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Reflection and refraction by uniaxial crystals

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Abstract. Explicit formulae are found for the electric field vectors of the ordinary and extraordinary modes produced when plane waves of p or s polarization are incident on an arbitrary face of a uniaxial crystal. The angle of incidence is unrestricted, and the anisotropic medium may be absorbing. The reflection amplitudes r_{pp}, r_{ps}, r_{ss}, r_{sp}, the transmission amplitudes t_{po}, t_{pe}, t_{so}, t_{se}, and the wavevector and ray directions are then determined in terms of the direction cosines of the optic axis relative to the laboratory axes.

1. Introduction

The aim of this paper is to produce formulae that enable ellipsometric and reflectance properties to be calculated, for reflection from a planar surface that has an arbitrary orientation relative to the crystallographic axes. An extensive literature deals with this problem, based mainly on a 4×4 matrix formalism (Teitler and Henvis 1970, Berreman 1971, Azzam and Bahshara 1977, Yeh 1979, 1988). One difficulty in the application of this formalism is that it is left to the user to transform the dielectric tensor from the principal-axes frame to the laboratory frame, and to solve the associated eigenvalue problem. This is done explicitly here, and formulae are derived for the reflection and transmission amplitudes in terms of the optical constants of the medium and the direction cosines of the optic axis relative to the laboratory axes.

The laboratory x, y, z axes are defined as follows. The reflecting surface is the xy plane, and the plane of incidence is the zx plane, with the z axis normal to the surface and directed into it. When a plane wave is incident, there will be a reflected plane wave, and (in general) two transmitted plane waves. All components of the electric and magnetic field vectors $\boldsymbol{E}$ and $\boldsymbol{B}$ then have x and t dependence contained in the factor $\exp \mathrm{i}(Kx - \omega t)$, where ω is the angular frequency and K is the tangential component of all the wave vectors. (The notation is that used in a recent monograph on reflection (Lekner 1987).) There is no y dependence, because of the translational symmetry in the y direction. Within the anisotropic medium (assumed non-magnetic) the two curl equations of Maxwell read, after differentiations with respect to time are performed,

$$\nabla \times \boldsymbol{E} = \mathrm{i}k\boldsymbol{B} \qquad \nabla \times \boldsymbol{B} = -\mathrm{i}k\boldsymbol{D} \tag{1}$$

where $k = \omega/c$ and $\boldsymbol{D}$ is found from $\boldsymbol{E}$ via the dielectric tensor ε_{ij}:

$$\begin{pmatrix} D_x \\ D_y \\ D_z \end{pmatrix} = \begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{pmatrix} \begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix}. \tag{2}$$

(We will see later that $\varepsilon_{ij} = \varepsilon_{ji}$.) The six equations (1) are, for the geometry specified above,

$$\begin{aligned} -\partial E_y/\partial z &= \mathrm{i}kB_x & -\partial B_y/\partial z &= -\mathrm{i}kD_x \\ \partial E_x/\partial z - \mathrm{i}KE_z &= \mathrm{i}kB_y & \partial B_x/\partial z - \mathrm{i}KB_z &= -\mathrm{i}kD_y \\ \mathrm{i}KE_y &= \mathrm{i}kB_z & \mathrm{i}KB_y &= -\mathrm{i}kD_z. \end{aligned} \tag{3}$$

When we eliminate $\boldsymbol{B}$, we are left with three coupled differential equations in $\boldsymbol{E}$:

$$\partial^2 E_x/\partial z^2 - \mathrm{i}K\,\partial E_z/\partial z + k^2 D_x = 0 \tag{4}$$

$$\partial^2 E_y/\partial z^2 - K^2 E_y + k^2 D_y = 0 \tag{5}$$

$$-\mathrm{i}K\,\partial E_x/\partial z - K^2 E_z + k^2 D_z = 0. \tag{6}$$

We note in passing that iK times (4) plus $\partial/\partial z$ times (6) gives a simple equation linking D_z with D_x:

$$\partial D_z/\partial z + \mathrm{i}KD_x = 0. \tag{7}$$

In the isotropic case (ε_{ij} diagonal), E_y is decoupled from E_x and E_z.

From the differential equations (4) to (6) we can deduce the boundary conditions to be satisfied at a discontinuity in the medium. The derivative of a discontinuous function would give a delta function, which cannot be cancelled by any other term in the equation. Also a derivative of a delta function is not allowed. Thus from (4) it follows that $\partial E_x/\partial z - \mathrm{i}KE_z$ and E_x are continuous (the continuity of E_x is also implied by (6)), and from (5) that $\partial E_y/\partial z$ and E_y are continuous. Thus, with reference to (3), we see that the boundary conditions are the continuity of the tangential components of $\boldsymbol{E}$ and $\boldsymbol{B}$, as expected. From (7) we deduce that the normal component of $\boldsymbol{D}$ is continuous, also a familiar result.

2. Propagation in a homogeneous anisotropic material

The above equations are for an arbitrary z-stratified anisotropic material. We now specialize to uniform anisotropic media (crystals). We need to find the normal modes, that is those fields that propagate as plane waves in the medium. Such fields have all components with the z-dependence $\exp(\mathrm{i}qz)$, q being the component of the wave vector normal to the surface. Substitution of this dependence into (4), (5) and (6) gives the equations

$$-q^2 E_x + qKE_z + k^2 D_x = 0 \tag{8}$$

$$-(q^2 + K^2)E_y + k^2 D_y = 0 \tag{9}$$

$$qKE_x - K^2E_z + k^2D_z = 0. \tag{10}$$

A solution for $\boldsymbol{E}$ is possible if the determinant of coefficient is zero, that is if

$$\begin{vmatrix} \varepsilon_{xx} - q^2/k^2 & \varepsilon_{xy} & \varepsilon_{xz} + qK/k^2 \\ \varepsilon_{yx} & \varepsilon_{yy} - (K^2 + q^2)/k^2 & \varepsilon_{yz} \\ \varepsilon_{zx} + qK/k^2 & \varepsilon_{zy} & \varepsilon_{zz} - K^2/k^2 \end{vmatrix} = 0. \tag{11}$$

Equation (11) gives a quartic in q, with solutions (eigenvalues) that depend on the tensor elements ε_{ij}.

We now consider how ε_{ij} are determined in terms of the three dielectric constants ε_a, ε_b, ε_c, which are the diagonal elements of ε_{ij} in the principal-axes coordinate system of the crystal. Denote the principal axes by unit vectors $\boldsymbol{a}$, $\boldsymbol{b}$, $\boldsymbol{c}$, and the laboratory frame by the unit vectors $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z}$. There are various ways of transforming from one orthogonal coordinate frame to another, the usual one being by means of a coordinate rotation matrix expressed in terms of the Euler angles (Yeh 1988). For our purposes it is more convenient to work with an orthogonal transformation expressed in terms of direction cosines (Goldstein 1959, ch 4). We have

$$\begin{aligned} \boldsymbol{x} &= \alpha_1\boldsymbol{a} + \alpha_2\boldsymbol{b} + \alpha_3\boldsymbol{c} \\ \boldsymbol{y} &= \beta_1\boldsymbol{a} + \beta_2\boldsymbol{b} + \beta_3\boldsymbol{c} \\ \boldsymbol{z} &= \gamma_1\boldsymbol{a} + \gamma_2\boldsymbol{b} + \gamma_3\boldsymbol{c} \end{aligned} \tag{12}$$

where $\alpha_1 = \boldsymbol{x}\cdot\boldsymbol{a}$ is the cosine of the angle between $\boldsymbol{x}$ and $\boldsymbol{a}$, etc. The inverse transformation is

$$\begin{aligned} \boldsymbol{a} &= \alpha_1\boldsymbol{x} + \beta_1\boldsymbol{y} + \gamma_1\boldsymbol{z} \\ \boldsymbol{b} &= \alpha_2\boldsymbol{x} + \beta_2\boldsymbol{y} + \gamma_2\boldsymbol{z} \\ \boldsymbol{c} &= \alpha_3\boldsymbol{x} + \beta_3\boldsymbol{y} + \gamma_3\boldsymbol{z}. \end{aligned} \tag{13}$$

Note that the matrix of the coefficients of the inverse transformation is the transpose of the matrix of the original transformation.

The nine direction cosines $\alpha_1 \ldots \gamma_3$ are not independent: the orthonormality conditions $\boldsymbol{x}\cdot\boldsymbol{x} = 1$ and $\boldsymbol{x}\cdot\boldsymbol{y} = 0$ (for example) imply

$$\alpha_1^2 + \alpha_2^2 + \alpha_3^2 = 1 \qquad \alpha_1\beta_1 + \alpha_2\beta_2 + \alpha_3\beta_3 = 0. \tag{14}$$

There are six such conditions, and six more (not independent of the first six) arising from $\boldsymbol{a}\cdot\boldsymbol{a} = 1$, $\boldsymbol{a}\cdot\boldsymbol{b} = 0$, etc. Only three independent parameters are required to specify the transformation (for example the three Euler angles).

We are now ready to transform from the principal axes to the laboratory frame to find ε_{ij}, since it is known (Nye 1957) that the elements of the dielectric function form a second-rank tensor, which transforms according to

$$T'_{ij} = \sum_k \sum_l a_{ik}a_{jl}T_{kl}. \tag{15}$$

The elements a_{ik} of the transformation are given by the coefficients in (12), and we have just seen that the inverse transformation is the transpose of this, so that (15) can be written as a similarity transformation

$$T'_{ij} = \sum_k \sum_l a_{ik} T_{kl} \tilde{a}_{lj} \tag{16}$$

where the tilde denotes a transpose. Thus the tensor ε_{ij} in (2) is to be found from

$$\begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{pmatrix} = \begin{pmatrix} \alpha_1 & \alpha_2 & \alpha_3 \\ \beta_1 & \beta_2 & \beta_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix} \begin{pmatrix} \varepsilon_a & 0 & 0 \\ 0 & \varepsilon_b & 0 \\ 0 & 0 & \varepsilon_c \end{pmatrix} \begin{pmatrix} \alpha_1 & \beta_1 & \gamma_1 \\ \alpha_2 & \beta_2 & \gamma_2 \\ \alpha_3 & \beta_3 & \gamma_3 \end{pmatrix}$$

$$= \begin{pmatrix} \varepsilon_a\alpha_1^2 + \varepsilon_b\alpha_2^2 + \varepsilon_c\alpha_3^2 & \varepsilon_a\alpha_1\beta_1 + \varepsilon_b\alpha_2\beta_2 + \varepsilon_c\alpha_3\beta_3 & \varepsilon_a\alpha_1\gamma_1 + \varepsilon_b\alpha_2\gamma_2 + \varepsilon_c\alpha_3\gamma_3 \\ \varepsilon_a\alpha_1\beta_1 + \varepsilon_b\alpha_2\beta_2 + \varepsilon_c\alpha_3\beta_3 & \varepsilon_a\beta_1^2 + \varepsilon_b\beta_2^2 + \varepsilon_c\beta_3^2 & \varepsilon_a\beta_1\gamma_1 + \varepsilon_b\beta_2\gamma_2 + \varepsilon_c\beta_3\gamma_3 \\ \varepsilon_a\alpha_1\gamma_1 + \varepsilon_b\alpha_2\gamma_2 + \varepsilon_c\alpha_3\gamma_3 & \varepsilon_a\beta_1\gamma_1 + \varepsilon_b\beta_2\gamma_2 + \varepsilon_c\beta_3\gamma_3 & \varepsilon_a\gamma_1^2 + \varepsilon_b\gamma_2^2 + \varepsilon_c\gamma_3^2 \end{pmatrix}. \tag{17}$$

We note the $\varepsilon_{ij} = \varepsilon_{ji}$ symmetry of the dielectric tensor follows from the transformation properties and the assumption of diagonal form for ε in some cartesian frame. Born and Wolf (1970, section 14.1) show that the symmetry of the dielectric tensor is related to the form taken by conservation of energy in the electromagnetic field, and that this symmetry implies the existence of principal axes in which the dielectric tensor is diagonal.

3. Dielectric tensor and normal modes in uniaxial crystals

In uniaxial crystals two of the principal dielectric constants ε_a, ε_b and ε_c are equal. Let us denote by $\varepsilon_o = n_o^2$ the common value of ε_a and ε_b, and by $\varepsilon_e = n_e^2$ the value of ε_c. The subscripts o and e stand for ordinary and extraordinary. It is convenient to define the anisotropy as $\Delta\varepsilon = \varepsilon_e - \varepsilon_o$, and set $\varepsilon_e = \varepsilon_o + \Delta\varepsilon$ in (17). Then use of the six orthonormality conditions of the type shown in (14) reduces the dielectric tensor in the laboratory frame to

$$\begin{pmatrix} \varepsilon_o + \alpha^2\Delta\varepsilon & \alpha\beta\Delta\varepsilon & \alpha\gamma\Delta\varepsilon \\ \alpha\beta\Delta\varepsilon & \varepsilon_o + \beta^2\Delta\varepsilon & \beta\gamma\Delta\varepsilon \\ \alpha\gamma\Delta\varepsilon & \beta\gamma\Delta\varepsilon & \varepsilon_o + \gamma^2\Delta\varepsilon \end{pmatrix}. \tag{18}$$

Here α, β and γ stand for α_3, β_3 and γ_3, the direction cosines of the optic axis (denoted as the $\boldsymbol{c}$ axis above) in the laboratory frame. The other direction cosines have dropped out, and the suffix 3 will be suppressed from now on. We note that the dielectric tensor is equal to ε_o times the unit tensor of second rank, plus $\Delta\varepsilon$ times a symmetric tensor whose elements are bilinear in the direction cosines α, β and γ. The remaining constraints on the direction cosines are

$$\alpha^2 + \beta^2 + \gamma^2 = 1 \qquad -1 \leqslant \alpha, \beta, \gamma \leqslant 1 \tag{19}$$

(the first relation comes from $\boldsymbol{c} \cdot \boldsymbol{c} = 1$).

We are now ready to find the normal modes, the eigenvalues of which are given by substituting the elements ε_{ij} from (18) into (11):

$$\begin{vmatrix} \varepsilon_o+\alpha^2\Delta\varepsilon-q^2/k^2 & \alpha\beta\Delta\varepsilon & \alpha\gamma\Delta\varepsilon+qK/k^2 \\ \alpha\beta\Delta\varepsilon & \varepsilon_o+\beta^2\Delta\varepsilon-(K^2+q^2)/k^2 & \beta\gamma\Delta\varepsilon \\ \alpha\gamma\Delta\varepsilon+qK/k^2 & \beta\gamma\Delta\varepsilon & \varepsilon_o+\gamma^2\Delta\varepsilon-K^2/k^2 \end{vmatrix} = 0. \tag{20}$$

This quartic in q can be factored into two quadratics: we note that $q = \pm q_o$, where

$$q_o^2 = \varepsilon_o k^2 - K^2 \tag{21}$$

are solutions of (20). After factoring out $q^2 - q_o^2$, the remaining quadratic is

$$(\varepsilon_o + \gamma^2\Delta\varepsilon)q^2 + (2\alpha\gamma K\Delta\varepsilon)q - [\varepsilon_o\varepsilon_e k^2 - K^2(\varepsilon_o + \alpha^2\Delta\varepsilon)] = 0 \tag{22}$$

with roots

$$q_e = (\pm\sqrt{d} - \alpha\gamma K\Delta\varepsilon)/(\varepsilon_o + \gamma^2\Delta\varepsilon) \tag{23}$$

(the positive sign corresponds to propagation into the crystal), where the discriminant d is given by

$$d = \varepsilon_o[\varepsilon_e(\varepsilon_o + \gamma^2\Delta\varepsilon)k^2 - (\varepsilon_e - \beta^2\Delta\varepsilon)K^2]. \tag{24}$$

From (22) it follows that

$$[(\varepsilon_o+\gamma^2\Delta\varepsilon)/\Delta\varepsilon](q_e^2-q_o^2) = \beta^2\varepsilon_o k^2+(\alpha q_o-\gamma K)^2+2\alpha\gamma K(q_o-q_e). \tag{25}$$

The right-hand side is non-negative, with zero as minimum value, attained when $\alpha q_o = \pm\gamma K$ and $\beta = 0$ (optic axis in the plane of incidence). The maximum value $\varepsilon_o k^2$ occurs when $\beta^2 = 1$ (and $\alpha, \gamma = 0$), the optic axis then being perpendicular to the plane of incidence. Thus q_e^2 is bounded by $q_o^2 = \varepsilon_o k^2 - K^2$ and $q_o^2 + \Delta\varepsilon k^2 = \varepsilon_e k^2 - K^2$, these bounds being reached under the conditions just given.

The ordinary and extraordinary modes have wave vector normal components q_o and q_e, and electric field vectors $\boldsymbol{E}^o$ and $\boldsymbol{E}^e$. To find $\boldsymbol{E}^o$ and $\boldsymbol{E}^e$ we substitute q_o and q_e for q in the equations (8) to (10), and obtain three sets of equations of the form $\Sigma_j b_{ij}E_j = 0$, where b_{ij} are the elements in the matrix corresponding to the determinant in (20). The corresponding eigenstates have $\boldsymbol{E}$ components proportional to each of the following parallel vectors:

$$\begin{array}{lll} (b_{22}b_{33}-b_{23}^2, & b_{13}b_{23}-b_{12}b_{33}, & b_{12}b_{33}-b_{13}b_{22}) \\ (b_{12}b_{23}-b_{13}b_{22}, & b_{12}b_{13}-b_{11}b_{23}, & b_{11}b_{22}-b_{12}^2) \\ (b_{13}b_{23}-b_{12}b_{33}, & b_{11}b_{33}-b_{13}^2, & b_{12}b_{13}-b_{11}b_{23}). \end{array} \tag{26}$$

Thus $\boldsymbol{E}^o$ is obtained by substituting $q = q_o$ in the array of equation (20). We find

$$\boldsymbol{E}^o = N_o(-\beta q_o, \alpha q_o - \gamma K, \beta K) \tag{27}$$

where N_o is a normalization factor. We note that the electric field vector of the ordinary mode is always perpendicular to the optic axis $\boldsymbol{c} = (\alpha, \beta, \gamma)$. The extraordinary electric field vector is obtained similarly by substituting $q = q_e$ in the array of equation (20), and using (26). Its components are

$$\begin{aligned} E_x^e/N_e &= \alpha q_o^2 - \gamma q_e K \\ E_y^e/N_e &= \beta\varepsilon_o k^2 \\ E_z^e/N_e &= \gamma(\varepsilon_o k^2 - q_e^2) - \alpha q_e K \end{aligned} \tag{28}$$

where N_e is the normalization factor for the extraordinary wave.

The scalar product of the ordinary and extraordinary electric field eigenvectors is

$$E^{o} \cdot E^{e} = \beta K(\alpha K + \gamma q_e)(q_o - q_e)N_o N_e. \tag{29}$$

The electric fields are orthogonal when the optic axis lies in the plane of incidence ($\beta = 0$), at normal incidence ($K = 0$), in the isotropic limit ($q_o = q_e$), and also when $\alpha K + \gamma q_e = 0$. When the last condition is satisfied, the extraordinary wavevector and ray direction (given by (31)) are both that of $(\gamma, 0, -\alpha)$, and thus perpendicular to the optic axis (α, β, γ).

The wavevector, giving the direction of the normal to the surface of constant phase, is given by $(K, 0, q)$ with $q = q_o$ or q_e for the two modes. The ray direction is given by

$$kE \times B = K(E_y^2 + E_z^2) - qE_zE_x, -E_y(KE_x + qE_z), q(E_x^2 + E_y^2) - KE_zE_x. \tag{30}$$

For the ordinary mode this has the same direction as the wavevector. For the extraordinary mode the ray direction is that of

$$\begin{aligned} &(\alpha q_e - \gamma K)[\alpha q_e K - \gamma(\varepsilon_o k^2 - q_e^2)] + \beta^2 K \varepsilon_o \\ &\beta(\alpha K + \gamma q_e)(q_e^2 - q_o^2) \\ &(\alpha q_e - \gamma K)(\alpha q_o^2 - \gamma q_e K) + \beta^2 q_e \varepsilon_o k^2. \end{aligned} \tag{31}$$

The extraordinary ray and wave vector are coplanar with the optic axis. Further discussion of ray direction in special geometries will be given in section 5.

4. The reflection and transmission amplitudes

To calculate the reflection and transmission of an incoming wave plane-polarized in an arbitrary direction, we decompose the incoming field into its s and p components, where E_s is perpendicular to the plane of incidence (the zx plane) and E_p lies in the plane of incidence. We consider the s polarization first. The z-dependence of the electric field components is

$$\begin{aligned} &\text{incoming:} && (0, \exp(iq_1z), 0) \\ &\text{reflected:} && (r_{sp}\cos\theta\exp(-iq_1z), r_{ss}\exp(-iq_1z), r_{sp}\sin\theta\exp(-iq_1z)) \\ &\text{transmitted:} && t_{so}\exp(iq_0z)(E_x^o, E_y^o, E_z^o) + t_{se}\exp(iq_ez)(E_x^e, E_y^e, E_z^e) \end{aligned} \tag{32}$$

where θ is the angle of incidence, q_1 is the z-component of the incoming wave vector, and r_{ss}, r_{sp}, t_{so} and t_{se} are the reflection and transmission amplitudes for an incoming s wave. At the end of section 1 we deduced the boundary conditions to be applied, namely the continuity of E_x, E_y, $\partial E_x/\partial z - iKE_z$, and $\partial E_y/\partial z$. At the reflecting plane ($z = 0$) these give

$$\begin{aligned} &r_{sp}\cos\theta = t_{so}E_x^o + t_{se}E_x^e \\ &1 + r_{ss} = t_{so}E_y^o + t_{se}E_y^e \\ &-q_1r_{sp}\cos\theta - Kr_{sp}\sin\theta = q_ot_{so}E_x^o + q_et_{se}E_x^e - K(t_{so}E_z^o + t_{se}E_z^e) \\ &q_1(1 - r_{ss}) = q_ot_{so}E_y^o + q_et_{se}E_y^e. \end{aligned} \tag{33}$$

These four equations may be solved for the four unknowns r_{ss}, r_{sp}, t_{so}, t_{se}. We find

$$r_{ss} = [(q_1 - q_e)AE_y^e - (q_1 - q_o)BE_y^o]/D$$
$$r_{sp} = 2n_1k(AE_x^e - BE_x^o)/D \tag{34}$$
$$t_{so} = -2q_1B/D \qquad t_{se} = -2q_1A/D$$

where $n_1 = \varepsilon_1^{1/2}$ is the refractive index of the medium of incidence, and

$$A = (q_o + q_1 + K\tan\theta)\,E_x^o - KE_z^o$$
$$B = (q_e + q_1 + K\tan\theta)\,E_x^e - KE_z^e \tag{35}$$
$$D = (q_1 + q_e)AE_y^e - (q_1 + q_o)BE_y^o.$$

The isotropic limit is obtained by letting $\Delta\varepsilon \to 0$. We find that the isotropic limit of $\boldsymbol{E}^e$ is

$$\boldsymbol{E}^e \to N_e(q_o(\alpha q_o - \gamma K), \beta\varepsilon_o k^2, -K(\alpha q_o - \gamma K)). \tag{36}$$

This $\boldsymbol{E}^e$ is perpendicular to $\boldsymbol{E}^o$, in accord with (29). The reflection and transmission amplitudes in the isotropic limit tend to

$$r_{ss} \to (q_1 - q_o)/(q_1 + q_o) \qquad r_{sp} \to 0$$
$$t_{so} \to [2q_1/(q_1 + q_o)](\alpha q_o - \gamma K)N_o \qquad t_{se} \to [2q_1/(q_1 + q_o)]\beta\varepsilon_o k^2 N_e. \tag{37}$$

The reflection amplitude for s to s polarization reproduces the Fresnel equation (see for example Lekner (1987), equations 1.13 and 1.14). The transmission amplitudes are such that the transmitted field is pure s in this isotropic limit, with the usual Fresnel amplitude:

$$t_{se}\boldsymbol{E}^o + t_{se}\boldsymbol{E}^e \to [2q_1/(q_1 + q_o)](0, 1, 0). \tag{38}$$

This result follows from (27), (36) and the fact that

$$N_o^{-2} = \beta^2\varepsilon_o k^2 + (\alpha q_o - \gamma K)^2 \qquad N_e^2 \to N_o^2/\varepsilon_o k^2. \tag{39}$$

We next turn to the reflection of the p wave. The z-dependence of the electric field components is, for incidence at θ to the surface normal,

$$\begin{aligned}
&\text{incoming:} && (\cos\theta\exp(\mathrm{i}q_1 z), 0, -\sin\theta\exp(\mathrm{i}q_1 z)) \\
&\text{reflected:} && (r_{pp}\cos\theta\exp(-\mathrm{i}q_1 z), r_{ps}\exp(-\mathrm{i}q_1 z), r_{pp}\sin\theta\exp(-\mathrm{i}q_1 z)) \\
&\text{transmitted:} && t_{po}\exp(\mathrm{i}q_o z)(E_x^o, E_y^o, E_z^o) + t_{pe}\exp(\mathrm{i}q_e z)(E_x^e, E_y^e, E_z^e).
\end{aligned} \tag{40}$$

The continuity of E_x, E_y, $\partial E_x/\partial z - \mathrm{i}KE_z$ and $\partial E_y/\partial z$ at $z = 0$ gives

$$\begin{aligned}
&\cos\theta(1 + r_{pp}) = t_{po}E_x^o + t_{pe}E_x^e \\
&r_{ps} = t_{po}E_y^o + t_{pe}E_y^e \\
&n_1k(1 - r_{pp}) = q_o t_{po}E_x^o + q_e t_{pe}E_x^e - K(t_{po}E_z^o + t_{pe}E_z^e) \\
&-q_1 r_{ps} = q_o t_{po}E_y^o + q_e t_{pe}E_y^e
\end{aligned} \tag{41}$$

(we have used the fact that $q_1\cos\theta + K\sin\theta = n_1k = \varepsilon_1^{1/2}k$). The solution of (41) is

$$\begin{aligned}
&r_{pp} = (2q_1/D)[(q_1 + q_e)E_x^o E_y^e - (q_1 + q_o)E_x^e E_y^o] - 1 \\
&r_{ps} = 2n_1k(q_e - q_o)E_y^o E_y^e/D \\
&t_{po} = 2n_1k(q_1 + q_e)E_y^e/D \\
&t_{pe} = -2n_1k(q_1 + q_o)E_y^o/D.
\end{aligned} \tag{42}$$

The denominator D is as defined in (35), and

$$q_t = q_1 + K\tan\theta = \varepsilon_1 k^2/q_1. \tag{43}$$

(The reader is reminded that $q_1 = kn_1\cos\theta$, $K = kn_1\sin\theta$.)

In the isotropic limit we find, using the notation $Q_1 = q_1/\varepsilon_1$, $Q_o = q_o/\varepsilon_o$,

$$\begin{aligned} &r_{pp} \to (Q_o - Q_1)/(Q_o + Q_1) \qquad r_{ps} \to 0 \\ &t_{po} \to -[2Q_1/(Q_1 + Q_o)]k^2 n_1 n_o \beta N_e \\ &t_{pe} \to [2Q_1/(Q_1 + Q_o)](n_1/n_o)(\alpha q_o - \gamma K)N_o. \end{aligned} \tag{44}$$

The reflection and transmission amplitudes are in accord with the known results for isotropic media: see for example Lekner (1987), equation (1.31). Note that the transmitted electric field amplitude is

$$\boldsymbol{E} \to [2Q_1/(Q_1 + Q_o)](n_1/\varepsilon_o k)(q_o, 0, -K) \tag{45}$$

which has magnitude

$$|E| \to [2Q_1/(Q_1 + Q_o)](n_1/n_o) \tag{46}$$

and (from (3)) corresponds to a magnetic field along the y axis.

The s to p and p to s reflection amplitudes may be factored to show the conditions under which they are zero:

$$\begin{aligned} r_{sp} &= 2\beta(\alpha q_o + \gamma K)(q_e - q_o)k^3 n_1 \varepsilon_o N_o N_e/D \\ r_{ps} &= 2\beta(\alpha q_o - \gamma K)(q_e - q_o)k^3 n_1 \varepsilon_o N_o N_e/D. \end{aligned} \tag{47}$$

Both are zero when the optic axis lies in the plane of incidence. The difference

$$r_{sp} - r_{ps} = 4\beta\gamma K(q_e - q_o)k^3 n_1 \varepsilon_o N_o N_e/D \tag{48}$$

is also zero when the optic axis lies in the reflecting plane ($\gamma = 0$), and at normal incidence ($K = 0$).

5. Special geometries

The reflection and transmission amplitudes for electromagnetic waves incident on an arbitrary face of a uniaxial anisotropic medium are given by (34) and (42) for incident s and p polarizations. We now look at some important special configurations.

5.1. Reflection from a basal plane (one perpendicular to the optic axis)

When the normal to the reflecting surface coincides with the optic axis, the system has azimuthal symmetry. The direction cosines are $\gamma = \pm 1$, $\alpha = 0 = \beta$. The eigenvalues for the normal component of the wave vector are given by $q_o^2 = \varepsilon_o k^2 - K^2$ (as always) and

$$q_e^2 = \varepsilon_o k^2 - (\varepsilon_o/\varepsilon_e)K^2. \tag{49}$$

The eigenstates are (taking $\gamma = -1$, with the optic axis out from, and z axis into the reflecting plane),

$$\boldsymbol{E}^o = (0, 1, 0) \qquad \boldsymbol{E}^e = N_e(q_e, 0, -(\varepsilon_o/\varepsilon_e)K) \tag{50}$$

The cross reflection amplitudes r_{ps} and r_{sp} are zero, and

$$r_{ss} = (q_1 - q_o)/(q_1 + q_o) \qquad r_{pp} = (Q - Q_1)/(Q + Q_1) \tag{51}$$

where $Q = q_e/\varepsilon_o$, and $Q_1 = q_1/\varepsilon_1$ as before. In the absence of absorption the r_{pp} coefficient is zero at a Brewster angle given by

$$\tan^2\theta_B = \varepsilon_e(\varepsilon_o - \varepsilon_1)/\varepsilon_1(\varepsilon_e - \varepsilon_1) \tag{52}$$

(note that a real θ_B will not exist when ε_1 lies between ε_o and ε_e). These results have been given previously (Lekner 1987, section 7–1; see also Azzam and Bashara 1977, pp 354–355 for formulae and references relevant to this and the next subsection). The transmission amplitudes are

$$t_{so} = 2q_1/(q_1 + q_o) \qquad t_{se} = 0 \qquad t_{po} = 0 \qquad t_{pe} = [(2Q_1/(Q_1 + Q)](n_1/\varepsilon_o k N_e). \tag{53}$$

5.2. *Reflection from a plane parallel to the optic axis*

The optic axis now lies in the reflecting plane (an example is reflection from a prism face of ice). Let φ be the angle between the optic axis and the x axis. In terms of the azimuthal angle φ, the direction cosines are $\alpha = \cos\varphi$, $\beta = \pm\sin\varphi$, $\gamma = 0$. The q eigenvalues are given by $q_o^2 = \varepsilon_o k^2 - K^2$ and

$$q_e^2 = q_o^2 + (\Delta\varepsilon/\varepsilon_o)(\varepsilon_o k^2 - \alpha^2 K^2). \tag{54}$$

The eigenvectors are

$$\begin{aligned} &\boldsymbol{E}^o = N_o(-\beta q_o, \alpha q_o, \beta K) \qquad \boldsymbol{E}^e = N_e(\alpha q_o^2, \beta\varepsilon_o k^2, -\alpha q_e K) \\ &N_o^{-2} = \varepsilon_o k^2 - \alpha^2 K^2 \qquad N_e^{-2} = N_o^{-2}(\varepsilon_o k^2 + (\Delta\varepsilon/\varepsilon_o)\alpha^2 K^2) \end{aligned} \tag{55}$$

with

$$\boldsymbol{E}^o \cdot \boldsymbol{E}^e = \alpha\beta K^2 N_o N_e (q_0 - q_e). \tag{56}$$

The extraordinary ray direction is that of $(K(\varepsilon_o + \alpha^2\Delta\varepsilon), \alpha\beta K\Delta\varepsilon, q_e\varepsilon_o)$.

We now look at the reflection amplitudes, starting with the cross terms, since these are simpler. Using the fact that (for $\gamma = 0$)

$$A = -\beta N_o(\varepsilon_o k^2 + q_o q_1) \qquad B = \alpha N_e(\varepsilon_o k^2 q_e + q_o^2 q_1) \tag{57}$$

we find that

$$r_{sp} = r_{ps} = 2\alpha\beta q_o(q_o - q_e)n_1 k/D' \tag{58}$$

where

$$\begin{aligned} D' = -\frac{D}{\varepsilon_o k^2 N_o N_e} &= (q_1 + q_o)\left(\frac{Q_o}{Q_1} + 1\right)(\varepsilon_o k^2 - \alpha^2 K^2) \\ &+ (q_e - q_o)\left(\varepsilon_o k^2 - \alpha^2 K^2 + \frac{q_o}{q_1}(\varepsilon_1 k^2 - \alpha^2 K^2)\right) \end{aligned} \tag{59}$$

with $Q_1 = q_1/\varepsilon_1$ as before, and $Q_o = q_o/\varepsilon_o$. Note that the cross reflection amplitudes are zero when the optic axis is parallel or perpendicular to the plane of incidence. The direct reflection amplitudes are given by

$$
\begin{aligned}
D'r_{ss} &= (q_1 - q_o)\left(\frac{Q_o}{Q_1} + 1\right)(\varepsilon_o k^2 - \alpha^2 K^2) - (q_e - q_o) \\
&\quad \times \left(\varepsilon_o k^2 - \alpha^2 K^2 + \frac{q_o}{q_1}[\varepsilon_1 k^2 - \alpha^2(2\varepsilon_1 k^2 - K^2)]\right) \\
D'r_{pp} &= (q_1 + q_o)\left(\frac{Q_o}{Q_1} - 1\right)(\varepsilon_o k^2 - \alpha^2 K^2) - (q_e - q_o) \\
&\quad \times \left(\varepsilon_o k^2 - \alpha^2 K^2 - \frac{q_o}{q_1}[\varepsilon_1 k^2 - \alpha^2(2\varepsilon_1 k^2 - K^2)]\right).
\end{aligned}
\tag{60}
$$

The s to s and p to p reflection amplitudes depend on $\alpha^2 = \cos^2\varphi$. As a function of the azimuthal angle φ they will thus have extrema when $\cos^2\varphi = 1$ or 0, that is when the optic axis is parallel or perpendicular to the plane of incidence. In these special configurations the cross reflection amplitudes are zero; in the parallel case $q_e = q_o n_e/n_o$, and

$$
\left.\begin{array}{l} c \parallel x \\ \varphi = 0 \quad \text{or} \quad \pi \\ \alpha = \pm 1, \beta = 0 \end{array}\right\} \qquad \begin{array}{l} r_{ss} = (q_1 - q_o)/(q_1 + q_o) \\ r_{pp} = (Q_e - Q_1)/(Q_e + Q_1) \end{array} \tag{61}
$$

where $Q_e = q_o/n_o n_e = q_e/\varepsilon_e$. The p to p reflection amplitude is zero at a Brewster angle of incidence given by

$$\tan^2\theta_B = \varepsilon_o(\varepsilon_e - \varepsilon_1)/\varepsilon_1(\varepsilon_o - \varepsilon_1). \tag{62}$$

As in the case above (see equation (52)), a real θ_B does not exist when ε_1 lies between ε_o and ε_e.

When the optic axis is perpendicular to the plane of incidence, $q_e^2 = \varepsilon_e k^2 - K^2$ and

$$
\left.\begin{array}{l} c \perp x \\ \varphi = \pi/2 \quad \text{or} \quad 3\pi/2 \\ \alpha = 0, \beta = \pm 1 \end{array}\right\} \qquad \begin{array}{l} r_{ss} = (q_1 - q_e)/(q_1 + q_e) \\ r_{pp} = (Q_o - Q_1)/(Q_o + Q_1). \end{array} \tag{63}
$$

The p to p reflection amplitude is zero at a Brewster angle given by

$$\tan^2\theta_B = \varepsilon_o/\varepsilon_1 \qquad \text{or} \qquad \tan\theta_B = n_o/n_1. \tag{64}$$

The results for the special configurations where the optic axis is parallel or perpendicular to the plane of incidence are in agreement with those of Elshazly-Zaghoul and Azzam (1982).

5.3. *Optic axis in the plane of incidence*

For the geometry used throughout this paper, the plane of incidence is the zx plane. Thus in this subsection the optic axis is perpendicular to the y axis, and $\beta = 0$. The eigenvalues of the normal component of the wave vector are q_o, and q_e as given by (23), with

$$d = \varepsilon_o \varepsilon_e (q_o^2 + \gamma^2 \Delta\varepsilon k^2). \tag{65}$$

The plane-wave propagating modes are orthogonal in this configuration:

$$\boldsymbol{E}^o = N_o(0, \alpha q_o - \gamma K, 0) \qquad \boldsymbol{E}^e = N_e(q_e K + \alpha\gamma\Delta\varepsilon k^2, 0, q_e^2 - \varepsilon_o k^2 - \alpha^2 \Delta\varepsilon k^2). \tag{66}$$

The extraordinary ray lies in the plane of incidence: its direction is that of $(\alpha q_e K - \gamma(\varepsilon_o k^2 - q_e^2), 0, \alpha q_o^2 - \gamma q_e K)$. The s to p and p to s reflection amplitudes are zero, and

$$r_{ss} = (q_1 - q_o)/(q_1 + q_o) \tag{67}$$

as expected. The p to p reflection amplitude is

$$r_{pp} = \frac{K(q_e q_t - \varepsilon_o k^2) - \alpha\Delta\varepsilon[\gamma(q_e - q_t) + \alpha K]k^2}{K(q_e q_t + \varepsilon_o k^2) + \alpha\Delta\varepsilon[\gamma(q_e + q_t) + \alpha K]k^2} \tag{68}$$

where $q_t = q_1 + K \tan\theta = \varepsilon_1 k^2/q_1 = k^2 Q_1^{-1}$ as before. This expression reduces to (51) when $\alpha = 0$ (reflection from a basal plane) and to (61) when $\alpha = 1$ (optic axis in reflecting plane and in plane of incidence).

5.4. Normal incidence

The final special configuration we consider is that of radiation incident perpendicularly onto the reflecting surface ($\theta = 0$). When $K = kn_1 \sin\theta$ is set to zero in our general formulae, the eigenvalues and eigenvectors become

$$q_o = kn_o \qquad q_e = kn_o n_e/n_\gamma \tag{69}$$

$$\boldsymbol{E}^o = N_o(-\beta, \alpha, 0) \qquad \boldsymbol{E}^e(\alpha, \beta, -\gamma(1-\gamma^2)\Delta\varepsilon/\varepsilon_\gamma) \tag{70}$$

where $n_\gamma^2 = \varepsilon_\gamma = \varepsilon_o + \gamma^2\Delta\varepsilon$ (ε_γ ranges from ε_o to ε_e, taking the value ε_o when the optic axis lies in the reflecting plane, and ε_e when the optic axis coincides with the surface normal). The ray direction is given by $(\alpha\gamma\Delta\varepsilon, \beta\gamma\Delta\varepsilon, \varepsilon_\gamma)$. For various orientations of the crystal axes the rays lie within a circular cone with the inward normal as axis, and half-angle equal to $\arctan(|\Delta\varepsilon|/2n_o n_e)$. Maximum deviation from the normal occurs when $\gamma^2 = \varepsilon_o/(\varepsilon_o + \varepsilon_e)$.

The reflection amplitudes are found from (34) and (42):

$$r_{ss} = \frac{\alpha^2(n_1 - n_o)(n_1 n_\gamma + n_o n_e) + \beta^2(n_1 + n_o)(n_1 n_\gamma - n_o n_e)}{(\alpha^2 + \beta^2)(n_1 + n_o)(n_1 n_\gamma + n_o n_e)} \tag{71}$$

$$r_{pp} = \frac{\alpha^2(n_1 + n_o)(n_1 n_\gamma - n_o n_e) + \beta^2(n_1 - n_o)(n_1 n_\gamma + n_o n_e)}{(\alpha^2 + \beta^2)(n_1 + n_o)(n_1 n_\gamma + n_o n_e)} \tag{72}$$

$$r_{sp} = r_{ps} = \frac{2\alpha\beta n_1 n_o(n_\gamma - n_e)}{(\alpha^2 + \beta^2)(n_1 + n_o)(n_1 n_\gamma + n_o n_e)}. \tag{73}$$

When the optic axis lies in the reflecting plane ($\gamma = 0$, $\alpha^2 + \beta^2 = 1$), these formulae reduce to

$$r_{ss} = \alpha^2 \frac{n_1 - n_o}{n_1 + n_o} + (1 - \alpha^2) \frac{n_1 - n_e}{n_1 + n_e} = \frac{(n_1 + n_o)(n_1 - n_e) + 2\alpha^2 n_1 (n_e - n_o)}{(n_1 + n_o)(n_1 + n_e)} \tag{74}$$

$$r_{pp} = \alpha^2 \frac{n_1 - n_e}{n_1 + n_e} + (1 - \alpha^2) \frac{n_1 - n_o}{n_1 + n_o} = \frac{(n_1 - n_o)(n_1 + n_e) - 2\alpha^2 n_1 (n_e - n_o)}{(n_1 + n_o)(n_1 + n_e)} \tag{75}$$

$$r_{sp} = r_{ps} = \frac{2\alpha\beta n_1 (n_o - n_e)}{(n_1 + n_o)(n_1 + n_e)}. \tag{76}$$

These results agree with those of subsection (b) above, when K is set to zero in the formulae (58) to (60). The $\gamma = 0$ results also agree with Yeh 1988, equations 9.6–48 to 50, but not with his r_{pp} expression.

The transmission amplitude depend on the factors N_o and N_e which normalize $\boldsymbol{E}^o$ and $\boldsymbol{E}^e$ to unit magnitude. These are given by

$$N_o^{-2} = 1 - \gamma^2 \qquad N_e^{-2} = N_o^{-2}[1 + \gamma^2(1 - \gamma^2)(\Delta\varepsilon/\varepsilon_\gamma)^2]. \tag{77}$$

From (34) and (42) we find

$$t_{so} = \frac{\alpha}{\sqrt{\alpha^2 + \beta^2}} \frac{2n_1}{n_1 + n_o} \qquad t_{se} = \frac{\beta N_e^{-1}}{\alpha^2 + \beta^2} \frac{2n_1 n_\gamma}{n_1 n_\gamma + n_o n_e} \tag{78}$$

$$t_{po} = -\frac{\beta}{\sqrt{\alpha^2 + \beta^2}} \frac{2n_1}{n_1 + n_o} \qquad t_{pe} = \frac{\alpha N_e^{-1}}{\alpha^2 + \beta^2} \frac{2n_1 n_\gamma}{n_1 n_\gamma + n_o n_e}. \tag{79}$$

When the reflection is from a plane parallel to the optic axis ($\gamma = 0$) these formulae simplify to

$$t_{so} = \alpha\, 2n_1/(n_1 + n_o) \qquad t_{se} = \beta\, 2n_1/(n_1 + n_e) \tag{80}$$

$$t_{po} = -\beta\, 2n_1/(n_1 + n_o) \qquad t_{pe} = \alpha\, 2n_1/(n_1 + n_e). \tag{81}$$

The $\gamma = 0$ subset is consistent with that of Yeh (1988), p 237.

6. Summary and discussion

We have presented explicit formulae for the reflection and transmission amplitudes for the s and p polarized electromagnetic waves incident on an arbitrary face of a uniaxial crystal. The results are expressed in terms of the direction cosines of the optic axis relative to the laboratory axes, where xy is the reflecting surface, and zx is the plane of incidence. The ordinary and extraordinary electric fields, wavevectors and ray directions are also determined explicitly.

Some special configurations of practical interest were considered. These help also in providing counter-examples to conjectures one might make, for example that the cross-reflection terms r_{ps} and r_{sp} are zero whenever $\boldsymbol{E}^o$ and $\boldsymbol{E}^e$ are orthogonal (this is not true in general, since $\boldsymbol{E}^o \cdot \boldsymbol{E}^e = 0$ at normal incidence (from (70)), but r_{ps} and r_{sp} are not zero). It is not even true that $r_{ps} = r_{sp}$ whenever $\boldsymbol{E}^o \cdot \boldsymbol{E}^e = 0$. Another expectation, that the Brewster angle θ_B will lie between arctan (n_o/n_1) and arctan (n_e/n_1), is also false. In fact zero reflectance of the p polarization need not exist in some circumstances, in contrast to reflection from non-absorbing isotropic media. But arctan (n_o/n_1) is an upper or lower bound for θ_B in some special geometries; see for example subsection 5.2.

Gaussian units have been used for simplicity, and to avoid confusion between ε_o $(=n_o^2)$ and ε_0 (the permittivity of the vacuum). All formulae from equation (11) on are unchanged in SI units, provided the dielectric constants are interpreted as the dimensionless ratios $\varepsilon/\varepsilon_0$.

In numerical work it is convenient to use n_o/n_1 and n_e/n_1 as the effective ordinary and extraordinary refractive indices, and also to set $k = \omega/c = 1$, in which case q_1 and K may be set equal to $\cos\theta$ and $\sin\theta$ respectively.

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