NEW FORMS OF NORMAL EQUATION FOR BIAXIALLY ANISOTROPIC MEDIA

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In solving problems of inclined incidence and reflection of light at the interface between two media, it is usually necessary to determine the normal components η_i of the refraction vector from the normal equation [1]

$$\mathbf{m}_i = \mathbf{b} + \eta_i \mathbf{q}. \tag{1}$$

In a number of cases (for isotropic media and uni- and biaxial crystals, and when the incidence plane of the light coincides with the symmetry plane of the crystal), the normal equation breaks down into two factors, which means that it is simple to solve. However, on passing to low-symmetry biaxial and also gyrotropic crystals, the normal equation becomes a complete fourth-order equation in terms of the components η_i, generally speaking, and this produces well-known mathematical difficulties for analytical solution. Therefore, in [1], an iterative method of calculating the refraction vectors of the reflected and refracted waves, using an axial representation of the tensor ε^{-1}, was proposed for nonmagnetic media. Essentially, in this method, η_i are calculated first in the approximation of an isotropic medium neglecting the anisotropy of the tensor ε^{-1}, and then the influence of anisotropy, since it is small, is taken into account by the sample method of successive approximation.

In [2], a new covariant form of the normal equation was obtained for anisotropic media characterized by a symmetric tensor ε and, on this basis, another, more effective, method of calculating η_i was proposed.

The fruitful idea of [2] — the expediency of isolating two factors giving approximate values of the roots in the normal equation — may be realized in various ways. This idea is used here, with some modifications, for a medium characterized by asymmetric tensors ε^{-1} and μ describing, for example, the optical properties of a series of magnetically ordered crystals in the near infrared region of the spectrum.

The refraction vectors $\mathbf{m}_i$ of the intrinsic plane monochromatic waves in such biaxially anisotropic media satisfy the normal equation [3]

$$\det(1 + \tau_c + \overline{\tau}_c) = 0, \quad \tau = \mu^{-1}\mathbf{m}^{\times}\varepsilon^{-1}\mathbf{m}^{\times}. \tag{2}$$

Note that, with inclined incidence of light on the crystal, three vectors are physically distinct: $\mathbf{n}$, the unit vector of the normal of the light vector of the wave, $\mathbf{a} = [\mathbf{mq}]$ and $[\mathbf{na}]$. Therefore, it is expedient to write the tensor τ in an orthonormalized basis $\{\mathbf{a}_1 = \mathbf{a}/|\mathbf{a}|, [\mathbf{na}_1], [\mathbf{n}]\}$. Then calculating Eq. (2), the normal equation is obtained, after some manipulation, in the form

$$([\mathbf{ma}_1]\,\mu^{-1}\mathbf{m}^{\times}\varepsilon^{-1}\mathbf{a}_1 - 1)(\mathbf{a}_1\mu^{-1}\mathbf{m}^{\times}\varepsilon^{-1}\mathbf{a}_1^{\times}\mathbf{m} - 1) = \mathbf{a}_1\mu^{-1}\mathbf{m}^{\times}\varepsilon^{-1}\mathbf{a}_1\cdot\mathbf{ma}_1^{\times}\mu^{-1}\mathbf{m}^{\times}\varepsilon^{-1}\mathbf{a}_1^{\times}\mathbf{m}. \tag{3}$$

When $\mu = 1$, Eq. (3) may be somewhat simplified. Using the identity

$$\mathbf{n}(\varepsilon_c^{-1} - \varepsilon^{-1})\,\mathbf{n} = [\mathbf{a}_1\mathbf{n}]\,\varepsilon^{-1}[\mathbf{a}_1\mathbf{n}] + \mathbf{a}_1\varepsilon^{-1}\mathbf{a}_1 \tag{4}$$

and taking into account that, on the other hand, the anisotropic medium is characterized by the normal equation [3]

$$\mathbf{m}^2\cdot\mathbf{m}\overline{\varepsilon^{-1}}\mathbf{m} + \mathbf{m}(\varepsilon^{-1} - \varepsilon_c^{-1})\,\mathbf{m} + 1 = 0, \tag{5}$$

Eq. (3) transforms to give

$$(\mathbf{m}\overline{\varepsilon^{-1}}\mathbf{m} - \mathbf{a}_1\varepsilon^{-1}\mathbf{a}_1)(m^2\cdot\mathbf{a}_1\varepsilon^{-1}\mathbf{a}_1 - 1) = [\mathbf{a}_1\mathbf{m}]\,\varepsilon^{-1}\mathbf{a}_1\cdot\mathbf{a}_1\varepsilon^{-1}[\mathbf{a}_1\mathbf{m}], \tag{6}$$

which coincides with Eq. (13) of [2] when $\varepsilon = \tilde{\varepsilon}$.

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Turning to Eq. (3), this form of the normal equation differs from the standard version [3, 4] in that the left-hand side of Eq. (3) breaks down into two factors: quadratic equations in η_i. The right-hand side is a small quantity which vanishes when the anisotropy and gyrotropy of the tensors ε^{-1} and μ^{-1} is neglected. More precisely, the right-hand side of Eq. (3) is a quantity of second-order smallness with respect to anisotropy and gyrotropy. In particular, if the plane of incidence of the light is the symmetry plane of the crystal, i.e., $\mathbf{a}_1$ is the eigenvector of the tensors μ^{-1} and ε^{-1}, then the right-hand side of Eq. (3) vanishes and Eq. (3) breaks down into factors accurately rather than approximately.

It will be shown below that the form of the normal equation found for biaxially anisotropic media in Eq. (3) allows the simple method of successive approximation to be used to calculate the components η_i of the refraction vectors with fast obligatory convergence.

It is known [3] that, in uniaxial crystals (where $\mu = 1$ or $\mu \neq 1$) the normal equation may break down accurately into factors. However, such direct resolution of Eqs. (3) and (6) in this way is difficult. Therefore, another invariant form of the normal equation that is free from this deficiency is obtained for biaxially anisotropic media.

Preliminarily, the tensor τ is written in the form

$$\tau = \mathbf{d}^{\times}\gamma\mathbf{m}^{\times}, \quad \mathbf{d} = \mathbf{m}\overline{\mu^{-1}}, \quad \gamma = \tilde{\mu}\varepsilon^{-1}, \tag{7}$$

and then Eq. (2) takes the form

$$1 + \mathbf{m}(\gamma - \gamma_c)\mathbf{d} + \mathbf{m}\overline{\gamma}\mathbf{d}\cdot\mathbf{d}\mathbf{m} = 0, \tag{2a}$$

which is equivalent to that proposed earlier in [4].

To resolve Eq. (2) approximately into factors, Eq. (2a) is multiplied by some scalar a_C and the result is added to the right-hand side of the identity

$$\mathbf{m}\overline{\gamma}\mathbf{d} = \mathbf{m}(\overline{\gamma - a_C})\mathbf{d} - a_C\mathbf{m}(\gamma - \gamma_c)\mathbf{d} - a_C^2\cdot\mathbf{d}\mathbf{m}. \tag{8}$$

After elementary transformations, one more form of the normal equation for biaxially anisotropic media is finally obtained

$$(1 - a_C\mathbf{d}\mathbf{m})(\mathbf{m}\overline{\gamma}\mathbf{d} - a_C) = \mathbf{m}(\overline{\gamma - a_C})\mathbf{d}. \tag{9}$$

Now suppose that a_C is some eigenvalue of the tensor $\gamma = \tilde{\mu}\varepsilon^{-1}$, that is

$$\gamma\mathbf{u}_C = a_C\mathbf{u}_C, \tag{10}$$

which means that $\overline{\gamma - a_C}$ and hence the right-hand side of Eq. (9) are again quantities of second-order smallness with respect to the anisotropy and/or gyrotropy. In the zero approximation, it follows from Eq. (9) that

$$\mathbf{m}\overline{\varepsilon^{-1}}\mathbf{m} = a_C, \tag{11}$$

$$\mathbf{m}\overline{\mu^{-1}}\mathbf{m} = 1/a_C, \tag{12}$$

while $\mathbf{m}(\overline{\gamma - a_C})\mathbf{d} = \mathbf{m}(\overline{\varepsilon^{-1} - a_C\tilde{\mu}^{-1}})\mathbf{m}$.

Suppose that the tensor $\gamma = \tilde{\mu}\varepsilon^{-1}$ is uniaxial, i.e., has a double eigenvalue a_C. Then as is known [3], $\overline{\gamma - a_C} = 0$ and therefore for uniaxial crystals Eq. (9) "automatically" breaks down into factors, i.e., in such cases, Eqs. (11) and (12) are accurate normal equations for each of the intrinsic waves. This corresponds to the results for uniaxial crystals outlined in [3] (Sec. 5).

If the plane of incidence of the light is the symmetry plane of the crystal, it is most expedient to take a_C corresponding to the eigenvector $\mathbf{u}_C = \mathbf{a}_1$ in Eq. (9). Then $\mathbf{m}(\overline{\gamma - a_C})\mathbf{d} = 0$ and again Eq. (9) breaks down accurately into factors.

Now consider the question of iterative methods of calculating the normal components η_i of the refraction wave vectors of the intrinsic waves on the basis of the new forms of the normal equation obtained in Eqs. (3) and (9). Since Eqs. (3) and (9) are of identical structure, it is sufficient to limit consideration to Eq. (9). In accordance with Eq. (9), Eqs. (11) and (12) are quadratic with respect to η_i and give zero approximations for the desired roots $\eta_i \equiv x_i$ ($i = 1$-4). Therefore, Eq. (9) may be written in the form proposed in [2]

$$f(x) = (x - x_1^{(0)})(x + x_3^{(0)})(x - x_2^{(0)})(x + x_4^{(0)}) - \delta(x) = 0, \tag{13}$$

where $(x_1^{(0)}, -x_3^{(0)})$ and $(x_2^{(0)}, -x_4^{(0)}$ are the zero-approximation roots of Eqs. (11) and (12) and $x_i^{(0)} \geq 0$.

In [2], an effective method of refining the roots obtained by an iterative formula (IF) of Newton tangents

$$x^{(n+1)} = \varphi(x^{(n)}) \equiv x^{(n)} - f(x^{(n)})/f'(x^{(n)}), \tag{14}$$

with quadratic convergence, generally speaking. However, when the normals of the refracted waves approach the optical axes of the crystal, the roots of Eq. (9) become multiple. This sharply retards the convergence of the sequence $x^{(0)}$, $x^{(1)}$, $x^{(2)}$, ... in the calculations. In addition, since $f/f' \to 0/0$ in this case, the computational process in Eq. (14) becomes unstable and sensitive to rounding errors, etc. Therefore, in such cases it is more expedient, in our view, to use the following method. Writing Eq. (13) in the form

$$\begin{gathered}(x - x_1^{(0)})(x - x_2^{(0)}) = \delta(x)/\psi(x), \\ \psi(x) = (x + x_3^{(0)})(x + x_4^{(0)}),\end{gathered} \tag{15}$$

it is seen that the desired roots x_1, x_2 are easily found by the iterative scheme in Eq. (16) which is analogous to that proposed in [5]

$$2x_{1,2}^{(n+1)} = 2\varphi_{1,2}(x_{1,2}^{(n)}) \equiv x_1^{(0)} + x_2^{(0)} \pm [(x_1^{(0)} - x_2^{(0)})^2 + 4\delta(x_{1,2}^{(n)})/\psi(x_{1,2}^{(n)})]^{1/2}. \tag{16}$$

The other two roots x_3 and x_4 are calculated ab analogously.

The convergence rates for the IF defined by Eqs. (14) and (16) are now estimated. According to [6], if $|\varphi'(x)| < 1$, then the IF $x^{(n+1)} = \varphi(x^{(n)})$ converges and the relation

$$C = \lim_{x^{(n)} \to x} \frac{|x^{(n+1)} - x|}{|x^{(n)} - x|^p} \tag{17}$$

may be used to introduce the following IF characteristics: p, the order of convergence; C, the constant of the error asymptote.

The Newton IF in Eq. (14) has quadratic (p = 2) convergence when $|f''/(f')^2| < 1$, while $C = |f''(2f')|$ [6]. In the case of a multiple root, however, very slow (C = 0.5) linear (p = 1) convergence is obtained.

This situation is different for the convergence of the IF in Eq. (16), which has linear but fast (C << 1) convergence. In fact, suppose that the parameter α characterizes the anisotropy of the tensor γ, i.e., $(\gamma - a_C) \sim \alpha$. Then $\delta(x) \sim \alpha^2$, $\varphi(x) \sim \alpha^2$, and the error-asymptote constant of the IF in Eq. (16) is of the following order of magnitude, regardless of the multiplicity of the root.

$$C = |\varphi'_{1,2}| = \left| \frac{(\delta/\psi)'}{2x_{1,2} - x_1^{(0)} - x_2^{(0)}} \right| \sim \alpha. \tag{18}$$

Suppose, for example, that the anisotropy parameter $\alpha \sim 10^{-3}$. Then each iteration in Eq. (16) gives an extra three accurate decimal places of the root.

Applying the IF in Eq. (16) instead of that in Eq. (14) in calculating a multiple root sharply accelerates the convergence, by a factor

$$k = -\lg a/\lg 2. \tag{19}$$

Thus, when $a \sim 10^{-2}$–10^{-3}, it is found that k ~ 7-10.

It is also significant that the convergence of the IF in Eq. (16) remains as before close to the angle of total internal reflection, when some of the roots $x_i \to 0$. Finally, if there are zero roots, then $\delta(x) = 0$ and therefore all the roots are determined at once.

Thus, Eqs. (3) and (9) are the desired new forms of the normal equation for biaxially anisotropic media, allowing a simple prosedure to be used for their solution with rapid linear convergence even in the case of multiple roots. Note that Eq. (9) is somewhat simpler than the first version of Eq. (3), since it does not depend on the vector $\mathbf{a}_1$. The zero approximations with respect to Eqs. (3) and (9) are equivalent to the symmetry plane and uniaxial approximations, respectively.

In conclusion, note also that the approach here proposed remains in force in the presence of absorption, and may be generalized for crystals of other types, taking account of possible phenomena of optical activity and the magnetoelectric effect.

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OPTOACOUSTIC GAS ANALYZERS WITH HIGH SELECTIVITY

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Optoacoustic (OA) automatic gas analyzers are widely applied in various branches of industry for analyzing complex processing mixtures. A basic OA gas analyzer is an OA detector filled with a gas; its special characteristics coincide with the absorption spectrum of the gas being analyzed in the mixture. This feature explains the high selectivity of an OA gas analyzer: however, the instrument does not contain a monochromator or any other dispersive element typically included in spectral devices.

Fundamental characteristics of OA gas analyzers were considered in [1], of which the sensitivity to the main component as a function of the parameters of the OA detector is of primary importance. However, sufficient attention has not been devoted to studying selectivity or sensitivity to interference components. One of the reasons for this could be the complexity in describing IR absorption spectra and the absence of a simple mathematical model. For a consideration of sensitivity to the main component, one can use the integral absorption function in exponential, square root, or any other sufficiently simple form. However, this method is inadequate for investigating selectivity, and a spectral approach is necessary. In [2], a combined model was proposed for the spectrum of an absorption band for studying selectivity of an OA gas analyzer with detector chambers positioned in a parallel manner. This approach allows one to investigate more complex OA gas analyzers with separated absorbing layers that are more selective in relation to interference components.

OA Gas Analyzer Schematic with Detection Chambers Positioned in a Parallel Manner. Fundamental Relations. We will consider the most widely used schematic for an OA gas analyzer with beam detector chambers positioned in a parallel fashion (Fig. 1a). The schematic contains two radiation sources, a comparison and working cell, a radiation flow modulator, a differential symmetric beam detector with a condenser microphone, and a system for converting the electric signal to a unified output signal. A mixture containing main and interference components is placed in the working cell, while the comparison cell is filled with an inert gas that does not absorb IR radiation. Both beam detection chambers are filled with the main component and have equivalent spectral characteristics.

The output signal for this schematic is given by the expression [2]

$$\Psi(u_x, u_y, v) = B[A(v, 0) - A(v + u_x, u_y) + A(u_x, u_y)], \quad (1)$$

where $u_x = c_x l_k$, and $u_y = c_y l_k$ are the optical depths of the main and interference components in the measurement cell; $v = c_d l_d$ is the optical depth of the main component in the OA detector, B is a proportionality coefficient that accounts for the intensity of the IR radiation flow, the thermal and acoustic resistance of the detector, and the conversion of the acoustic signal into the output electric signal of the gas analyzer.

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