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Eigenequations and Compact Algorithms for Bulk and Layered Anisotropic Optical Media: Reflection and Refraction at a Crystal-Crystal Interface*

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Eigenequations leading to compact algorithms for computing the optical properties of anisotropic media that may be stratified in the x-direction are described. For each medium a 4×4 matrix $\hat{F}$ of basis field vectors is determined as the eigenvectors of a 4×4 matrix form of Fresnel's equation. A minimum sort of the columns of $\hat{F}$ that is necessary for a birefringent cover or substrate separates basis vectors that carry power in the positive and negative x-directions respectively. A sorting procedure is discussed for the most complicated refractive index section in which the outer and inner sheets do not touch and the outer sheet has a well defined cusp. MATLAB code is provided for the implementation of basic routines.

1. INTRODUCTION

Birefringent materials are used extensively for measuring or changing the polarization state of light. When the materials are used with coherent light interference effects caused by multiple reflections have a significant effect on overall properties. Thus the exact phase retardation of a wave plate in a laser beam depends on the interferometric thickness of the plate.

Current developmental work on the deposition and characterization of birefringent optical coatings requires access to computer routines which are both robust and flexible. For example, computation of reflectance and transmittance at an arbitrary angle of incidence may be required in one application, computation of phase retardation in a second application, and modelling of transmission in a planar biaxial waveguide in another.

Several authors have contributed to the development of 4×4 matrix theories for describing propagation in anisotropic media [1–3], and the matrix method has been applied to thin films [4], waveguides [5], and macroscopic devices such as birefringent filters for tuning the output wavelength of lasers [6]. However, these papers have a theoretical direction rather than a computing focus, and the reader is left with a significant amount of work to do in order to develop a useful computer program. Thus there remains a need for simple algorithms for computing optical properties resulting from propagation in anisotropic media.

In this article we derive compact algorithms that are based on the solution of eigenequations derived from Maxwell's equations. We begin by reviewing the relevant properties of anisotropic media, develop the algorithms, and then discuss a procedure for sorting the eigenvalues and eigenvectors by considering the most complicated example. Finally, implementation code for MATLAB [7] is listed in an appendix.

2. MATERIAL AND PROPAGATION AXES

2.1. *Material Principal Axes*

We consider a general linear biaxial dielectric medium that is nonmagnetic and not optically active. Such a medium has three mutually orthogonal principal dielectric axes, which we label 1, 2, 3 as shown in Fig. 1, and three associated principal refractive indices n_1, n_2, n_3. Thus n_1 is the refractive index "seen" by light travelling with its electric field $\mathbf{E}$ parallel to the 1-axis. For more general directions of propagation the polarization of the light is determined by the electric displacement, $\mathbf{D}$, which is related to the electric field by the dielectric permittivity, $\mathbf{D} = \varepsilon_0 \boldsymbol{\varepsilon} \mathbf{E}$, where $\boldsymbol{\varepsilon}$ is a symmetric tensor of rank 2.

In general we shall represent a field such as $\mathbf{E}$ by a column vector formed from the components of $\mathbf{E}$. To make equations easier to read, a right overarrow symbol $\rightarrow$ is used to identify a column vector and the hat symbol ˆ indicates a matrix. Thus,

$$\vec{E}_{123} = \begin{bmatrix} E_1 \\ E_2 \\ E_3 \end{bmatrix} \tag{1}$$

represents the electric field of a travelling wave in the

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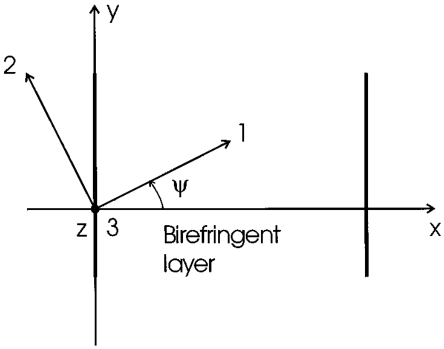

FIG. 1. The axes 1, 2, 3 are the principal axes, with associated principal refractive indices n_1, n_2, n_3, of the biaxial medium. Light propagates in the x–y plane and layer interfaces are parallel to the y–z plane. The orientation of the biaxial medium is determined by the rotation ψ of the medium about the z-axis shown in the figure, followed by a rotation ξ about the x-axis.

material frame. The components E_1, E_2, E_3 are amplitudes that may be signed or complex, but note that the complex exponential spatial and temporal phase terms of the wave, which we write as $\exp(ik\alpha x)$, $\exp(ik\beta y)$, $\exp(-i\omega t)$ with $k = 2\pi/\lambda = \omega/c$, $\alpha = n \cos\theta$, $\beta = n \sin\theta$, are implied but not included explicitly.

The relative permittivity is represented by a diagonal matrix in the material frame,

$$\hat{\varepsilon}_{123} = \begin{bmatrix} \varepsilon_1 & 0 & 0 \\ 0 & \varepsilon_2 & 0 \\ 0 & 0 & \varepsilon_3 \end{bmatrix}, \tag{2}$$

where $\varepsilon_1 = n_1^2$, $\varepsilon_2 = n_2^2$, and $\varepsilon_3 = n_3^2$.

2.2. *Light Propagation Axes*

We shall assume, without loss of generality, that light propagates in the x–y plane, as shown in Fig. 2. As a

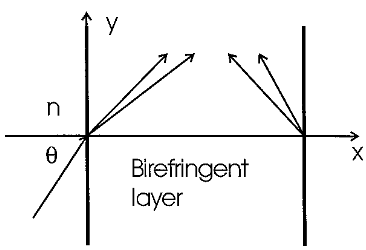

FIG. 2. An incident plane wave establishes four travelling waves in a biaxial layer. Multiple reflections between the interfaces and interference effects are included. All five waves have the same value of $\beta = n \sin\theta$, and hence, the y-components of the five wavevectors are equal as illustrated. The values of $\alpha = n \cos\theta$, and hence, the x-components of the wavevectors are different, in general.

consequence the z-component of the wavenormal is zero, and we can write a column vector for the wavenormal in the form $\vec{s} = \{s_x\ s_y\ 0\} = \{\cos\theta \sin\theta\ 0\}$, where θ, the angle of incidence, is the angle between the wavenormal and the x-axis. Note that, by default, column vectors and matrices are assumed to be referenced to the propagation axes.

The relative directions of the material axes and the propagation axes are specified by starting with aligned axes and rotating the material in turn about x, z, and x again. Transformations between axes are readily carried out using the rotation matrices

$$\hat{S}_x(\phi) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\phi & -\sin\phi \\ 0 & \sin\phi & \cos\phi \end{bmatrix} \tag{3}$$

and

$$\hat{S}_z(\phi) = \begin{bmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{4}$$

For a tilted columnar thin film [5] it is sufficient to rotate the material by an angle ψ about z to establish the column angle in the deposition plane, followed by a rotation of ξ about x to establish the relative azimuth angle between the deposition plane and the propagation plane. As an example of the use of the rotation matrices (for the thin film case), the symmetric relative permittivity matrix for the propagation frame,

$$\hat{\varepsilon} = \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{xy} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{xz} & \varepsilon_{yz} & \varepsilon_{zz} \end{bmatrix}, \tag{5}$$

can be computed using the equation

$$\hat{\varepsilon} = \hat{S}_x(\xi)\hat{S}_z(\psi)\hat{\varepsilon}_{123}\hat{S}_z(-\psi)\hat{S}_x(-\xi). \tag{6}$$

3. PROPAGATION IN BULK BIAXIAL MEDIA

3.1. *Maxwell's Equations*

In this section we consider solutions for the two basis waves that can travel in the same direction in a biaxial medium. Each basis wave satisfies the vector form of Maxwell's equations for plane harmonic waves listed for SI units in the left side of Table I; $z_0 = (\mu_0/\varepsilon_0)^{1/2} \approx 377\ \Omega$ is

TABLE I
Maxwell's Equations for Plane Harmonic Waves

Vector form	Column vector form	Matrix form
$n_s\mathbf{s}\times\mathbf{E} = z_0\mathbf{H}$	$n_s\hat{s}\vec{E} = z_0\vec{H}$	$\hat{s}\hat{E}\hat{n}_s = z_0\hat{H}$
$n_s\mathbf{s}\times\mathbf{H} = -\frac{1}{z_0}\boldsymbol{\varepsilon}\mathbf{E}$	$n_s\hat{s}\vec{H} = -\frac{1}{z_0}\hat{\varepsilon}\vec{E}$	$\hat{s}\hat{H}\hat{n}_s = -\hat{\varepsilon}\hat{E}/z_0$
$\mathbf{s.D} = 0$	$\vec{s}'\vec{D} = 0$	$\vec{s}'\hat{D} = 0$
$\mathbf{s.H} = 0$	$\vec{s}'\vec{H} = 0$	$\vec{s}'\hat{H} = 0$

known as the impedance of free space. The middle column of the table shows a column vector form of Maxwell's equations for individual plane waves propagating in the x–y plane. These equations are derived from the equations in the right-hand column of the table by using the matrix

$$\hat{s} = \begin{bmatrix} 0 & 0 & s_y \\ 0 & 0 & -s_x \\ -s_y & s_x & 0 \end{bmatrix} \tag{7}$$

for $\vec{s}\times$; the row vector $\vec{s}' = [s_x\ s_y\ 0]$ is the simple transpose of $\vec{s}$. Note that the matrix $\hat{s}$ is singular, $|\hat{s}| = 0$. Hence, care is needed with matrix algebra involving $\hat{s}$.

The right side of Table I lists Maxwell's equations in matrix form. Here all solutions to the problem of plane wave propagation in a common direction are combined together. Thus $\hat{E}$, a 3×3 matrix, is formed using the $\vec{E}$'s as columns and $\hat{n}_s$ is a 3×3 diagonal matrix formed from the n_s's associated with the individual plane waves.

3.2. *Fresnel's Equation*

Note that the n's can be determined directly from the quadratic equation,

$$\begin{aligned}(s_1^2\varepsilon_1 + s_2^2\varepsilon_2 + s_3^2\varepsilon_3)n^4 \\ - [(s_1^2 + s_2^2)\varepsilon_1\varepsilon_2 + (s_2^2 + s_3^2)\varepsilon_2\varepsilon_3 \\ + (s_3^2 + s_1^2)\varepsilon_3\varepsilon_1]n^2 + \varepsilon_1\varepsilon_2\varepsilon_3 = 0,\end{aligned} \tag{8}$$

which is a form of Fresnel's equation [8]; s_1, s_2, and s_3 are required for this purpose and can be calculated using the rotation matrices, i.e., $\vec{s}_{123} = \hat{S}_z(-\psi)\hat{S}_x(-\xi)\vec{s}$.

3.3. *Eigenequations for Normalized Fields*

Matrix solutions to the problem of propagation in a common direction in a biaxial medium can be obtained from the column vector form of Maxwell's equations (middle row of Table I) in the following way. It is assumed that the relative permittivity $\hat{\varepsilon}$ is known and the wave propagation direction $\vec{s}$ is specified for the x–y propagation plane. The refractive indices $n_s = \varepsilon_s^{1/2}$ associated with the two waves and the fields $\vec{E}$, $\vec{D}$, $\vec{H}$ that appear in the equations, together with the magnetic induction $\vec{B} = \mu_0\vec{H}$, are the unknowns.

The first two equations in the middle row of Table I can be combined simultaneously, to eliminate $\vec{H}$. This leaves an equation for $\vec{E}$ which we organize as a generalized eigenequation, $\hat{I}\vec{E} = \varepsilon_s(-\hat{\varepsilon}^{-1}\hat{s}^2)\vec{E}$. Here $\hat{I}$ is an identity matrix (which is omitted later), the electric field $\vec{E}$ is an eigenvector and ε_s is an eignevalue. The outcome of this is that both the electric fields (which are normalized) and the refractive indices can be obtained by making a single call to the MATLAB eig function.

In practice the MATLAB call $[\hat{E}, \hat{\varepsilon}_s] = \mathrm{eig}(\hat{I}, -\hat{\varepsilon}^{-1}\hat{s}^2)$ yields a matrix $\hat{E}$ in which the columns are the $\vec{E}$'s and a diagonal eigenvalue matrix $\hat{\varepsilon}_s$ in which the nonzero elements are the ε_s's; $\hat{E}$ and $\hat{\varepsilon}_s$ satisfy the equation $\hat{E} = -\hat{\varepsilon}^{-1}\hat{s}^2\hat{E}\hat{\varepsilon}_s$. A summary of similar equations for the four fields is given in Table II.

One of the eigenvector/eigenvalue pairs for each line in Table II represents a trivial solution and is returned as $\vec{s}$ for the eigenvector and a large value for the eigenvalue. A suitable procedure, such as the one shown in outline below, (i) recognizes and removes this pair, (ii) reduces $\hat{E}$ and $\hat{n}_s$ to 3×2 and 2×2 matrices, respectively, and (iii) completes the solution for the indices and all the fields:

Given $\hat{\varepsilon}_{123}$, and $\vec{s}$ in the propagation frame

$\Downarrow$

Use rotation matrices to calculate $\hat{\varepsilon}$

$\Downarrow$

Call the eig function with $[\hat{E}, \hat{\varepsilon}_s] = \mathrm{eig}(\hat{I}, -\hat{\varepsilon}^{-1}\hat{s}^2)$

$\Downarrow$

Identify the trivial solution

$\Downarrow$

Reduce order of $\hat{E}$ to 3×2 and $\hat{\varepsilon}_s$ to 2×2

$\Downarrow$

TABLE II
Propagation in a Common Direction in a Crystal

Eigenequation	MATLAB solution	Equation satisfied
$\vec{E} = \varepsilon_s(-\hat{\varepsilon}^{-1}\hat{s}^2)\vec{E}$	$[\hat{E}, \hat{\varepsilon}_s] = \mathrm{eig}(I, -\hat{\varepsilon}^{-1}\hat{s}^2)$	$\hat{E} = -\hat{\varepsilon}^{-1}\hat{s}^2\hat{E}\hat{\varepsilon}_s$
$\vec{D} = \varepsilon_s(-\hat{s}^2\hat{\varepsilon}^{-1})\vec{D}$	$[\hat{D}, \hat{\varepsilon}_s] = \mathrm{eig}(I, -\hat{s}^2\hat{\varepsilon}^{-1})$	$\hat{D} = -\hat{s}^2\hat{\varepsilon}^{-1}\hat{D}\hat{\varepsilon}_s$
$\vec{H} = \varepsilon_s(-\hat{s}\hat{\varepsilon}^{-1}\hat{s})\vec{H}$	$[\hat{H}, \hat{\varepsilon}_s] = \mathrm{eig}(I, -\hat{s}\hat{\varepsilon}^{-1}\hat{s})$	$\hat{H} = -\hat{s}\hat{\varepsilon}^{-1}\hat{s}\hat{H}\hat{\varepsilon}_s$
$\vec{B} = \varepsilon_s(-\hat{s}\hat{\varepsilon}^{-1}\hat{s})\vec{B}$	$[\hat{B}, \hat{\varepsilon}_s] = \mathrm{eig}(I, -\hat{s}\hat{\varepsilon}^{-1}\hat{s})$	$\hat{B} = -\hat{s}\hat{\varepsilon}^{-1}\hat{s}\hat{B}\hat{\varepsilon}_s$

Calculate

$$\hat{n}_s = \hat{\varepsilon}_s^{1/2}$$
$$\hat{D} = \varepsilon_0 \hat{\varepsilon} \hat{E}$$
$$\hat{H} = \hat{s} \hat{E} \hat{n}_s / z_0$$
$$\hat{B} = \mu_0 \hat{H}$$

4. PROPAGATION IN LAYERED BIAXIAL MEDIA

We begin by considering a plane wave propagating in the x–y plane and incident on a single parallel-sided layer of biaxial material, as illustrated in Fig. 2. In general, such a plane wave will initiate four plane waves in the biaxial layer, two forward-travelling waves in the x–y plane, and two backward-travelling waves in the same plane. The four waves are linearly polarized, in directions specified by the D fields, and share a common values of the Snell's law quantity $\beta = n \sin \theta$ with the incident wave. In most practical situations the value of β is set by free choice of the angle of incidence, and so it is reasonable to regard β as a known quantity.

The wave propagation angles θ of the four waves established in the biaxial layer are all different, in general, as are the four effective refractive indices n and the four values of α. Recall that $\alpha = n \cos \theta$, and notice that knowledge of the four α's amounts to knowledge of the four n's and the four θ's because, for each wave, $n = (\alpha^2 + \beta^2)^{1/2}$ and $\theta = \sin^{-1} (\beta/n)$.

Now we can state the problem to be solved in the following way: given the principal refractive indices n_1, n_2, n_3, the column angle ψ, the angle ξ between the deposition and propagation planes, and the common Snell's law quantity β, how can the four α's and the field components of the four waves be calculated?

4.1. *Fresnel's Quartic Equation*

As in the previous section, the n's can be obtained from Fresnel's equation. However, in this case explicit solutions are not practical because the recast Fresnel's equation is a quartic in α.

4.2. *Eigenequation Solution*

The upper pair of equations in the middle column of Table I can be written in the form

$$\begin{bmatrix} 0 & 0 & \beta \\ 0 & 0 & -\alpha \\ -\beta & \alpha & 0 \end{bmatrix} \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix} = z_0 \begin{bmatrix} H_x \\ H_y \\ H_z \end{bmatrix} \tag{9}$$

and

$$\begin{bmatrix} 0 & 0 & \beta \\ 0 & 0 & -\alpha \\ -\beta & \alpha & 0 \end{bmatrix} \begin{bmatrix} H_x \\ H_y \\ H_z \end{bmatrix} = -\frac{1}{z_0} \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{xy} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{xz} & \varepsilon_{yz} & \varepsilon_{zz} \end{bmatrix} \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix}. \tag{10}$$

Six equations are implied here and two of them,

$$E_x = -(\varepsilon_{xy} E_y + \varepsilon_{xz} E_z + \beta z_0 H_z)/\varepsilon_{xx}, \tag{11}$$
$$H_x = (\beta/z_0) E_z, \tag{12}$$

may be used to eliminate the field components E_x and H_x that are normal to interfaces and not required for boundary condition matching. This leads to the eigenequation

$$\begin{bmatrix} -\dfrac{\beta\varepsilon_{xy}}{\varepsilon_{xx}} & z_0 - \dfrac{z_0\beta^2}{\varepsilon_{xx}} & -\dfrac{\beta\varepsilon_{xz}}{\varepsilon_{xx}} & 0 \\ \dfrac{\varepsilon_{yy}}{z_0} - \dfrac{\varepsilon_{xy}^2}{z_0\varepsilon_{xx}} & -\dfrac{\beta\varepsilon_{xy}}{\varepsilon_{xx}} & \dfrac{\varepsilon_{yz}}{z_0} - \dfrac{\varepsilon_{xy}\varepsilon_{xz}}{z_0\varepsilon_{xx}} & 0 \\ 0 & 0 & 0 & -z_0 \\ -\dfrac{\varepsilon_{yz}}{z_0} + \dfrac{\varepsilon_{xy}\varepsilon_{xz}}{z_0\varepsilon_{xx}} & \dfrac{\beta\varepsilon_{xz}}{\varepsilon_{xx}} & \dfrac{\beta^2}{z_0} + \dfrac{\varepsilon_{xz}^2}{z_0\varepsilon_{xx}} - \dfrac{\varepsilon_{zz}}{z_0} & 0 \end{bmatrix} \begin{bmatrix} E_y \\ H_z \\ E_z \\ H_y \end{bmatrix} = \alpha \begin{bmatrix} E_y \\ H_z \\ E_z \\ H_y \end{bmatrix}, \tag{13}$$

which we abbreviate as $\hat{M}_\beta \vec{F} = \alpha \vec{F}$. Hence solutions to both the n's and the basis fields can be obtained by a single MATLAB call

$$[\hat{F}, \hat{\alpha}] = \mathrm{eig}(M_\beta). \tag{14}$$

The 4×4 basis field matrix $\hat{F}$ contains the basis fields as columns,

$$\hat{F} = \begin{bmatrix} E_{y1}^+ & E_{y1}^- & E_{y2}^+ & E_{y2}^- \\ H_{z1}^+ & H_{z1}^- & H_{z2}^+ & H_{z2}^- \\ E_{z1}^+ & E_{z1}^- & E_{z2}^+ & E_{z2}^- \\ H_{y1}^+ & H_{y1}^- & H_{y2}^+ & H_{y2}^- \end{bmatrix}. \tag{15}$$

Here the plus and minus superscripts indicate waves that are positive-going and negative-going with respect to the

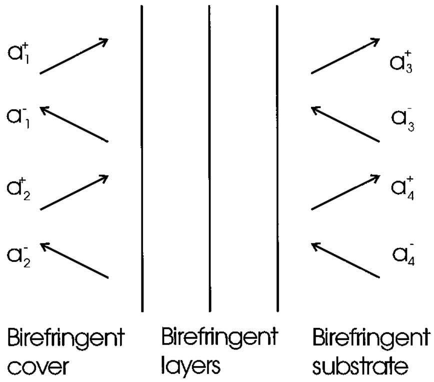

FIG. 3. Labelling scheme used for the amplitudes of the four basis vectors that propagate in the cover and the amplitudes of the four basis vectors in the substrate.

x-axis. The exact meaning of these terms and the pairing implied by the subscripts 1 and 2 is discussed in Section 6.

4.3. *Field Transfer Matrices*

The y and z components of the total anharmonic field $\vec{m} = \{E_y\ H_z\ E_z\ H_y\}$ at a point in a layered medium can be expressed as a linear sum of the four harmonic travelling wave basis fields, $\vec{m} = \hat{F}\vec{a}$. We shall refer to the column vector $\vec{a} = \{a_1^+\ a_1^-\ a_2^+\ a_2^-\}$ that provides the complex coefficients for the linear sum as the travelling wave field coefficients (see Fig. 3) and to $\vec{m}$ as the total field. Thus, the matrix $\hat{F}$ has the property of transforming the travelling wave field coefficients to the total field at the same point in a layered biaxial medium and, similarly, $\hat{F}^{-1}$ transforms the total field to the travelling wave field coefficients at the same point.

The other 4×4 matrices, $\hat{M}$ and $\hat{A}$, provide useful transformations. The phase matrix,

$$\hat{A}_d = \begin{bmatrix} \exp[-i\phi_1^+] & 0 & 0 & 0 \\ 0 & \exp[-i\phi_1^-] & 0 & 0 \\ 0 & 0 & \exp[-i\phi_2^+] & 0 \\ 0 & 0 & 0 & \exp[-i\phi_2^-] \end{bmatrix}, \tag{16}$$

where $\phi_{1,2}^{\pm} = k\alpha_{1,2}^{\pm}d$, is a special case of $\hat{A}$ and transforms the travelling wave field coefficients from one point (at $x = x_0$, say) to the travelling wave field coefficients at another point (at $x = x_0 - d$). The field transfer matrix $\hat{M} = \hat{F}\hat{A}_d\hat{F}^{-1}$ transforms the total field from one point to the total field at another point, such as across the interfaces of a single layer. For N layers stacked between the cover and the substrate the field transfer matrix is the product $\hat{M} = \hat{M}_1\hat{M}_2 \cdots \hat{M}_N$. Finally, the system matrix $\hat{A} = \hat{F}_C^{-1}\hat{M}\hat{F}_S$ transforms the travelling wave field coefficients from a point just inside the substrate to a point just inside the cover.

However, before leaving this section we wish to reinforce the fact that all matrix transformations discussed in this section satisfy Maxwell's equations and electromagnetic field boundary conditions. The matrix transformations between the interfaces of a single layer, for example, give the same result that could be obtained by superposing an infinite set of multiply reflected beams.

5. REFLECTANCE AND TRANSMITTANCE

Methods for computing the reflectance and transmittance coefficients are developed in this section. MATLAB code for implementing the procedures is listed in Appendix A.

5.1. *General Case*

The boundary conditions at the interfaces of a stack of anisotropic films sandwiched between an anisotropic cover and an anisotropic substrate are satisfied, provided the total field $\hat{F}_C\vec{a}_C$ at the cover is equal to the result of transferring the total field $\hat{F}_S\vec{a}_S$ in the substrate to the cover, i.e., $\hat{F}_C\vec{a}_C = \hat{M}\hat{F}_S\vec{a}_S$. Rearranging and using $\hat{A} = \hat{F}_C^{-1}\hat{M}\hat{F}_S$ yields the condition $\vec{a}_C = \hat{A}\vec{a}_S$, i.e.,

$$\begin{bmatrix} a_1^+ \\ a_1^- \\ a_2^+ \\ a_2^- \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & A_{24} \\ A_{31} & A_{32} & A_{33} & A_{34} \\ A_{41} & A_{42} & A_{43} & A_{44} \end{bmatrix} \begin{bmatrix} a_3^+ \\ a_3^- \\ a_4^+ \\ a_4^- \end{bmatrix}. \tag{17}$$

Note the use of subscripts 1, 2 in the cover and 3, 4 in the substrate, as illustrated in Fig. 3.

Next we rearrange this equation so that it has the form *output waves* = *matrix* x *input waves,*

$$\begin{bmatrix} a_1^- \\ a_2^- \\ a_3^+ \\ a_4^+ \end{bmatrix} \equiv \hat{r} \begin{bmatrix} a_1^+ \\ a_2^+ \\ a_3^- \\ a_4^- \end{bmatrix}, \tag{18}$$

with the result

$$\hat{r} \equiv \begin{bmatrix} r_{11} & r_{12} & t_{13} & t_{14} \\ r_{21} & r_{22} & t_{23} & t_{24} \\ t_{31} & t_{32} & r_{33} & r_{34} \\ t_{41} & t_{42} & r_{43} & r_{44} \end{bmatrix} = \begin{bmatrix} 0 & 0 & -A_{11} & -A_{13} \\ 1 & 0 & -A_{21} & -A_{23} \\ 0 & 0 & -A_{31} & -A_{33} \\ 0 & 1 & -A_{41} & -A_{43} \end{bmatrix}^{-1} \begin{bmatrix} -1 & 0 & A_{12} & A_{14} \\ 0 & 0 & A_{22} & A_{24} \\ 0 & -1 & A_{32} & A_{34} \\ 0 & 0 & A_{42} & A_{44} \end{bmatrix}. \tag{19}$$

Here $\hat{r}$ is to be regarded as an intermediary matrix, because its elements are ratios of the a's, rather than ratios of actual field coefficients. The (irradiance) reflectance and transmittance coefficients,

$$\hat{R} = \begin{bmatrix} R_{11} & R_{12} & T_{13} & T_{14} \\ R_{21} & R_{22} & T_{23} & T_{24} \\ T_{31} & T_{32} & R_{33} & R_{34} \\ T_{41} & T_{42} & R_{43} & R_{44} \end{bmatrix}, \tag{20}$$

are defined in terms of ratios of power flow in the x-direction. Thus $R_{12} = P_1^-/P_2^+ = |a_1^-|^2|p_1^-|/|a_2^+|^2 p_2^+| = |r_{12}|^2|p_1^-/p_2^+|$ etc., where the p's are the Poynting power fluxes carried by the basis vectors along the x-axis and p may be found from

$$p = \tfrac{1}{2}\mathscr{R}(E_y H_z^* - E_z H_y^*). \tag{21}$$

Finally, the reflectance and transmittance coefficients are given by

$$\hat{R} = \begin{bmatrix} |r_{11}|^2|p_1^-/p_1^+| & |r_{12}|^2|p_1^-/p_2^+| & |t_{13}|^2|p_1^-/p_3^-| & |t_{14}|^2|p_1^-/p_4^-| \\ |r_{21}|^2|p_2^-/p_1^+| & |r_{22}|^2|p_2^-/p_2^+| & |t_{23}|^2|p_2^-/p_3^-| & |t_{24}|^2|p_2^-/p_4^-| \\ |t_{31}|^2|p_3^+/p_1^+| & |t_{32}|^2|p_3^+/p_2^+| & |r_{33}|^2|p_3^+/p_3^-| & |r_{34}|^2|p_3^+/p_4^-| \\ |t_{41}|^2|p_4^+/p_1^+| & |t_{42}|^2|p_4^+/p_2^+| & |r_{43}|^2|p_4^+/p_3^-| & |r_{44}|^2|p_4^+/p_4^-| \end{bmatrix}. \tag{22}$$

5.2. *Crystal–Crystal Interface*

In the absence of films $\hat{M} = \hat{I}$ and, hence, $\hat{A} = \hat{F}_C^{-1}\hat{F}_S$. Thus the general equations developed above are applicable to the crystal–crystal interface. Alternatively, the boundary conditions for the crystal–crystal interface can be expressed by the equation $\hat{F}_C\vec{a}_C = \hat{F}_S\vec{a}_S$, i.e.,

$$\begin{bmatrix} E_{y1}^+ & E_{y1}^- & E_{y2}^+ & E_{y2}^- \\ H_{z1}^+ & H_{z1}^- & H_{z2}^+ & H_{z2}^- \\ E_{z1}^+ & E_{z1}^- & E_{z2}^+ & E_{z2}^- \\ H_{y1}^+ & H_{y1}^- & H_{y2}^+ & H_{y2}^- \end{bmatrix} \begin{bmatrix} a_1^+ \\ a_1^- \\ a_2^+ \\ a_2^- \end{bmatrix} = \begin{bmatrix} E_{y3}^+ & E_{y3}^- & E_{y4}^+ & E_{y4}^- \\ H_{z3}^+ & H_{z3}^- & H_{z4}^+ & H_{z4}^- \\ E_{z3}^+ & E_{z3}^- & E_{z4}^+ & E_{z4}^- \\ H_{y3}^+ & H_{y3}^- & H_{y4}^+ & H_{y4}^- \end{bmatrix} \begin{bmatrix} a_3^+ \\ a_3^- \\ a_4^+ \\ a_4^- \end{bmatrix}, \tag{23}$$

and then a procedure similar to that used above leads to

$$\hat{r} = \begin{bmatrix} E_{y1}^- & E_{y2}^- & -E_{y3}^+ & -E_{y4}^+ \\ H_{z1}^- & H_{z2}^- & -H_{z3}^+ & -H_{z4}^+ \\ E_{z1}^- & E_{z2}^- & -E_{z3}^+ & -E_{z4}^+ \\ H_{y1}^- & H_{y2}^- & -H_{y3}^+ & -H_{y4}^+ \end{bmatrix}^{-1} \begin{bmatrix} -E_{y1}^+ & -E_{y2}^+ & E_{y3}^- & E_{y4}^- \\ -H_{z1}^+ & -H_{z2}^+ & H_{z3}^- & H_{z4}^- \\ -E_{z1}^+ & -E_{z2}^+ & E_{z3}^- & E_{z4}^- \\ -H_{y1}^+ & -H_{y2}^+ & H_{y3}^- & H_{y4}^- \end{bmatrix}. \tag{24}$$

Thus in the direct method $\hat{r}$ is defined in terms of the columns of $\hat{F}$ rather than the columns of $\hat{A}$.

6. SORTING COLUMNS OF $\hat{F}$

In general it is not necessary to sort the basis vectors associated with anisotropic layers, because $\hat{M}$ for a film does not depend on the order of the columns of $\hat{F}$. However, a minimum sort of the cover and substrate basis vectors is necessary because the equations leading to the reflectance and transmittance coefficients require identification of the positive-going (+) and negative-going (−) basis waves. In the remaining part of this section we explain the various situations that arise and need to be addressed by considering the most complicated numerical example.

Consider first the plot of α versus β shown in the left-hand part of Fig. 4 for an anisotropic substrate specified by $n_1 = 2.4$, $n_2 = 1.55$, $n_3 = 2.0$, $\psi = -45°$, $\xi = 0°$. In this case the eigenvectors are decoupled and propagate with p (transverse magnetic, TM) and s (transverse electric, TE) polarizations. Thus, in this special situation ($\xi = 0°$) it would be natural to sort the α's according to polarization. However, for refractive index sections in which ξ is not exactly zero the inner and outer sheets of the refractive index surface do not touch, and sorts based on polarization

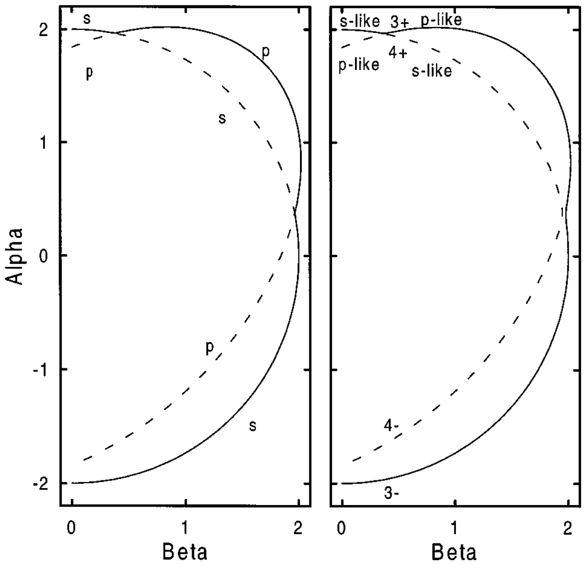

FIG. 4. Plots of $\alpha = n \cos \theta$ versus $\beta = n \sin \theta$ for a biaxial medium with $n_1 = 2.4$, $n_2 = 1.55$, $n_3 = 2.0$, $\psi = -45°$, and $\xi = 0°$ (left), $\xi = 2°$ (right). The cusp in the outer sheet of the refractive index surface provides the most complicated example for sorting and matching α's determined as eigenvalues with optical features.

lead to discontinuities in plotted curves of reflectance and transmittance as functions of angle of incidence or β.

Figure 4 (right) shows the outer sheet (solid line) and inner sheet (broken line) for the anisotropic substrate with $\xi = 2°$. For a given β the four associated values of α can be determined by drawing a vertical line in the figure, and the directions of the component of the Poynting vector in the x–y plane obtained by drawing normals to the curves. The positive α direction in Fig. 4 corresponds to the x-axis shown normal to the substrate in Fig. 2. It is clear that the sign of α (and, hence, the sign of the x-component of the wavevector) is not a reliable indicator of the sense of power flow along the x-axis. For this reason we take the terms positive-going (+) and negative-going (−) to refer to positive and negative senses of power flow along the x-axis for nonevanescent waves. In the case of evanescent waves, which carry no average power along x, the terms positive-going and negative-going are conveniently associated with the sign of the imaginary part of α, as this implies exponentially decreasing field strengths for waves moving away from the interface(s).

Apart from the necessary sort of cover and substrate basis vectors considered above, matching of the subscript pairs 1, 2 and 3, 4 with optical characteristics of the cover and substrate media is desirable to prevent fragmentation in plotted curves such as R_{11} versus θ. To illustrate suitable procedures we consider the above substrate (with $\xi = 2°$), together with an air ($n_1 = n_2 = n_3 = 1$) cover. For small values of β the "optical characteristic" used is simply association with the refractive index outer sheet (label 1 for an anisotropic cover and label 3 for the substrate) or the inner sheet (label 2 for an anisotropic cover and label 4 for the substrate).

In this particular example the cover is isotropic and normal practice dictates that the basis vectors should represent p and s polarizations. For such cases we use

$$\hat{F} = \begin{bmatrix} 1 & 1 & 0 & 0 \\ \gamma_p & -\gamma_p & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & \gamma_s & -\gamma_s \end{bmatrix} \tag{25}$$

with $\gamma_p = H_z^+/E_y^+ = -H_z^-/E_y^- = n/z_0 \cos \theta$ and $\gamma_s = H_y^+/E_z^+ = -H_y^-/E_z^- = -n \cos \theta/z_0$. The subscripts 1 and 2 in previous equations translate to p and s in the cover, and 3 and 4 would translate to p and s in an isotropic substrate.

The first column of the matrix $\hat{R}$ is plotted in Fig. 5 as a function of β, for the range $0 \le \beta \le 1$ corresponding to $0 \le \theta_C \le 90°$. For each of these curves the incident light is the 1+ (p) wave in the cover. The upper part of the figure shows a Brewster angle reflection for $R_{11} \equiv R_{pp}$. For small values of β the incident light excites p-like (4+)

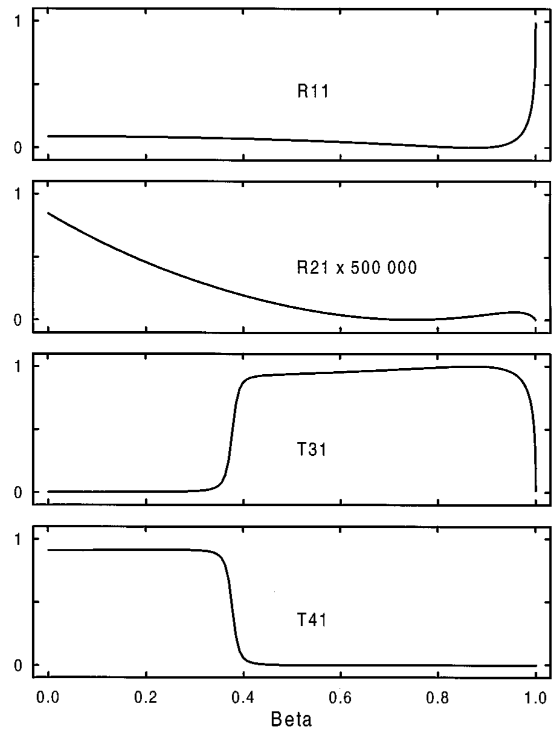

FIG. 5. Four of the 16 R–T coefficients plotted as functions of $\beta = n \sin \theta$ for an air cover medium and the biaxial substrate specified by $n_1 = 2.4$, $n_2 = 1.55$, $n_3 = 2.0$, $\psi = -45°$, and $\xi = 2°$.

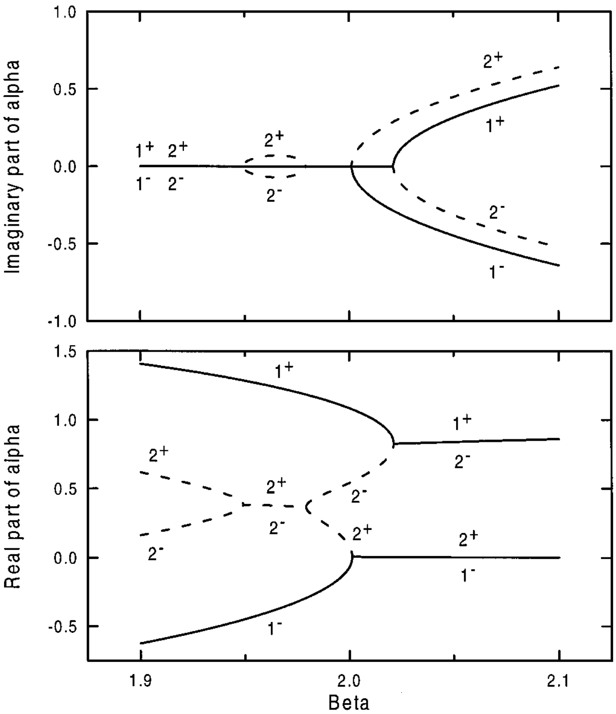

FIG. 6. Real and imaginary parts of α near the cusp described in Fig. 4. The labelling scheme both satisfies the minimum sorting requirement and prevents fragmentation in plotted reflectance and transmittance curves.

waves in the substrate, and hence T_{41} is large. The sudden fall in T_{41} and the corresponding rapid rise in T_{31} is caused by the switches in polarization character from p-like to s-like and s-like to p-like shown by the labels on Fig. 4(right).

Unfortunately, pairs of α's cannot always be identified with the outer and inner sheets of the refractive index surface, and our example has been chosen to illustrate this point. Suppose that a line of constant β is moved from the left-hand side to the right-hand side of Fig. 6, in which both real and imaginary parts of α are plotted as functions of β. The intersections made can be classed as (i) outer sheet (two real), inner sheet (two real); (ii) outer sheet (two real), inner sheet (pair of compex conjugates); (iii) outer sheet (four real); (iv) outer sheet (two pairs of complex conjugates). In each case the four positions on the refractive index surface can be identified by considering the numerical order of the real parts of α, together with the sign of the x-component of the Poynting vector or the sign of the imaginary part of α. The labels in Fig. 6, which result from such a sorting procedure, ensure both identification and continuity of reflectance and transmittance curves for this complicated example. In specific (and more usual) cases in which a cusp is not present in the outer sheet, sorting is correspondingly simpler.

7. CONCLUSIONS

The eigenequation approach yields a simple method for calculating the optical properties of anisotropic media. When the substrate and the cover are both isotropic, the adoption of presorted basis field matrices means that no further sorting of eigenfunctions is necessary for calculations of reflectance and transmittance.

Identification of the four eigenvectors propagating in an anisotropic cover or substrate is necessary for reflectance and transmittance calculations and can be achieved for the simple case of real alpha's by association with the outer and inner sheets of the refractive index surface. In the most complicated case, which includes a cusp in the outer refractive index sheet, the alpha's are sorted by real parts, together with the sign of the normal component of the Poynting vector or the imaginary part of the complex conjugate pair.

The main advantage of the method is economy of computer code, compared to traditional methods in which a quartic for α is solved and the fields are obtained by back-substitution. When the method is used with a numerical computation software package, such as MATLAB, only a few lines of code are required for the determination of the reflectance and transmittance coefficients.

APPENDIX A: MATLAB CODE

```
% The eigenvector method has the advantage of yielding compact MATLAB code for comput-
% ing the coefficients of reflectance and transmittance from stratified birefringent me-
% dia. To begin the dielectric tensor e is determined for the propagation x, y, z
% frame using Eqs. (2–6). Then the 4x4 matrix F and the alpha's associated with each
% medium are found from Eq.(14),

[F,Alpha]=eig([
                 -b*exy/exx       (1-b*b/exx)*z0       -b*exz/exx          0
             (eyy-exy^2/exx)/z0    -b*exy/exx    (eyz-exy*exz/exx)/z0    0
                     0                  0                    0             -z0
  (-eyz+exy*exz/exx)/z0 b*exz/exx (b^2+exz^2/exx-ezz)/exx/z0]-Z0);
```

```
alpha=[Alpha(1,1) Alpha(2,2) Alpha(3,3) ... alpha(4,4)];

% The powers pc and ps of the four cover basis waves and the four substrate basis
% waves are determined using Eq.(21),

p=real([F(1,:).*conj(F(2,:))-F(3,:) ... *conj(F(4,:))])/2;

% Fc and Fs require sorting by columns into + - + - pairs. Calculation of the system
% matrix A is straightforward (Sect. 4.3) and the intermediary matrix r is computed
% using Eq.(19),

r=inv([I(:,2) I(:,4) -A(:,1) -A(:,3)])* ... [-I(:,1) -I(:,3) A(:,2) A(:,4)];

% If there are no layers then for the crystal–crystal interface it is simpler to use
% Eq.(24),

r=inv([Fc(:,2)Fc(:,4) -Fs(:,1) -Fs(:,3)])* ... [-Fc(:,1) -Fc(:,3) Fs(:,2) Fs(:,4)];

% Finally the matrix R holding the eight reflectances and eight transmittances is de-
% termined from Eq. (22),

R=abs([pc(2) pc(4) ps(1) ps(3)]'* ... [1/pc(1) 1/pc(3) 1/ps(2) 1/ps(4)])...
*abs(r).^2;
```

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