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Algorithm to visualize a 3D normal surface in anisotropic crystals and the polarization states of the o- and e-waves in uniaxial crystals.

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Abstract

Of the many topics generally taught in undergraduate or graduate optics courses, the propagation of light through crystals with electrical anisotropy is one of the most difficult for students and for teachers who do not work in this field. In particular, the mathematics and equations are complex vectorial equations, and this complicates the visualization of the implications of the theory. Also, the standard textbooks and papers on the subject have led to some misconceptions on this problem by presenting results only for specific cases of the theory in graphical form. For example, it is a general belief that after refraction of an incident wave on the crystal, the polarization state of the two waves propagating inside the crystal, given by their displacement vectors **D**, are always orthogonal to each other. However, this is not the case, as explained and illustrated for uniaxial crystals in J. Opt. Soc. Am. A **33**(4), 677–682, (2016). The purpose of this paper is to help students and teachers visualize the solution to Maxwell's equations in electrical anisotropic crystals. An algorithm has been written in Mathematica so the reader can use it to visualize the normal surface in uniaxial and biaxial crystals. This algorithm can be used as the basis of computational projects for students to better understand the equations involved, or as a visualization tool for teachers in class.

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I. INTRODUCTION

In our experience one of the most difficult topics for undergraduate and graduate students in the area of optics is the propagation of light in anisotropic crystals, such as calcite and quartz. The complex vectorial equations required to understand this topic make it difficult for students to visualize the physical properties of the propagation and how it is affected by the polarization of light .¹ Additionally, there are misconceptions that are widely accepted in the optics community, even among teachers, on this subject. In this paper we present the equations and an algorithm to visualize the propagation of light in anisotropic crystals, which can be used as a computational project for students, to help them understand the results of the equations, or as a visualization tool for teachers, to help them explain the physical phenomenon in class.

In the 17th century, scientists including Isaac Newton and Christian Huygens knew about double refraction in crystals such as calcite or quartz. It took many years, however, before scientists were able to understand and explain the presence of the two polarized waves propagating inside these crystals. The existence of these two waves and their state of polarization is a consequence of applying Maxwell's equations on the boundary condition and inside a medium with electrical anisotropy. Additionally, due to this electrical anisotropy, the phase velocity of these two waves depends on their state of polarization and the direction of propagation of the wave inside the crystal. Depending on the type of anisotropy, crystals are divided in uniaxial or biaxial crystals. In uniaxial crystals there is only one direction within the crystal along which the two waves propagate with the same phase velocity and in biaxial crystals there are two directions; the direction along which the two waves propagate with the same phase velocity is called the crystal axis. In both types of crystals the two waves are polarized. In uniaxial crystals, one wave is called the ordinary wave because it satisfies Snell's law, and the other wave is called the extraordinary wave because in general it does not satisfy Snell's law. In biaxial crystals, in general, neither of the two waves satisfies Snell's law. To study the propagation of light inside these crystals, Maxwell's equations and the particular boundary conditions have to be used. For the propagation of light through uniaxial crystals, Huygens's principle can also be used.^{2,3} When Maxwell's equations are used, the solution to these equations gives the normal surface which consists of two shells that give the two wave vectors that can propagate inside the crystal. To visualize the 3D-

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normal surface is not easy, and, in textbooks and in the literature, the normal surface is generally only plotted in three planes called the principal planes.⁴ When the two waves propagate in the same direction, the polarization states for the displacement vector, \mathbf{D} , are always mutually orthogonal.⁴ But when the two waves do not propagate in the same direction, as happens after refraction and for oblique incidence, the polarization states for \mathbf{D} are no longer orthogonal,^{5,6} except if the two waves propagate on the principal planes, which are the cases that are normally plotted in textbooks and in the literature. This may be one of the reasons why there is a general belief among students and teachers⁷ that the polarization states for the two waves, \mathbf{D}_o (the ordinary wave o-), and \mathbf{D}_e , (the extraordinary wave e-), are **always** mutually orthogonal, i.e., $\mathbf{D}_o \cdot \mathbf{D}_e = 0$.

Another possible reason for this general misconception is that the deviation angle, θ_d , where $\cos(\theta_d) = \mathbf{D}_o \cdot \mathbf{D}_e$, in the most common crystals such as calcite or quartz is very small. The polarization states for the ordinary \mathbf{D}_o and extraordinary waves \mathbf{D}_e in calcite and quartz crystals were calculated by Alemán-Castañeda and Rosete-Aguilar,⁸ for the case when the crystal axis lies parallel to the interface between air and the crystal. It was shown that θ_d is larger in calcite than in quartz and it has a maximum value of about 1.68°, while quartz has a maximum value of about 0.09°. In this paper, we present the equations and an algorithm to calculate the normal surface and the corresponding o- and e- polarization states inside crystals. Many different programming languages are suitable for this problem, but we used Mathematica, and we present the results of our algorithm to illustrate that the two polarization states are not always orthogonal to each other after refraction, as an example application.

II. NORMAL SURFACE

In anisotropic media the phase velocity of light depends on its state of polarization as well as on its direction of propagation. If the anisotropic medium is a dielectric we can neglect the magnetic properties and focus on its electrical ones such as its permittivity. The permittivity in these materials is given by a tensor called the dielectric permittivity tensor.⁴

To conserve energy, the dielectric permittivity tensor must be symmetric, i.e, $\epsilon_{ij} = \epsilon_{ji}$. The symmetry of the dielectric permittivity tensor is a direct consequence of assuming that the permittivity is a real dielectric tensor. Therefore the eigenvalues, ϵ_{xx} , ϵ_{yy} , and ϵ_{zz} are

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real and their corresponding eigenvectors are orthogonal which define a coordinate system. In this coordinate system, the dielectric permittivity tensor is a diagonal matrix given by the eigenvalues which are called the principal dielectric constants. If the three principal dielectric constants are equal, $\epsilon_{xx} = \epsilon_{yy} = \epsilon_{zz}$, then the medium is isotropic and only one wave propagates in the medium with a phase velocity which is the same regardless of the direction of propagation. This wave is called the ordinary wave and satisfies Snell's law. If two principal dielectric constants are equal and one is different, $\epsilon_{xx} = \epsilon_{yy} \neq \epsilon_{zz}$, the medium is anisotropic and two waves, called the ordinary (o-) and extraordinary (e-) waves, can propagate in the medium with different phase velocity except along the so-called crystal axis; this crystal is called uniaxial. Finally, if the three principal dielectric constants are different, $\epsilon_{xx} \neq \epsilon_{yy} \neq \epsilon_{zz}$, two waves can propagate in the anisotropic medium with different phase velocity except along two directions called the crystal axes where the two waves propagate with the same phase velocity; this crystal is called biaxial

To study the propagation of light waves in anisotropic media requires the solution of the following equation which is derived from Maxwell's equations in a dielectric medium free of electric charges⁴

$$\mathbf{k} \times (\mathbf{k} \times \mathbf{E}) + \omega^2 \mu \epsilon \mathbf{E} = 0. \tag{1}$$

where $\mathbf{E} = (E_x, E_y, E_z)$ is the electric field, $\mathbf{k} = (k_x, k_y, k_z)$ is the wave propagation vector, ω is the angular frequency of the electric field, μ is the permeability of the medium and ϵ is its dielectric permittivity tensor given by the eigenvalues as follows:

$$\epsilon = \begin{pmatrix} \epsilon_{xx} & 0 & 0 \\ 0 & \epsilon_{yy} & 0 \\ 0 & 0 & \epsilon_{zz} \end{pmatrix} \tag{2}$$

Substituting the electric field, E, the wave propagation vector, k, and the dielectric permittivity tensor, ϵ , in Eq. (1), we get:

$$\begin{pmatrix} \omega^{2} \mu \epsilon_{xx} - k_{y}^{2} - k_{z}^{2} & k_{x} k_{y} & k_{x} k_{z} \\ k_{x} k_{y} & \omega^{2} \mu \epsilon_{yy} - k_{x}^{2} - k_{z}^{2} & k_{y} k_{z} \\ k_{x} k_{z} & k_{y} k_{z} & \omega^{2} \mu \epsilon_{zz} - k_{x}^{2} - k_{y}^{2} \end{pmatrix} \begin{pmatrix} E_{x} \\ E_{y} \\ E_{z} \end{pmatrix} = 0$$
 (3)



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To solve Eq. (3) it is necessary that the determinant of the system must vanish; that is,

$$\det \begin{vmatrix} \omega^{2}\mu\epsilon_{xx} - k_{y}^{2} - k_{z}^{2} & k_{x} k_{y} & k_{x} k_{z} \\ k_{x} k_{y} & \omega^{2}\mu\epsilon_{yy} - k_{x}^{2} - k_{z}^{2} & k_{y} k_{z} \\ k_{x} k_{z} & k_{y} k_{z} & \omega^{2}\mu\epsilon_{zz} - k_{x}^{2} - k_{y}^{2} \end{vmatrix} = 0$$
 (4)

Eq. (4) can be represented by a three-dimensional surface in \mathbf{k} space (momentum-space) which is known as the normal surface.

For a particular direction of a wave vector inside the crystal, a line with this direction and passing through the origin of the coordinate system is plotted. This line will intersect the two shells of the normal surface in two points. These two points give the magnitude of the wave vectors allowed in the crystal for that particular direction. The phase velocities of the two waves can easily be evaluated from the magnitude of the wave vectors using $v = \omega/k$.

We have developed an algorithm in Mathematica, as described in Section III, to draw the normal surface of an uniaxial or biaxial crystal to visualize the solution given by Eq. (4). Results for uniaxial and biaxial crystals are described in the following sections.

ALGORITHM IMPLEMENTATION

The algorithm consists of the following steps:

1. Rewrite Eq. (4) as follows:

$$(-k_y^2 - k_z^2 + \omega^2 \mu \epsilon_{xx})[(-k_x^2 - k_z^2 + \omega^2 \mu \epsilon_{yy})(-k_x^2 - k_y^2 + \omega^2 \mu \epsilon_{zz}) - k_y^2 k_z^2]$$

$$-(k_x k_y)[(k_x k_y)(-k_x^2 - k_y^2 + \omega^2 \mu \epsilon_{zz}) - k_x k_y k_z^2]$$

$$+(k_x k_z)[(k_x k_y^2 k_z) - (k_x k_z)(-k_x^2 - k_z^2 + \omega^2 \mu \epsilon_{yy})] = 0$$
 (5)

2. After doing some algebra to Eq. (5), the solutions for $k_z = f(k_x, k_y)$ are given by

$$k_z = \pm \sqrt{\frac{-b \pm \sqrt{b^2 - 4ac}}{2a}} \tag{6}$$

where

$$a = \epsilon_{zz} \tag{7}$$

$$b = k_x^2 (\epsilon_{xx} + \epsilon_{zz}) + k_y^2 (\epsilon_{yy} + \epsilon_{zz}) - \omega^2 \mu \epsilon_{zz} (\epsilon_{xx} + \epsilon_{yy})$$
(8)

$$c = (k_x^2 + k_y^2)(k_x^2 \epsilon_{xx} + k_y^2 \epsilon_{yy})$$

$$-\omega^{2}\mu[k_{x}^{2}\epsilon_{xx}(\epsilon_{yy}+\epsilon_{zz})+k_{y}^{2}\epsilon_{yy}(\epsilon_{xx}+\epsilon_{zz})-\omega^{2}\mu\epsilon_{xx}\epsilon_{yy}\epsilon_{zz}]$$
(9)

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- 3. Assign values to the principal dielectric constants (e.g. $\epsilon_{xx} = 3$, $\epsilon_{yy} = 2$, $\epsilon_{zz} = 1$).
- 4. With a symbolic algebra interpreter such as Mathematica, plot the normal surface as four explicit functions $k_z = f(k_x, k_y)$ (Eq. (6)).
- To define the crystal axis or axes A, solve the normal surface equation when the shells have the same solution.
- 6. To analyse the polarization states (for uniaxial crystals), define a ray going through the crystal and use Eqs. (10) and (11) given in Section IV.

All the codes necessary to perform the work presented in this article are available in the supplementary material to this article. 9

IV. UNIAXIAL CRYSTALS

Uniaxial crystals can be seen as a particular case of biaxial crystals, where two of the eigenvalues are equal. We have assumed that $\epsilon_{xx} = \epsilon_{yy} \neq \epsilon_{zz}$. The normal surface is formed by two shells, a sphere and an ellipsoid, that touch in two points. The line that joins these two points and passes through the origin is known as the crystal axis, named as vector A, which is the direction along which the ordinary and extraordinary waves propagate with the same phase velocity. Uniaxial crystals are classified as positive if $\epsilon_{xx} > \epsilon_{zz}$, see Fig. 1a, or negative if $\epsilon_{xx} < \epsilon_{zz}$, see Fig. 1b. The crystal axis is along the k_z -axis, see Fig. 1. For uniaxial crystals, there are only two principal refractive indices given by $n_x = c\sqrt{\mu\epsilon_{xx}}$ and $n_z = c\sqrt{\mu\epsilon_{zz}}$. For the negative uniaxial crystal shown in Fig. 1b, the sphere has a radius given by $r = \omega n_x/c$. Any solution over the sphere gives the ordinary wave vector, k_o , and the refractive index given by n_x is called the ordinary refractive index, n_o , i.e., $n_o = n_x$. The name ordinary is because any wave mode solution over the sphere propagates with the phase velocity c/n_o regardless of the direction of propagation and this wave refracts satisfying Snell's law. The ellipsoid has two principal axes and any wave-mode solution over the ellipsoid is called the extraordinary wave. The ellipsoid has two principal refractive indices, n_x and n_z , which are the refractive indices along the semi-axes of the ellipsoid. n_x is the ordinary refractive index and n_z is called the extraordinary refractive index, so $n_o = n_x$

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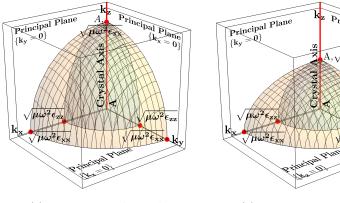
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and $n_e = n_z$. The phase velocity for the extraordinary wave depends on the angle of the wave vector \mathbf{k} and the crystal axis \mathbf{A} .

Principal Plane

Principal Plane

Principal Plane



(a) Positive uniaxial crystal.

(b) Negative uniaxial crystal.

FIG. 1: Normal surface representations for uniaxial crystals.

A. Polarization states of the electric displacement in uniaxial crystals

Consider the case usually shown in textbooks of a single ray propagating inside the crystal, with a direction given by the unit wave vector $\hat{\mathbf{k}}$. Two possible wave modes, the ordinary, $k_o\hat{\mathbf{k}}$, and the extraordinary, $k_e\hat{\mathbf{k}}$, can propagate in the medium. k_o and k_e are given by the intersection of the line that passes through the origin with direction $\hat{\mathbf{k}}$, and the sphere and the ellipsoid, respectively. These two waves are polarized and the direction of the electric displacement field-vector \mathbf{D}_o for the ordinary wave is given by the unit vector $\hat{\mathbf{d}}_o$ which is perpendicular to the plane defined by the crystal axis \mathbf{A} and the wave vector $\hat{\mathbf{k}}$, that is,

$$\hat{\mathbf{d}}_o = \frac{\hat{\mathbf{k}} \times \mathbf{A}}{|\hat{\mathbf{k}} \times \mathbf{A}|} \tag{10}$$

For the extraordinary wave, the direction of the electric displacement \mathbf{D}_e is given by the unit vector:

$$\hat{\mathbf{d}}_e = \frac{\hat{\mathbf{d}}_o \times \hat{\mathbf{k}}}{|\hat{\mathbf{d}}_o \times \hat{\mathbf{k}}|} \tag{11}$$

These two vectors, $\hat{\mathbf{d}}_o$ and $\hat{\mathbf{d}}_e$ are always orthogonal as shown in Fig. 2a for a positive unaxial crystal and Fig. 2b for a negative uniaxial crystal.

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Principal Plane

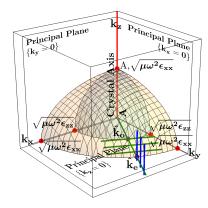
(ky 0)

(ky 0)

(kx 0)

(kx 0)

(kx 0)



- (a) Positive uniaxial crystal.
- (b) Negative uniaxial crystal.

FIG. 2: Polarization states of the electric displacement for the ordinary and extraordinary waves when the two waves propagate in the same direction, $\hat{\mathbf{k}}$.

However, a ray has to enter the crystal from outside, so let us now discuss the problem when a wave propagates in air with a wave vector, \mathbf{k}_i , and this wave is refracted at the interface between the air and the uniaxial crystal. Let $\hat{\mathbf{n}}$ be the normal to the interface at the point of incidence. It is necessary to use the boundary condition, $(\mathbf{k}_i - \mathbf{k}_{o,e}) \times \hat{\mathbf{n}} = 0$, to find the two refracted wave vectors, \mathbf{k}_o and \mathbf{k}_e , that can propagate inside the uniaxial crystal, see Fig. 3. These two wave vectors are refracted, in general, with different directions $\hat{\mathbf{k}}_o$ and $\hat{\mathbf{k}}_e$ inside the crystal. A misunderstanding in textbooks and in the literature is that the electric displacement vectors of the refracted o-wave and e-wave are always orthogonal; this, however, is not always the case but only for special cases discussed below.^{5,6}

The direction of the electric displacement for the ordinary ray, \mathbf{D}_o , is given by the unit vector, $\hat{\mathbf{d}}_o$, as:

$$\hat{\mathbf{d}}_o = \frac{\hat{\mathbf{k}}_o \times \mathbf{A}}{|\hat{\mathbf{k}}_o \times \mathbf{A}|} = \frac{\hat{\mathbf{k}}_o \times \mathbf{A}}{\sqrt{1 - (\hat{\mathbf{k}}_o \cdot \mathbf{A})^2}}.$$
 (12)

The direction of the electric displacement for the extraordinary wave, \mathbf{D}_e , is given by the unit vector, $\hat{\mathbf{d}}_e$, as:

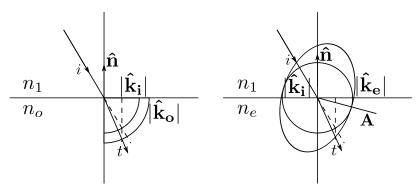
$$\hat{\mathbf{d}}_e = \frac{\hat{\mathbf{k}}_e \times (\hat{\mathbf{k}}_e \times \mathbf{A})}{|\hat{\mathbf{k}}_e \times (\hat{\mathbf{k}}_e \times \mathbf{A})|} = \frac{(\hat{\mathbf{k}}_e \cdot \mathbf{A})\hat{\mathbf{k}}_e - \mathbf{A}}{\sqrt{1 - (\hat{\mathbf{k}}_e \cdot \mathbf{A})^2}}$$
(13)

where we have used the vector identity $\mathbf{A} \times (\mathbf{B} \times \mathbf{C}) = (\mathbf{A} \cdot \mathbf{C})\mathbf{B} - (\mathbf{A} \cdot \mathbf{B})\mathbf{C}$.

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(a) For the ordinary wave.

(b) For the extraordinary wave.

FIG. 3: Boundary condition.

For the two electric displacement field vectors, \mathbf{D}_o and \mathbf{D}_e , of the refracted waves to be orthogonal it is required that,

$$\hat{\mathbf{d}}_o \cdot \hat{\mathbf{d}}_e = 0 \tag{14}$$

That is,

$$\left[\hat{\mathbf{k}}_{\mathbf{o}} \times \mathbf{A}\right] \cdot \left[(\hat{\mathbf{k}}_{\mathbf{e}} \cdot \mathbf{A}) \hat{\mathbf{k}}_{\mathbf{e}} - \mathbf{A} \right] = 0 \tag{15}$$

The second term in Eq. (15) is equal to zero; that is, $(\hat{\mathbf{k}}_{\mathbf{o}} \times \mathbf{A}) \cdot \mathbf{A} = 0$, so Eq. (15) simplifies as follows:

$$\begin{bmatrix} \hat{\mathbf{k}}_{\mathbf{o}} \times \mathbf{A} \end{bmatrix} \cdot \begin{bmatrix} (\hat{\mathbf{k}}_{\mathbf{e}} \cdot \mathbf{A}) \hat{\mathbf{k}}_{\mathbf{e}} \end{bmatrix} = \begin{bmatrix} \hat{\mathbf{k}}_{\mathbf{e}} \cdot \mathbf{A} \end{bmatrix} \begin{bmatrix} (\hat{\mathbf{k}}_{\mathbf{o}} \times \mathbf{A}) \cdot \hat{\mathbf{k}}_{\mathbf{e}} \end{bmatrix} = \begin{bmatrix} \hat{\mathbf{k}}_{\mathbf{e}} \cdot \mathbf{A} \end{bmatrix} \begin{bmatrix} \mathbf{A} \cdot (\hat{\mathbf{k}}_{\mathbf{e}} \times \hat{\mathbf{k}}_{\mathbf{o}}) \end{bmatrix} = 0$$
(16)

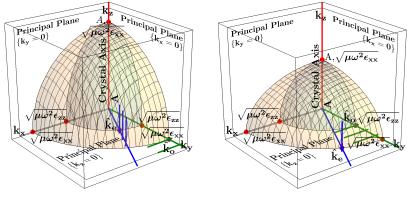
where we have used the vector identity $\mathbf{A} \cdot (\mathbf{B} \times \mathbf{C}) = \mathbf{B} \cdot (\mathbf{C} \times \mathbf{A})$.

The field vectors \mathbf{D}_{o} and \mathbf{D}_{e} are orthogonal for two cases that are visualized using our algorithm: 1) if the extraordinary wave, $\hat{\mathbf{k}}_{\mathbf{e}}$, is orthogonal to the crystal axis, \mathbf{A} , in which case $(\hat{\mathbf{k}}_{\mathbf{e}} \cdot \mathbf{A}) = 0$ (shown in Fig. 4a) or 2) if the crystal axis is coplanar with $\hat{\mathbf{k}}_{\mathbf{e}}$ and $\hat{\mathbf{k}}_{\mathbf{o}}$, in which case $\mathbf{A} \cdot (\hat{\mathbf{k}}_{\mathbf{e}} \times \hat{\mathbf{k}}_{\mathbf{o}}) = 0$ (shown in Fig. 4b).

For any other case, the field vectors \mathbf{D}_o and \mathbf{D}_e are non-orthogonal as shown in Figs. 5a and 5b using our algorithm for positive and negative uniaxial crystals, respectively, and their dot product is given by:

$$\cos(\theta_D) = \hat{\mathbf{d}}_o \cdot \hat{\mathbf{d}}_e = \frac{\left[\hat{\mathbf{k}}_e \cdot \mathbf{A}\right] \left[\mathbf{A} \cdot (\hat{\mathbf{k}}_e \times \hat{\mathbf{k}}_o)\right]}{\sqrt{1 - (\hat{\mathbf{k}}_o \cdot \mathbf{A})^2} \sqrt{1 - (\hat{\mathbf{k}}_e \cdot \mathbf{A})^2}} \neq 0$$
(17)

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(a) Case 1) $\hat{\bf k}_{\bf e} \cdot {\bf A} = 0$ in a positive uniaxial (b) Case 2) ${\bf A} \cdot (\hat{\bf k}_{\bf e} \times \hat{\bf k}_{\bf o}) = 0$ in a negative crystal.

FIG. 4: Polarization states of the electric displacement vectors for the ordinary and extraordinary waves when $\hat{\bf d}_o \cdot \hat{\bf d}_e = 0$

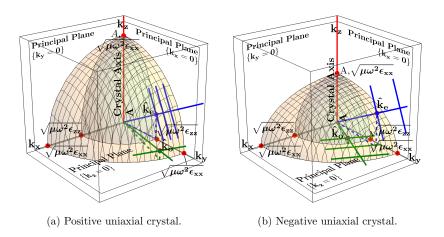


FIG. 5: Polarization states of the electric displacement for the ordinary and extraordinary waves when $\hat{\mathbf{d}}_o \cdot \hat{\mathbf{d}}_e \neq 0$ (when the two waves propagate in different direction after refraction in the interface air-crystal).

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V. BIAXIAL CRYSTALS

The normal surface is formed by two shells that, in general, have four points in common. Two lines that go through the origin of the coordinate system and these points are known as the crystals axes. The normal surface for a biaxial crystal is plotted in Fig. 6 and assuming that $\epsilon_{xx} > \epsilon_{yy} > \epsilon_{zz}$. In Fig. 6 one of the four common points is shown as point A on the plane $k_y = 0$. The red line that passes through the origin and point A is one of the crystal axes named as vector A. It can be seen in Fig. 6 that the outer normal surface concaves towards the inner surface because these two surfaces touch at point A where the vector \mathbf{k} has the same magnitude for the two surfaces which means that the two waves propagate with the same phase velocity. The planes $k_x = 0$, $k_y = 0$, and $k_z = 0$ are called principal planes. In Eq. (1) all the vectors are expressed in the coordinate system given by the eigenvectors which are called the principal axes. The wave vector can be written as $\mathbf{k} = (\omega n_x/c, \omega n_y/c, \omega n_z/c)$ where c is the velocity of light in vacuum and n_x , n_y , and n_z are the principal refractive indices of the crystal given by $n_x = c\sqrt{\mu\epsilon_{xx}}$, $n_y = c\sqrt{\mu\epsilon_{yy}}$, and $n_z = c\sqrt{\mu\epsilon_{zz}}$. All the points of the two shells are solutions of Eq. (1), so if a line with direction given by a wave propagation vector, k, is plotted in any direction in this diagram, starting from the origin, the intersection of this line with the shells gives two solutions which are the two waves that can propagate inside the crystal with different phase velocities except along the crystal axes. For example, if a line is drawn along the k_r -axis, there are two waves that can propagate inside the medium: 1) a wave with a wave vector given by $\mathbf{k}_1 = \left(\sqrt{\omega^2 \mu \epsilon_{xx}}, 0, 0\right)$ which propagates with a phase velocity $v_1 = 1/\sqrt{\mu \epsilon_{xx}}$ and 2) a wave with $\mathbf{k}_2 = (\sqrt{\omega^2 \mu \epsilon_{yy}}, 0, 0)$ which propagates with a phase velocity $v_2 = 1/\sqrt{\mu \epsilon_{yy}}$. The equations presented in Section IV were derived for uniaxial crystals.⁵ The calculation of the polarization states of the two waves in biaxial crystals is out of the scope of this paper.

Finally, in Fig. 7 a stereo pair figure of the normal surface in a biaxial crystal created using our algorithm is displayed so the reader can use a stereoscope to visualize a 3D image of the normal surface.



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$\begin{array}{c|c} Principal & Plane & k_z & Principal & Plane \\ \{k_y \geq 0\} & \{k_x \geq 0\} & \{k_x \geq 0\} \end{array}$

FIG. 6: Normal surface for a biaxial crystal.

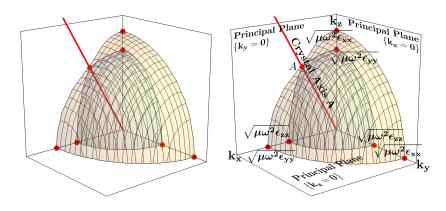


FIG. 7: Stereo pairs to visualize the normal surface for a biaxial crystal with $\epsilon_{xx}=3$, $\epsilon_{yy}=2$, and $\epsilon_{zz}=1$.

VI. CONCLUSION

An algorithm written in Mathematica has been presented in this paper and used to visualize the normal surface of uniaxial or biaxial crystals. A stereo pair of images are also plotted from our algorithm permitting students and teachers to use a stereoscope to visualize more clearly a 3D normal surface of a biaxial crystal. Additionally, the polarization states

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of the electric displacement for the ordinary (o-) an extraordinary (e-) waves in uniaxial crystals can be plotted using this algorithm. Figures can be displayed so students and teachers can visualize the polarization states of the electric displacement for the ordinary and extraordinary waves which are always orthogonal when the two waves propagate in the same direction. If the o- and e- waves do not propagate in the same direction, however, as it may happen after refraction of an incident wave on the crystal, their electric displacement vectors are not orthogonal to each other but only for particular cases discussed by Alemán-Castañeda and Martha Rosete-Aguilar, which can also be displayed in figures.

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¹ María C. Simon and Karin V. Gottschalk, "Waves and rays in uniaxial birefringent crystals," Optik 118(10), 457–470 (2007).

² Maximino Avendaño-Alejo, Orestes N. Stavroudis, and Ana Rosa Boyain y Goitia, "Huygens's principle and rays in uniaxial anisotropic media. I. Crystal axis normal to refracting surface," J. Opt. Soc. Am. A, 19(8), 1668–1673 (2002).

Maximino Avendaño-Alejo and Orestes N. Stavroudis, "Huygens's principle and rays in uniaxial anisotropic media. II. Crystal axis orientation arbitrary," J. Opt. Soc. Am. A, 19(8), 1674–1679 (2002).

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- ⁴ A. Yariv and P. Yev, Optical Waves in Crystals. Propagation and Control of Laser Radiation, 1st Ed. (John Wiley and Sons, Inc., 1984).
- ⁵ Luis A. Alemán-Castañeda and Martha Rosete-Aguilar, "Deviation from orthogonal polarization for ordinary and extraordinary rays in uniaxial crystals," J. Opt. Soc. Am. A 33(4), 677–682 (2016).
- ⁶ Luis A. Alemán-Castañeda, Trazo de rayos en lentes birrefringentes uniaxiales, Bachelor's Thesis (Universidad Nacional Autónoma de México, 2016).
- Maximino Avendaño-Alejo and Rufino Díaz-Uribe and Ivan Moreno, "Caustics caused by refraction in the interface between an isotropic medium and a uniaxial crystal," J. Opt. Soc. Am. A 25(7), 1586–1593 (2008).
- ⁸ Luis A. Alemán-Castañeda and Martha Rosete-Aguilar, "Study of orthogonal polarization approximation for ordinary and extraordinary rays in ray tracing for uniaxial crystals," in *Optical Modelling and Design IV*, edited by Frank Wyrowski, John T. Sheridan, and Youri Meuret [Proc. SPIE 9889 (2016)], pp. 410–419.
- ⁹ See the supplementary material at [URL will be inserted by AIP] for the Mathematica code.