (4.250), r_{01pp}, r_{12pp} and r_{01ss}, r_{12ss} are the reflection coefficients at the 0–1 (ambient-film) and 1–2 (film-substrate) interfaces for the p- and s-polarization, respectively. They can be obtained directly from eqs. (4.242) and (4.243), noting that $r_{12} = -r_{21}$, as follows

$$r_{01pp} = \frac{N_{1o}N_{1e}\cos\phi_0 - N_0(N_{1e}^2 - N_0^2\sin^2\phi_0)^{\frac{1}{2}}}{N_{1o}N_{1e}\cos\phi_0 + N_0(N_{1e}^2 - N_0^2\sin^2\phi_0)^{\frac{1}{2}}}, \tag{4.251}$$

$$r_{12pp} = \frac{-N_{1o}N_{1e}\cos\phi_2 + N_2(N_{1e}^2 - N_2^2\sin^2\phi_2)^{\frac{1}{2}}}{N_{1o}N_{1e}\cos\phi_2 + N_2(N_{1e}^2 - N_2^2\sin^2\phi_2)^{\frac{1}{2}}}, \tag{4.252}$$

$$r_{01ss} = \frac{N_0\cos\phi_0 - (N_{1o}^2 - N_0^2\sin^2\phi_0)^{\frac{1}{2}}}{N_0\cos\phi_0 + (N_{1o}^2 - N_0^2\sin^2\phi_0)^{\frac{1}{2}}}, \tag{4.253}$$

$$r_{12ss} = \frac{-N_2\cos\phi_2 + (N_{1o}^2 - N_2^2\sin^2\phi_2)^{\frac{1}{2}}}{N_2\cos\phi_2 + (N_{1o}^2 - N_2^2\sin^2\phi_2)^{\frac{1}{2}}}, \tag{4.254}$$

where N_0, N_2 are the refractive indices of the isotropic ambient and substrate, respectively, and N_{1o}, N_{1e} are the ordinary and extraordinary refractive indices of the uniaxial film. ϕ_0 is the angle of incidence in the ambient, ϕ_2 is the angle of refraction in the substrate and these two angles are interrelated by Snell's law

$$N_0\sin\phi_0 = N_2\sin\phi_2. \tag{4.255}$$

The phase thicknesses β_p and β_s for the p- and s-polarizations that appear in eqs. (4.249) and (4.250) are given by

$$\beta_p = 2\pi\left(\frac{d_1}{\lambda}\right)\left(\frac{N_{1o}}{N_{1e}}\right)(N_{1e}^2 - N_0^2\sin^2\phi_0)^{\frac{1}{2}}, \tag{4.256}$$

$$\beta_s = 2\pi\left(\frac{d_1}{\lambda}\right)(N_{1o}^2 - N_0^2\sin^2\phi_0)^{\frac{1}{2}}, \tag{4.257}$$

where d_1 is the film thickness and λ is the free-space wavelength of light.

Although we have considered above the case when the optic axis of the uniaxial film is perpendicular to its boundaries, analogous expressions can be similarly derived for the two other symmetrical orientations, when the optic axis is parallel to the film boundaries in or normal to the plane of incidence.

4.7.3.4. *Biaxially anisotropic film on an isotropic substrate in an isotropic ambient* [195]

Let two of the principal axes (x and y) of the biaxial film lie parallel to the film boundaries while the third (z) be perpendicular to them. Furthermore, let the plane of incidence be taken to coincide with the xz plane. In this symmetrical orientation, both interface and overall (three-phase) reflection matrices are diagonal. The three-phase diagonal reflection coefficients R_{pp} and R_{ss} are given by eqs. (4.249) and (4.250), but with the interface reflection coefficients determined from eqs. (4.247) and (4.248). Since the substitutions involved are quite straightforward, the results for this case will be left out. Note, however, that β_p and β_s are now given by

$$\beta_p = 2\pi\left(\frac{d_1}{\lambda}\right)\left(\frac{N_{1x}}{N_{1z}}\right)(N_{1z}^2 - N_0^2 \sin^2 \phi_0)^{\frac{1}{2}}, \tag{4.258}$$

$$\beta_s = 2\pi\left(\frac{d_1}{\lambda}\right)(N_{1y}^2 - N_0^2 \sin^2 \phi_0)^{\frac{1}{2}}, \tag{4.259}$$

where N_{1x}, N_{1y}, and N_{1z} are the principal indices of refraction associated with the principal axes x, y, and z of the biaxial film.

4.7.3.5. Uniaxial film on a uniaxial substrate in an isotropic ambient

When the optic axes of the uniaxial film and the uniaxial substrate are aligned in parallel, expressions for the reflection coefficients can be readily derived, provided that the common direction of the optic axes is either normal to the film boundaries, or parallel to them in or perpendicular to the plane of incidence [71]. Consider, for example, the case when the optic axes of the film and substrate are oriented normal to the film boundaries. Again, because of symmetry, both the interface and overall (three-phase) reflection matrices are diagonal. The three-phase diagonal reflection coefficients are given by eqs. (4.249) and (4.250). In the latter equations, notice that the 0–1 interface reflection coefficients (r_{01pp}, r_{01ss}) are the same as in eqs. (4.251) and (4.253), the phase thicknesses of the film β_p and β_s are the same as in eqs. (4.256) and (4.257), while the 1–2 interface reflection coefficients (r_{12pp}, r_{12ss}) are given by

$$r_{12pp} = \frac{N_{1o}N_{2e}\sin^2\phi_{1e}(N_{1e}^2 - N_0^2\sin^2\phi_0)^{\frac{1}{2}} - N_{2o}N_{1e}\sin^2\phi_{2e}(N_{2e}^2 - N_0^2\sin^2\phi_0)^{\frac{1}{2}}}{N_{1o}N_{2e}\sin^2\phi_{1e}(N_{1e}^2 - N_0^2\sin^2\phi_0)^{\frac{1}{2}} + N_{2o}N_{1e}\sin^2\phi_{2e}(N_{2e}^2 - N_0^2\sin^2\phi_0)^{\frac{1}{2}}}, \tag{4.260}$$

$$r_{12ss} = \frac{(N_{1o}^2 - N_0^2\sin^2\phi_0)^{\frac{1}{2}} - (N_{2o}^2 - N_0^2\sin^2\phi_0)^{\frac{1}{2}}}{(N_{1o}^2 - N_0^2\sin^2\phi_0)^{\frac{1}{2}} + (N_{2o}^2 - N_0^2\sin^2\phi_0)^{\frac{1}{2}}}. \tag{4.261}$$

In the above equations, N_0, (N_{1o}, N_{1e}), and (N_{2o}, N_{2e}) are the indices of refraction of the ambient (medium 0), film (medium 1), and substrate (medium 2), respectively. ϕ_0 is the angle of incidence in the ambient, ϕ_{1e} and ϕ_{2e} are the angles of refraction of the extraordinary (p-polarized) wave in the film and substrate respectively, and are given by [71]

$$\tan\phi_{1e} = (N_0N_{1e}/N_{1o})(N_{1e}^2 - N_0^2\sin^2\phi_0)^{-\frac{1}{2}}, \tag{4.262}$$

$$\tan\phi_{2e} = (N_0N_{2e}/N_{2o})(N_{2e}^2 - N_0^2\sin^2\phi_0)^{-\frac{1}{2}}. \tag{4.263}$$

4.8. Ellipsometry on surfaces covered with discontinuous films and on surfaces with rough boundaries

In the previous sections of this chapter we considered the reflection and transmission of light by multi-layer structures assuming that each layer is continuous and that interfaces between layers are perfectly smooth (plane) and parallel. In this section we briefly review studies of the effect of deviations from these idealizations on the interpretation of reflection ellipsometric data.

Discontinuous films often arise when they are prepared by the vacuum evaporation of film material onto a substrate. Especially in the early stages of evaporation, the film assumes the form of disconnected islands of film material separated by clear areas of the substrate. A simplified approach to deal with such films is to use the theory of Maxwell Garnett [196] which is based on the representation of the discontinuous film by a random distribution of small-diameter (compared to the wavelength of light) spherical particles of film material embedded in a dielectric ambient. Such an inhomogeneous system can then be proved to be equivalent to a homogeneous one with an *effective* complex refractive index N_e given by

$$\frac{N_e^2 - N_a^2}{N_e^2 + 2N_a^2} = q\frac{N_f^2 - N_a^2}{N_f^2 + 2N_a^2}, \tag{4.264}$$

where N_f and N_a are the refractive indices of the film and ambient materials, respectively, and q is the volume fraction occupied by the spherical particles in the discontinuous film. Often the ambient is vacuum or air so that $N_a = 1$ and eq. (4.264) becomes

$$\frac{N_e^2 - 1}{N_e^2 + 2} = q\frac{N_f^2 - 1}{N_f^2 + 2} \tag{4.265}$$

from which

$$N_e^2 = \frac{1 + 2fq}{1 - fq}, \qquad f = \frac{N_f^2 - 1}{N_f^2 + 2}. \tag{4.266}$$

A more exact approach to the reflection of light from substrates covered by discontinuous or sub-monolayer films is that of Strachan [197] and Sivukhin [198]. In this case, an island-like or sub-monolayer film is replaced by a two-dimensional distribution of Hertzian oscillators whose strength S per unit area of the substrate is

$$S = \sigma_x E_x + \sigma_y E_y + \sigma_z E_z, \tag{4.267}$$

where E_x, E_y, E_z are the components of the electric field of the light wave driving the oscillators along directions x, y (in the surface) and z (normal to