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LOCATION OF RAY PATHS FOR A KNOWN WAVE NORMAL IN BIAXIAL CRYSTALS

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Abstract

The values of the principal indices of refraction determine the properties of the optical indicatrix. The directions of the ray paths associated with a wave normal ultimately depend on the indices of refraction. The directions of the wave normal and ray paths need not coincide in anisotropic media. To find a ray path for a given wave normal, two items of information must be extracted from the properties of the indicatrix: the location of a vector representing a vibration direction or electric displacement vector, **D**, and the direction of the vector representing the electric field generated by the electromagnetic radiation, **E**. The angle $2V$ and optic sign, obtainable from the indices of refraction, are all the information needed to calculate vectors parallel to the vibration directions associated with a given wave normal. A second-rank tensor, with principal components inversely proportional to the squares of the principal indices of refraction of the crystal, relates vectors representing the vibration direction and the electric field, **D** and **E**. **E** is calculated from this relation. The angle between **D** and **E** equals the angle between the wave normal and the ray path. Maximum values of the angles between ray path and wave normal depend on the largest index of refraction, γ, and the birefringence of the crystal ($\gamma - \alpha$). For common rock-forming minerals, the maximum angle is approximately 0.5° – 2°. In crystals with extreme birefringence, such as aragonite and strontianite, the maximum angle approaches 6°. Wave normals and ray paths diverge most in sections cut parallel to the Y vibration direction and tilted with their normals between 45° and 50° from the Z vibration direction. The precise angle between the Z vibration direction and the normal to the section depends on γ and ($\gamma - \alpha$).

Keywords: optical mineralogy, ray path, wave normal, optical directions, vector algebra, indicatrix, Maxwell's equations, vibration direction, electric vector.

Sommaire

Les valeurs des principaux indices de réfraction déterminent les propriétés de l'ellipsoïde de propagation et de vibration optique. Les directions de propagation d'ondes associées avec un front d'onde dépendent finalement des indices de réfraction. Il n'est pas nécessaire que la direction perpendiculaire au front d'onde et les directions de propagation des ondes coïncident dans un milieu anisotrope. Pour trouver une direction de propagation d'onde pour un plan perpendiculaire à un front d'onde donné, il est nécessaire d'extraire deux pièces d'information des propriétés de l'ellipsoïde: la localisation du vecteur qui représente la direction de vibration ou le vecteur de déplacement électrique, **D**, et la direction du vecteur qui représente le champ électrique que génère le rayonnement électromagnétique, **E**. L'angle $2V$ et le signe optique, qui découlent des indices de réfraction, suffisent pour calculer les vecteurs parallèles aux directions de vibration associées à un plan perpendiculaire à un front d'onde donné. Un tenseur de deuxième rang, dont les composants principaux sont inversement proportionnels aux carrés des principaux indices de réfraction du cristal, font le lien entre les vecteurs représentant la direction de vibration et le champ électrique, **D** et **E**. On calcule **E** à partir de cette relation. L'angle entre **D** et **E** est égal à l'angle entre la perpendiculaire au front d'onde et la direction de propagation d'une onde. Les valeurs maximales de l'angle entre ces deux directions dépendent de la valeur de l'indice de réfraction le plus élevé, γ, et la biréfringence du cristal ($\gamma - \alpha$). Dans les cas des minéraux courants dans les roches, l'angle maximum se situe dans l'intervalle 0.5° – 2°. Dans les cas d'une biréfringence extrême, l'aragonite et la strontianite par exemple, l'angle maximum peut atteindre 6°. Les perpendiculaires aux fronts d'onde et les tracés d'ondes sont davantage divergents dans les sections parallèles à la direction de vibration Y et inclinées avec leurs perpendiculaires au front d'onde entre 45° et 50° de la direction de vibration Z. L'angle précis entre cette direction de vibration et la perpendiculaire à la section étudiée dépendrait de γ et de ($\gamma - \alpha$).

Mot-clés: minéralogie optique, tracé d'une onde, perpendiculaire à un front d'onde, directions optiques, algèbre vectorielle, ellipsoïde de propagation et de vibration, équations de Maxwell, direction de vibration, vecteur électrique.

INTRODUCTION

Three directions are associated with the transmission of normally incident light through crystals: two are ray paths, or directions of energy transfer, and the third is the wave normal, perpendicular to two directions of vibration of light normally incident on general sections through anisotropic crystals. The three directions need not coincide in anisotropic media. By and large, ray paths do not play a prominent role in the theory of optical crystallography (*e.g.*, Bloss 1961, Nesse 1991). It is the vibration directions that are important, and these are associated with the wave normal, not the ray path. In spite of the relative importance of ray paths and wave normals, students of optical mineralogy do ask about the location of ray paths. In addition, the location of ray paths is required for a complete description of interference figures. A completely rigorous and general mathematical description of the phenomena leading to interference figures has not been developed, even though research into the matter dates back to the late 1800s (Bethke & Birnie 1980). It is much easier to determine the wave normals than the ray paths. The latest model for describing interference figures (Bethke & Birnie 1980) assumes that wave normals are adequate approximations to the ray paths. This paper describes a method, using vector algebra, for finding the ray paths associated with a given wave normal. Consequently, a quantitative evaluation of the wave normal approximation follows. Bloss (1961, p. 77–78, 160–161), Wahlstrom (1979, Appendix B), and Nesse (1991, p. 56–57, 80–81) described graphical procedures for finding ray paths. Graphical procedures, however, are not always practical methods for finding numerical solutions to real problems. The vector-based method outlined in this paper results in an analytical expression for the angles between the wave normal and ray path.

MAXWELL'S EQUATIONS

Light is a form of electromagnetic radiation; there are two vectors associated with each kind of phenomenon, electricity and magnetism. The vectors associated with electricity will be labeled **E** and **D**. If a crystal is placed in an electric field described by the vector function **E**, then a current will tend to flow in the crystal parallel to **D** (see Bloss 1971, p. 361–371). If the crystal is isometric or if an anisotropic crystal is given a particular orientation with respect to **E**, then **D** will be parallel to **E**. In general, however, **D** and **E** are not parallel. When light is the source of the electric field, **E**, the field oscillates, causing **D** to oscillate as well. **D** is parallel to a vibration direction in the crystal. Inside the crystal, **E** presumably still exists, and it is the normal to **E** that constitutes the ray path. Energy is carried by the electric field in a direction of transfer normal to **E**. The wave normal, represented by the vector $\boldsymbol{w}$, is normal to **D**. Even though **D** is the direction along which an electric current tends to flow in response to **E**, there will be no net current if **E** is oscillating; as many electrons will try to flow along **+D** as along **–D**, thereby cancelling the flow of electricity.

Similar to the vectors describing the electrical properties of crystals are two vectors associated with their magnetic properties, **B** and **H**. Place a crystal in a sufficiently strong magnetic field, **B**, and it will acquire a magnetic direction parallel to **H**. The crystals that transmit light are found by experiment to be effectively isotropic in their magnetic behavior. Consequently, **B** and **H** are parallel in most rock-forming minerals.

Maxwell's equations relate **B**, **H**, **D** and **E**. They are partial differential vector equations and contain a complete classical description of electromagnetic phenomena (Schey 1973). The following relationships between the properties of electromagnetic waves result from solutions to Maxwell's equations (Nye 1957, p. 305–309):

$$\mathbf{H} = (\boldsymbol{w} \times \mathbf{E})/(\mu_o v) \quad (1)$$

$$\mathbf{D} = -\boldsymbol{w} \times (\boldsymbol{w} \times \mathbf{E})/(\mu_o v^2) = -(\boldsymbol{w} \times \mathrm{H})/v \quad (2)$$

$$\mathbf{R} = \mathbf{E} \times \mathbf{H} \quad (3)$$

R is a vector parallel to the direction of transmission of energy or ray path, μ_o is the permeability of a vacuum, and v is the speed of light in the substance. The geometrical relationships between the directions represented by these vectors are shown on Figure 1. **D**, **E**, $\boldsymbol{w}$, and **R** are coplanar, and all are normal to **H**. These geometrical relations are a consequence of Equations (1) – (3) and follow from Maxwell's equations. The angle θ, shown on Figure 1, is the deviation between the ray path, **R**, and the wave normal, $\boldsymbol{w}$. It is also the angle between **E** and **D**. Consequently, calculating the angle between **D** and **E** also gives the angle between **R** and $\boldsymbol{w}$. Figure 1 shows vectors representing the properties for only one ray path. In anisotropic crystals, there are generally two ray paths and two vibration directions.

Expand the triple product in Equation (2), with the result:

$$\mu_o v^2 \mathbf{D} + (\boldsymbol{w} \cdot \mathbf{E})\boldsymbol{w} - \mathbf{E} = \mathbf{0} \quad (4)$$

Equation (4) is a vector equation relating **D** and **E**. It has been derived for the general case, not for a specific optical symmetry. To find the ray path for a given wave normal, the location of the vibration direction parallel to **D**, and a relationship between **D** and **E**, are required.

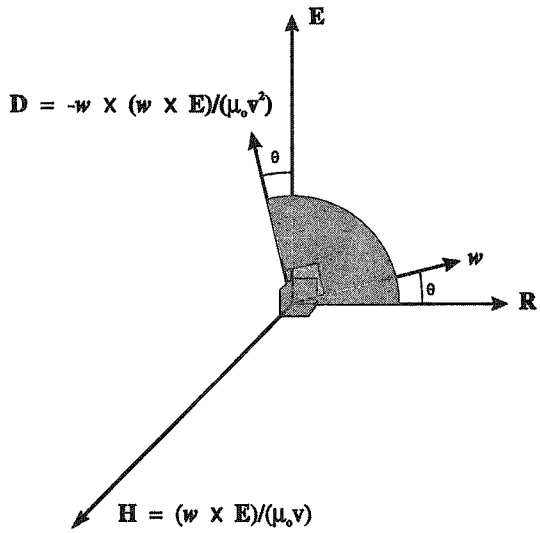


FIG. 1. Schematic diagram showing the relationships among electromagnetic vectors. **E** is the vector representing the electric field, **D** is parallel to a vibration direction, w is a unit vector parallel to the wave normal. **H** is normal to the plane defined by **E** and w. **R** is parallel to the ray path and is defined by **E** × **H**. **E**, **D** and w are coplanar.

LOCATION OF VIBRATION DIRECTIONS

The important directions in the indicatrix are the directions of principal vibration, X, Y, Z, the optic axes and, in any given section through the indicatrix, the two vibration directions of light and their wave normal. In orthoscopic light, the normal to a thin section is parallel to the wave normal vector, w. The law of Biot–Fresnel (see, *e.g.*, Bloss 1961, p. 161) states that a vibration direction bisects the angle between the two planes formed by the wave normal and each of the optic axes. To apply this law, the locations of the wave normal and the optic axes in a frame of reference are required. The indicatrix provides a convenient frame of reference for the location of vectors representing optical directions. The direction of the wave normal relative to the indicatrix axes is given. Consequently, an equation for a unit vector parallel to this direction is:

$$w = w_1 i + w_2 j + w_3 k \tag{5}$$

where i, j, and k are unit vectors parallel to the axes of the indicatrix, X, Y, and Z, respectively. The w_i, $i = 1, 2, 3$, are the components of w parallel to X, Y, and Z, in that order, and are given quantities. Because the components of a unit vector are the same as the direction cosines of the vector in the frame of reference, it is relatively simple to locate the wave

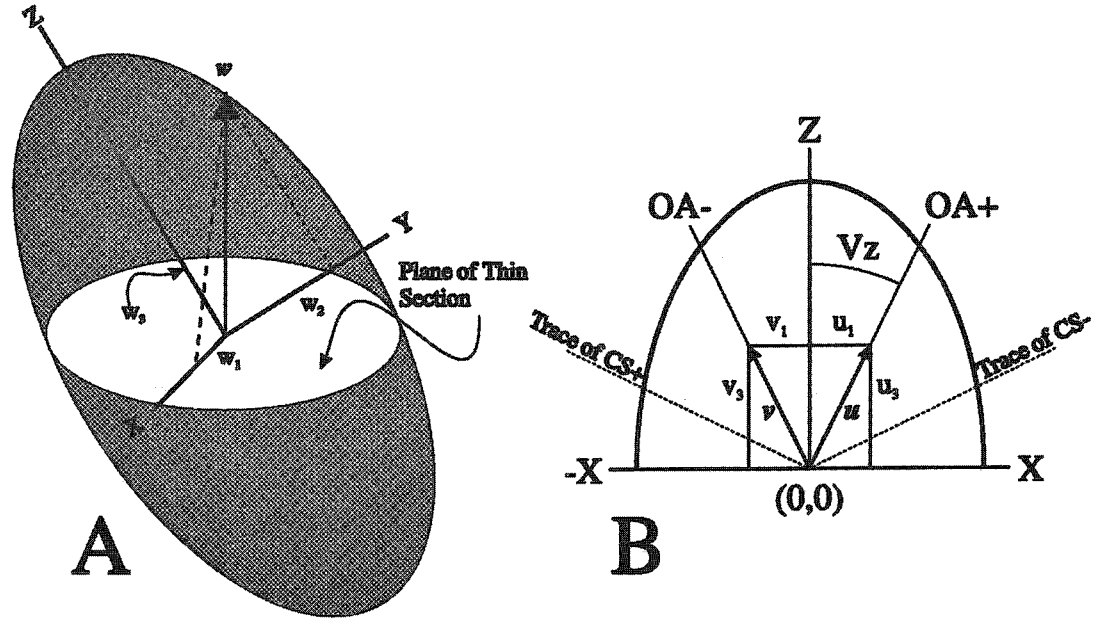


FIG. 2. A. Schematic illustration of a general wave normal in the frame of reference defined by the axes of the indicatrix. The projections of the unit vector parallel to the wave normal, w, on the axes are the components of w in this frame of reference. The w_i are equal to the cosines of the angles w makes with the axes of the indicatrix. B. Sketch of the optic axial plane through an indicatrix showing the unit vectors, u and v, parallel to the optic axes. The components of these vectors are u_1, u_2, u_3 and v_1, v_2, v_3. Constraints on these quantities are: $v_1 = -u_1$, $u_2 = v_2 = 0$, and $v_3 = u_3$. The positive end of the Y axis projects into the plane of the diagram for a right-hand system of coordinates.

normal vector by the angles it makes with the axes of the frame of reference (Fig. 2A).

The directions of the optic axes, relative to the indicatrix axes, are determined by the sign and $2V$ of the substance. A unit vector parallel to the optic axis that falls between positive X and positive Z is given by:

$$\boldsymbol{u} = \sin V_z \boldsymbol{i} + \cos V_z \boldsymbol{k} \quad (6)$$

or:

$$\boldsymbol{u} = u_1 \boldsymbol{i} + u_3 \boldsymbol{k} \quad (7)$$

where:

$$u_1 = \sin V_z$$
$$u_3 = \cos V_z \quad (8)$$

These vectors are illustrated on Figure 2B. The second optic axis will be parallel to a unit vector:

$$\boldsymbol{v} = -\sin V_z \boldsymbol{i} + \cos V_z \boldsymbol{k} \quad (9)$$

Note that:

$$\boldsymbol{v} = -u_1 \boldsymbol{i} + u_3 \boldsymbol{k} \quad (10)$$

The angle between the optic axes, $2V$, is a property of the indices of refraction (see, *e.g.*, Bloss 1961, p. 156). Consequently, the optic axis vectors, **u** and **v**, are themselves functions of and can be calculated from the indices of refraction.

A stereographic projection of the relationships among $\boldsymbol{w}$, $\boldsymbol{u}$, $\boldsymbol{v}$ and the sections (planes) normal to each vector is shown on Figure 3. A vector parallel to the line of intersection of the circular section normal to OA+ (CS+, Fig. 3) and the plane of the thin section will be normal to both OA+ and the wave normal. Label this vector $\boldsymbol{t}$. The same situation will hold for another vector parallel to the intersection of the second circular section (CS–, Fig. 3) and the plane of the thin section; label it $\boldsymbol{s}$. The vector $\boldsymbol{t}$ lies at 90° to $\boldsymbol{u}$ and $\boldsymbol{w}$; $\boldsymbol{s}$ lies at 90° to $\boldsymbol{v}$ and $\boldsymbol{w}$.

Calculate the components of the vectors parallel to the lines of intersection. The cross-product was designed to find such a vector, as it produces a new vector normal to two original ones. A vector parallel to the first intersection is:

$$\mathbf{T} = \boldsymbol{u} \times \boldsymbol{w} \quad (11)$$

and a vector parallel to the second intersection is:

$$\mathbf{S} = \boldsymbol{w} \times \boldsymbol{v} \quad (12)$$

Unit vectors parallel to the two lines of intersection are obtained by dividing by the magnitudes of the **T** and **S**:

$$\boldsymbol{t} = \boldsymbol{u} \times \boldsymbol{w} / [(\boldsymbol{u} \times \boldsymbol{w}) \cdot (\boldsymbol{u} \times \boldsymbol{w})]^{1/2} \quad (13)$$

$$\boldsymbol{s} = \boldsymbol{w} \times \boldsymbol{v} / [(\boldsymbol{w} \times \boldsymbol{v}) \cdot (\boldsymbol{w} \times \boldsymbol{v})]^{1/2} \quad (14)$$

Substitution of Equations (7) and (10) into Equations (13) and (14), plus the fact that the sum of

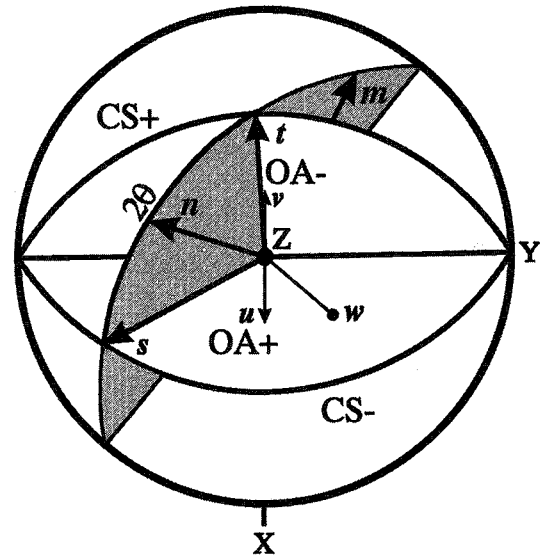


FIG. 3. Stereographic projection of the optical indicatrix and a Biot–Fresnel construction showing the relationship of the unit vector parallel to the wave normal, $\boldsymbol{w}$, to unit vectors parallel to the optic axes, $\boldsymbol{u}$ and $\boldsymbol{v}$, and to unit vectors parallel to the intersections of the circular sections with the plane of the thin section, $\boldsymbol{t}$ and $\boldsymbol{s}$. Unit vectors parallel to the vibration directions in the plane of the thin section, $\boldsymbol{n}$ and $\boldsymbol{m}$, bisect the angles between $\boldsymbol{t}$ and $\boldsymbol{s}$. The optic axes, OA+ and OA– emerge from the projection at the tips of the vectors $\boldsymbol{u}$ and $\boldsymbol{v}$ and are normal to the circular sections CS+ and CS–.

squares of the components of a unit vector is one, provides, after algebraic manipulation:

$$\boldsymbol{t} = [-u_3 w_2 \boldsymbol{i} + (u_3 w_1 - u_1 w_3)\boldsymbol{j} + u_1 w_2 \boldsymbol{k}] / [1 - (u_1 w_1 + u_3 w_3)^2]^{1/2} \quad (15)$$

$$\boldsymbol{s} = [u_3 w_2 \boldsymbol{i} - (u_3 w_1 + u_1 w_3)\boldsymbol{j} + u_1 w_2 \boldsymbol{k}] / [1 - (u_1 w_1 - u_3 w_3)^2]^{1/2} \quad (16)$$

Equations (15) and (16) are formulae for calculation. The w_i are given quantities, and the u_i can be calculated from $2V_z$ [Equation (8)].

According to the Law of Biot–Fresnel, one of the vibration directions in the plane of the thin section bisects the angle between $\boldsymbol{t}$ and $\boldsymbol{s}$, labeled 2θ on Figure 3. A unit vector parallel to this vibration direction is labeled $\boldsymbol{n}$. Because $\boldsymbol{n}$ bisects the angle between $\boldsymbol{t}$ and $\boldsymbol{s}$, and because $\boldsymbol{t}$ and $\boldsymbol{s}$ are of equal magnitude, being unit vectors, the parallelogram law of vector addition requires that:

$$\mathbf{G} = \boldsymbol{t} + \boldsymbol{s} \quad (17)$$

where **G** is a vector parallel to ***n***. It is then a simple matter to convert **G** into a unit vector by dividing by the magnitude of **G**:

$$\boldsymbol{n} = \mathbf{G}/[\mathbf{G} \cdot \mathbf{G}]^{1/2} \tag{18}$$

The second vibration direction, ***m***, is normal to both ***w*** and ***n***. As a result, the three vectors are related by the cross-product:

$$\boldsymbol{m} = \boldsymbol{n} \times \boldsymbol{w} \tag{19}$$

or, in component form:

$$\begin{aligned} m_1 &= n_2 w_3 - n_3 w_2 \\ m_2 &= n_3 w_1 - n_1 w_3 \\ m_3 &= n_1 w_2 - n_2 w_1 \end{aligned} \tag{20}$$

The foregoing contains the information needed to calculate the vibration directions in any section through a biaxial mineral, given the wave normal vector, ***w***, and the principal indices of refraction. An example of these calculations is given in Table 1.

TABLE 1. EXAMPLE OF THE CALCULATIONS

Given Values	w_1	w_2	w_3
Wave normal vector: *w*	0.57735	0.57735	0.57735
	α	β	γ
Indices of Refraction	1.60	1.62	1.70

Calculated Values

V_z (see Bloss 1961, p. 156) 27.618

	i	*j*	*k*		
Optic Axis Vector: *u*	0.46357	0.0	0.88606		
Optic Axis Vector: *v*	–0.46357	0.0	0.88606		
t: Eqn. (15)	–0.81620	0.38918	0.42703		
s: Eqn. (16)	0.52750	–0.80348	0.27598		
G = *t* + *s*: Eqn. (17)	–0.28871	–0.41430	0.70301		
n: Eqn. (18)	–0.33354	–0.47865	0.81219		
m: Eqn. (20)	–0.74526	0.66149	0.08378		
e_n: Eqn. (40)	–0.13029	–0.18238	0.28103	$e_n \cdot e_n$	0.12922
e_m	–0.29112	0.25205	0.02899	$e_m \cdot e_m$	0.14912
r_n: Eqn(42)	0.07222	0.07127	0.07974	$e_n \cdot w_n$	–0.01827
r_m	0.08440	0.08756	0.08626	$e_m \cdot w_m$	–0.00582
r_n: Unit Vector: Eqn. (43)	0.55966	0.55228	0.61788	$n \cdot e_n$	0.35901
r_m	0.56606	0.58725	0.57855	$m \cdot e_m$	0.38612
cos θ_n: Eqn. (46)	0.99871				
cos θ_m	0.99989				
θ_n =	2.91				
θ_m =	0.86				

The components of the unit vectors, *w, u, v, n, m,* and *r,* are equal to the direction cosines of the angles between the vector and the axes of the frame of reference, the indicatrix. The wave normal vector, *w,* was chosen to make equal angles with the axes of the indicatrix. The *m* and *n* subscripts refer to values calculated for the two vibration directions.

Relationship Between D and E

The relationship between **D** and **E** is most simple in isotropic media, where **D** and **E** are parallel. In that case, **E** is normal to ***w***, and the dot product in Equation (4) vanishes, to give:

$$\mathbf{E} = \mu_0 v^2 \mathbf{D} \tag{21}$$

The terms before **D** constitute a scalar, hence, Equation (21) states that the two vectors, **E** and **D**, are parallel, as they must be in isotropic media.

In anisotropic substances, **E** and **D** are not parallel, and a second-rank tensor is needed to describe the relationship between **D** and **E** (Bloss 1971, p. 361–372; Nye 1957, Ch. 1). The indicatrix is the geometrical representation of a tensor property, the reciprocal of the square of the index of refraction. In other words, the optical property, $1/N^2$, associated with a known vibration direction, ***n***, is a tensor property of the crystal that relates two vectors. A modification of the indicatrix tensor relates **D** and **E**. In an arbitrary frame of reference, the tensor equation that relates **D** and **E** is:

$$\begin{vmatrix} \kappa_{11} & \kappa_{12} & \kappa_{13} \\ \kappa_{21} & \kappa_{22} & \kappa_{23} \\ \kappa_{31} & \kappa_{32} & \kappa_{33} \end{vmatrix} \begin{vmatrix} E_1 \\ E_2 \\ E_3 \end{vmatrix} = \begin{vmatrix} D_1 \\ D_2 \\ D_3 \end{vmatrix} \tag{22}$$

where D_i and E_i are the components of **D** and **E** in the arbitrary frame of reference, and the κ_{ij} are the components, in this frame of reference, of the second-rank tensor that relates **D** and **E**.

An even simpler notation for the same set of equations is:

$$\underline{\kappa}\,\mathbf{E} = \mathbf{D} \tag{23}$$

where $\underline{\kappa}$ is short-hand for:

$$\begin{vmatrix} \kappa_{11} & \kappa_{12} & \kappa_{13} \\ \kappa_{21} & \kappa_{22} & \kappa_{23} \\ \kappa_{31} & \kappa_{32} & \kappa_{33} \end{vmatrix} \tag{24}$$

Second-rank tensors can be referred to a special set of axes such that Equation (22) can be written:

$$\begin{vmatrix} \kappa_1 & 0 & 0 \\ 0 & \kappa_2 & 0 \\ 0 & 0 & \kappa_3 \end{vmatrix} \begin{vmatrix} E_1 \\ E_2 \\ E_3 \end{vmatrix} = \begin{vmatrix} D_1 \\ D_2 \\ D_3 \end{vmatrix} \tag{25}$$

where the κ_i are nonzero components of $\underline{\kappa}$ in this new frame of reference. The details of obtaining the κ_i from the κ_{ij} are given in Nye (1957). $\underline{\kappa}$ is equally well represented by the form of the tensor in either Equation (22) or Equation (25). The differences are solely due to a change in the system of coordinates. Equation (25) can be written as:

$$\kappa_1 E_1 \boldsymbol{i} + \kappa_2 E_2 \boldsymbol{j} + \kappa_3 E_3 \boldsymbol{k} = \mathbf{D} \quad (26)$$

In order for Equation (26) to reduce to the isotropic case, Equation (21), the values for the κ_i would all have to be equal, say to κ:

$$\kappa \mathbf{E} = \mathbf{D} \quad (27)$$

Comparing Equations (22) and (28) gives:

$$\kappa = 1/(\mu_o v^2) \quad (28)$$

for isotropic substances. Optically isotropic substances are characterized by a uniform index of refraction, regardless of vibration direction. Because the index of refraction is inversely proportional to the speed of light in a substance, one expects the components of $\underline{\kappa}$ to be functions of the indices of refraction.

An index of refraction is the ratio of the speed of light in a vacuum to the speed in a substance. To relate speeds and indices of refraction, an expression for the speed of light in a vacuum is needed. Presumably, a vacuum is isotropic and uniform throughout the universe. Consequently, in a vacuum, **D** and **E** should be related by:

$$\mathbf{D} = \kappa_o \mathbf{E} \quad (29)$$

where κ_o, the permittivity of free space, is a universal scalar constant. Maxwell's achievement was to relate k_o and μ_o to the speed of light, c:

$$\nabla^2 \mathbf{E} = \mu_o \kappa_o \partial^2 \mathbf{E}/\partial t^2 \quad (30)$$

Equation (30) has the form of the classic wave equation if:

$$c^2 = 1/(\mu_o \kappa_o) \quad (31)$$

The two constants, μ_o and κ_o, can be experimentally determined. The reciprocal of their product equals the square of the measured speed of light in a vacuum.

Equation (31) suggests that the velocity of light vibrating in a particular direction parallel to **D** would have as its components in the frame of reference defined by Equation (25):

$$\begin{aligned} v_1^2 &= 1/(\mu_o \kappa_1) \\ v_2^2 &= 1/(\mu_o \kappa_2) \\ v_3^2 &= 1/(\mu_o \kappa_3) \end{aligned} \quad (32)$$

The nonzero components of $\underline{\kappa}$ can be written as:

$$\begin{aligned} \kappa_1 &= \kappa_o c^2/v_1^2 \\ \kappa_2 &= \kappa_o c^2/v_2^2 \\ \kappa_3 &= \kappa_o c^2/v_3^2 \end{aligned} \quad (33)$$

The set of Equations (33) relate the components of the tensor $\underline{\kappa}$ to three velocities of light through the crystal. There is one component that is the largest possible and one that is the smallest possible. If the *X* axis is the direction along which D_1 lies, then κ_1 is the tensor component of interest. If κ_1 is assigned the smallest value, then v_1 must be the fastest. But in that case, c^2/v_1^2 is equal to the square of the smallest index of refraction, α^2, and κ_1 is equal to $\kappa_o \alpha^2$. In a like manner, κ_2 is equal to $\kappa_o \beta^2$ and κ_3 is equal to $\kappa_o \gamma^2$, where β and γ are the intermediate and largest indices of refraction. Consequently, the equation relating **D** and **E** becomes:

$$\begin{vmatrix} \kappa_o\alpha^2 & 0 & 0 \\ 0 & \kappa_o\beta^2 & 0 \\ 0 & 0 & \kappa_o\gamma^2 \end{vmatrix} \begin{vmatrix} E_1 \\ E_2 \\ E_3 \end{vmatrix} = \begin{vmatrix} D_1 \\ D_2 \\ D_3 \end{vmatrix} \quad (34)$$

The relationship between n and **D** can be expressed:

$$\boldsymbol{n} = \mathbf{D}/[\mathbf{D} \cdot \mathbf{D}]^{1/2} \quad (35)$$

If a new vector **e** is defined in the following fashion:

$$\mathbf{e} = \kappa_o \mathbf{E}/[(\mathbf{D} \cdot \mathbf{D})^{1/2}] \quad (36)$$

Equation (25) becomes:

$$\underline{\mathbf{K}}\, \boldsymbol{n} = \mathbf{e} \quad (37)$$

where $\underline{\mathbf{K}}$ is the tensor:

$$\begin{vmatrix} 1/\alpha^2 & 0 & 0 \\ 0 & 1/\beta^2 & 0 \\ 0 & 0 & 1/\gamma^2 \end{vmatrix} \quad (38)$$

Notice, in particular, that **e** and **E** are parallel vectors because of Equation (36).

Nye (1957) showed that a tensor with positive principal components, such as $\underline{\mathbf{K}}$, can be geometrically represented by the triaxial ellipsoid:

$$X^2/\alpha^2 + Y^2/\beta^2 + Z^2/\gamma^2 = 1 \quad (39)$$

which is the equation for the indicatrix. Hence, Maxwell's Equations and the tensor relationship between **D** and **E** lead to an expression for the indicatrix.

The Indicatrix and Ray Paths

In order to calculate the ray path, first calculate **e** from the Equation (37):

$$\mathbf{e} = \underline{\mathbf{K}}\, \boldsymbol{n} = n_1/\alpha^2 \boldsymbol{i} + n_2/\beta^2 \boldsymbol{j} + n_3/\gamma^2 \boldsymbol{k} \quad (40)$$

the ray path is then parallel to a vector:

$$\mathbf{r} = \mathbf{e} \times (\boldsymbol{w} \times \mathbf{e}) \quad (41)$$

The location of the ray path with respect to the axes of the indicatrix is most easily calculated if a unit vector parallel to **r** is first calculated. To do this, expand the triple product in Equation (41) into a form that is easier to express in a numerical format:

$$\mathbf{r} = (\mathbf{e} \cdot \mathbf{e})\, \boldsymbol{w} - (\mathbf{e} \cdot \boldsymbol{w})\, \mathbf{e} \tag{42}$$

then calculate the unit vector from:

$$\boldsymbol{r} = \mathbf{r}/[\mathbf{r} \cdot \mathbf{r}]^{1/2} \tag{43}$$

Explicitly, the two dot products in Equation (42) are given by:

$$\mathbf{e} \cdot \mathbf{e} = n_1^2/\alpha^4 + n_2^2/\beta^4 + n_3^2/\gamma^4 \tag{44}$$

$$\mathbf{e} \cdot \boldsymbol{w} = w_1 n_1/\alpha^2 + w_2 n_2/\beta^2 + w_3 n_3/\gamma^2 \tag{45}$$

Equation (43) has the components of the wave normal vector and the principal indices of refraction as its primary variables; the n_i are functions of the w_i and the indices of refraction [see Equations (6), (10), (15), (16), and (18)]. It is the analytical expression for calculating the ray path. An example of the calculations is shown in Table 1.

In summary, to find the ray paths associated with the wave normal $\boldsymbol{w}$, first calculate the two vibration vectors, $\boldsymbol{m}$ and $\boldsymbol{n}$. Next calculate the two **e** vectors, $\underline{\mathbf{K}}\,\boldsymbol{n}$ and $\underline{\mathbf{K}}\,\boldsymbol{m}$. Finally, calculate the two ray paths with Equation (43).

Magnitude of the Angle Between $\boldsymbol{r}$ and $\boldsymbol{w}$

Optical crystallography texts state that the angle between the ray path and wave normal is small. We now have the capability of calculating this angle and determining how small it is. The angle between $\boldsymbol{w}$ and $\boldsymbol{r}$ will equal the angle between $\boldsymbol{n}$ and **e** because of the cross-product relationship shown on Figure 1. The angle between **e** and $\boldsymbol{n}$ is most easily obtained with the dot product:

$$\cos\theta = \boldsymbol{n} \cdot \mathbf{e}/[\mathbf{e} \cdot \mathbf{e}]^{1/2} \tag{46}$$

Explicitly, the dot product, $\boldsymbol{n} \cdot \mathbf{e}$, is given by:

$$\boldsymbol{n} \cdot \mathbf{e} = n_1^2/\alpha^2 + n_2^2/\beta^2 + n_3^2/\gamma^2 \tag{47}$$

Equation (43) can be obtained by a second method, from which some additional results follow. Consider the equation for the indicatrix written in the following fashion:

$$f(X,Y,Z) = X^2/\alpha^2 + Y^2/\beta^2 + Z^2/\gamma^2 = 1 \tag{48}$$

where $f(X,Y,Z)$ is a scalar function of position. The gradient of such a function is normal to surfaces on which the function $f(X,Y,Z)$ is constant (Schey 1973, p. 138). Hence a vector normal to the indicatrix is given by:

$$\nabla f = (2X/\alpha^2)\boldsymbol{i} + (2Y/\beta^2)\boldsymbol{j} + (2Z/\gamma^2)\boldsymbol{k} \tag{49}$$

A vector parallel to the vibration vector that stretches from the center of the indicatrix to a point (X,Y,Z) on the indicatrix is given by:

$$\mathbf{N} = \mathrm{N}\,\boldsymbol{n} \tag{50}$$

where N is a scalar that multiplies $\boldsymbol{n}$ and gives the magnitude of **N**. From the definition of the indicatrix, one concludes that value of N is equal to the index of refraction of the light vibrating parallel to $\boldsymbol{n}$. In component form, Equation (50) becomes:

$$X\boldsymbol{i} + Y\boldsymbol{j} + Z\boldsymbol{k} = \mathrm{N}\,n_1\boldsymbol{i} + \mathrm{N}\,n_2\boldsymbol{j} + \mathrm{N}\,n_3\boldsymbol{k} \tag{51}$$

from which it follows that:

$$\boldsymbol{n} = (X/\mathrm{N})\boldsymbol{i} + (Y/\mathrm{N})\boldsymbol{j} + (Z/\mathrm{N})\boldsymbol{k} \tag{52}$$

where N is the index of refraction of light vibrating parallel to $\boldsymbol{n}$. Substitution for X, Y and Z in Equation (48) gives:

$$\nabla f = 2\mathrm{N}\,[(n_1/\alpha^2)\boldsymbol{i} + (n_2/\beta^2)\boldsymbol{j} + (n_3/\gamma^2)\boldsymbol{k}] \tag{53}$$

Thus, the gradient, ∇f, is parallel to the electric vector **e**:

$$\nabla f = 2\mathrm{N}\,\mathbf{e} \tag{54}$$

Consequently, this parallelism means that the angle between $\boldsymbol{n}$ and **e** can be calculated from:

$$\cos\theta = \boldsymbol{n} \cdot \nabla f/|\nabla f| \tag{55}$$

Note that because ∇f is normal to the indicatrix surface, the electric vector, **E**, is also.

These relationships are illustrated in Figure 4. The evenly shaded, inclined plane is the plane of the thin section and contains the vibration vector $\boldsymbol{n}$. In this particular example, the thin section is parallel to the X axis. Consequently, the wave normal, $\boldsymbol{w}$, the vibration vector, $\boldsymbol{n}$, and the electric vector lie in the Y–Z plane, as does the ray path, parallel to **r**. Because ∇f is normal to the indicatrix surface, the ray path will be parallel to its tangent. As a result, the vibration vector, $\boldsymbol{n}$, and the ray path vector, **r**, are parallel to conjugate radii of the indicatrix, a fact that was described by Bloss (1961).

The factors that control the size of the angle between the vibration and electric vectors, θ, are the indices of refraction associated with the two vibration directions. Any central section through the indicatrix is an ellipse, including the section that contains the vibration,

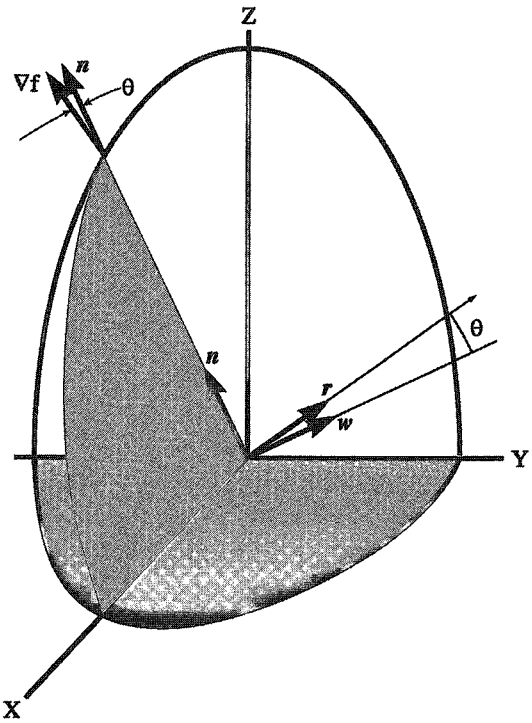


FIG. 4. Diagram showing the relationship among the gradient to the indicatrix, ∇f, a vibration direction, ***n***, and its associated wave normal, ***w***. The angle between the ray path, ***r***, and the wave normal equals the angle between ***n*** and ∇f (see text).

electric, and wave normal vectors, ***n***, ∇f, and ***w*** (Fig. 5A). This ellipse is not the plane of the thin section; rather, the plane of the thin section, the plane normal to ***w***, is perpendicular to the ellipse under discussion (Fig. 5A). Label the major and minor axes of the ellipse containing ***w***, ***n***, and ∇f as P and Q with unit vectors, ***p*** and ***q***, along these axes:

$$f(P,Q) = P^2/b^2 + Q^2/a^2 = 1 \qquad (56)$$

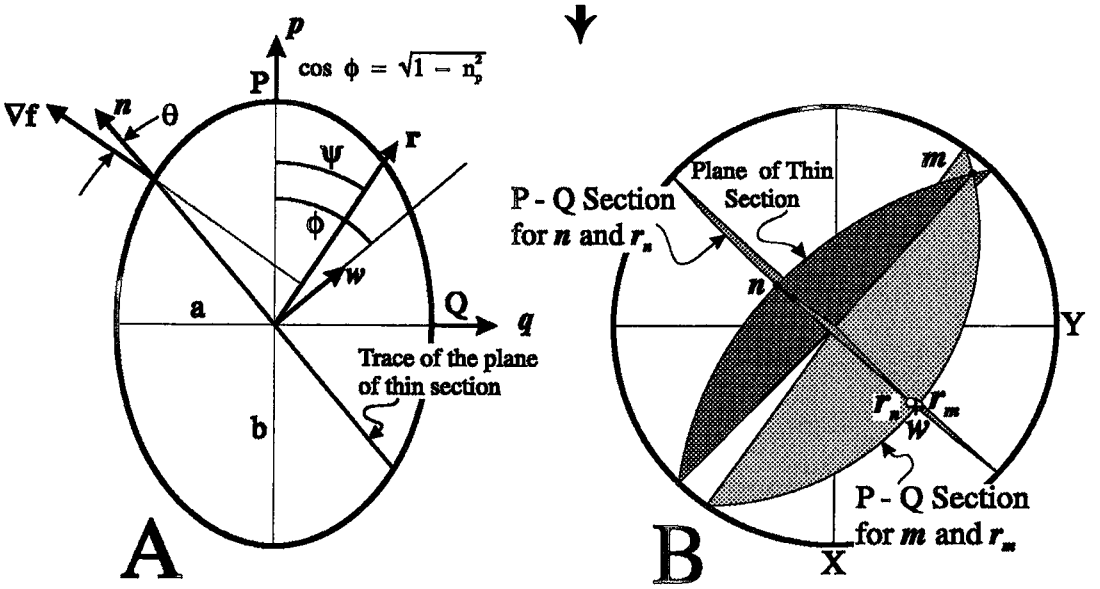
where a and b are the lengths of the minor and major axes of the ellipse. The gradient to f(P,Q) is:

$$\nabla f = (2P/b^2)\,\boldsymbol{p} + (2Q/a^2)\,\boldsymbol{q} \qquad (57)$$

In the plane containing ***n*** and ∇f, ***n*** can be written in the form:

$$\boldsymbol{n} = n_p\,\boldsymbol{p} + n_q\,\boldsymbol{q} \qquad (58)$$

FIG. 5. A. Diagram of an arbitrary section through the indicatrix. Major and minor axes of the elliptical section are P and Q, with lengths a and b. ∇f is the gradient of the equation of the ellipse, ***p*** and ***q*** are unit vectors parallel to the P and Q axes, ***w*** is a unit vector parallel to the wave normal, ***n*** is a unit vector parallel to the vibration direction in the plane of the ellipse, and ***r*** is parallel to the ray path. B. Stereographic projection of the wave normal vector, ***w***, the vibration vectors, ***n*** and ***m***, and the two ray path vectors, $\boldsymbol{r}_n$ and $\boldsymbol{r}_m$ associated with ***w***. The projection of ***w*** is shown with a cross between the two small open circles. Filled circles mark the projections of the vibration directions, and open circles mark the projections of the ray paths.



where $n_p = P/\sqrt{(P^2 + Q^2)}$
$n_q = Q/\sqrt{(P^2 + Q^2)}$

Next calculate the cosine of the angle between $\boldsymbol{n}$ and ∇f with the dot product. After some algebraic manipulations, the result is:

$$\cos\theta = [b^2 - n_p^2(b^2 - a^2)]/[b^4 - n_p^2(b^4 - a^4)]^{1/2} \quad (59)$$

The substitution of trigonometric identities into the equation for uniaxial ray paths (Wahlstrom 1979):

$$\tan\psi = \omega^2\tan\phi/\varepsilon^2 \quad (60)$$

will transform it into Equation (59) with ω replacing a and ε replacing b; ψ is the angle between the ray path and the major axis of the ellipse (Fig. 5A). The results of the calculations listed in Table 1 are plotted on Figure 5B. The wave normal vector, $\boldsymbol{w}$, is coplanar with the vibration vectors, **n** and $\boldsymbol{m}$, and with the two ray paths, r_n and r_m.

To find the maximum value of θ for the given ellipse, calculate the derivative of θ with respect to n_p in Equation (59) and set the result to zero. After some more algebraic manipulation, the result is:

$$n_{pm} = b/[a^2 + b^2]^{1/2} \quad (61)$$

$$\theta_m = \text{Arccos}\,[2ab/(a^2 + b^2)] \quad (62)$$

where θ_m is the maximum value of θ for the particular ellipse, and n_{pm} is the value of n_p for which θ is a maximum. One can check that θ_m is a maximum rather than a minimum by substituting one and zero for n_p in Equation (59). In both cases, θ will be zero. Because θ_m is greater than zero for positive values of a and b in Equation (62), θ_m must be a maximum. If ρ represents the ratio of b to a with ρ greater than one, Equation (62) becomes:

$$\theta_m = \text{Arccos}\,[2\rho/(1 + \rho^2)],\ \rho = b/a > 1 \quad (63)$$

One can show by several techniques that θ_m increases with increasing values of ρ. For any given crystal, ρ is largest if a is equal to α, and b is equal to γ. Hence, the maximum value for the angle between the ray path and wave normal for any given crystal is:

$$\theta_m = \text{Arccos}\,[2\alpha\gamma/(\alpha^2 + \gamma^2)] \quad (64)$$

Direction of the Wave Normal Farthest from the Ray Path

Because the largest angle between the ray path and the wave normal lies in the optic axial plane where the largest and smallest indices of refraction are γ and α, the thin section that shows this largest divergence will be normal to the optic axial plane and parallel to the *Y* vibration direction. In the optic axial plane, the unit

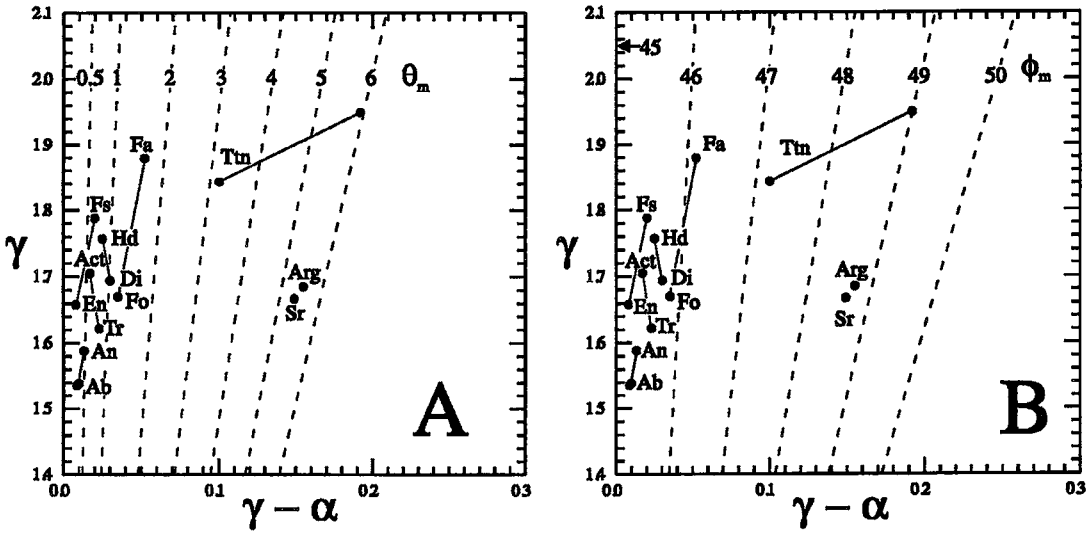


FIG. 6. A. Contours of the maximum angle, θ_m, between ray paths and wave normals as functions of the birefringence ($\gamma - \alpha$) and the refringence, γ. B. Contours of the angle, ϕ_m, between the wave normal associated with θ_m and the *Z* vibration direction of the indicatrix. Also plotted are values expected for common end-members and minerals. Symbols: Ttn: titanite, Fa: fayalite, Fo: forsterite, Fs: ferrosilite, En: enstatite, Hd: hedenbergite, Di: diopside, Act: actinolite, Tr: tremolite, An: anorthite, Ab: albite, Arg: aragonite, Sr: strontianite.

vectors corresponding to $\boldsymbol{p}$ and $\boldsymbol{q}$ are $\boldsymbol{k}$ and $\boldsymbol{i}$. The angle ϕ_m between the Z vibration direction and the wave normal associated with the ray path most divergent from the wave normal can be calculated with the dot product, with the result:

$$\cos \phi_m = \sqrt{(1 - n_{pm}^2)} = \alpha/\sqrt{(\alpha^2 + \gamma^2)} \qquad (65)$$

Examples and Applications

A plot of θ_m as a function of γ and birefringence $(\gamma - \alpha)$ is shown in Figure 6A. The common rock-forming minerals, olivine, pyroxene, amphibole, and plagioclase, have small angles between ray paths and wave normals (approximately 0.5° to 2°). Minerals with higher birefringences have larger angles (3° – 6°, titanite; 5.5°, strontianite and aragonite). Except for the calcium-bearing chain silicates, Fe-end members of solid-solution series have larger values of θ_m than do the Mg-end members. This relationship is reversed for the calcium-bearing chain silicates because of the lower birefringences of the Fe-end members.

A plot of χ_m, the angle between the Z vibration direction and the wave normal that diverges most from its associated ray path, as a function of γ and birefringence $(\gamma - \alpha)$ is shown on Figure 6B. The wave normal and ray path will diverge most in thin sections cut parallel to the Y vibration direction and with wave normals between 45° and 50° of the Z vibration direction. Crystals with larger birefringences show maximum divergence between wave normals and ray paths in sections closer to the Y–Z plane of the indicatrix.

For most rock-forming minerals, the ray path and wave normal will diverge by less than 2°. Consequently, the approximation that the wave normal and ray path are parallel is a good one. Vector algebra provides a convenient way to calculate optical directions in crystals.

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