# Tensors and matrices in optical mineralogy

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## Abstract

A series of matrix operations is described which enables the following optical data to be calculated for plane polarized light perpendicularly incident on a section of a transparent or opaque mineral: 1. vibration directions and refractive indices of anisotropic transparent minerals: 2. reflectivities and the state of polarization of light reflected from anisotropic opaque minerals. The data needed are the dielectric tensor, its orientation with respect to the crystal axes, the unit cell parameters and the direction of the incident light. The mathematical techniques involve the manipulation of matrices, the determination of eigenvalues and eigenvectors and, for opaque minerals, the manipulation of complex numbers. All operations can be carried out with the aid of some of the recent electronic calculators which have built-in matrix algebra procedures and complex arithmetic.

KEYWORDS: tensors, matrices, optical properties, olivine, diopside, covelline, stibnite

## Introduction

THE Biot–Fresnel construction has long been used in teaching optical mineralogy for finding vibration directions in sections of anisotropic transparent minerals. It forms a useful teaching aid in demonstrating the variation in extinction angles with composition in solid-solution series such as the plagioclase feldspars. However, the construction does not directly provide information as to the refractive indices of the vibrations, nor is it applicable to opaque minerals, since they have no optic axes. Some examples of calculations based on geometry and the Fletcher Indicatrix are to be found in the literature such as by Phemister (1954) dealing with transparent minerals and Berek (1937) for opaque minerals. But the equations are long, complicated and prone to blunder during calculation.

The procedures outlined in this paper are matrix methods. The complications of the analytical geometric methods are replaced by the complications of matrix algebra. They too would be rather tedious to apply by hand calculation, but modern electronic calculators have built-in matrix handling facilities. Several electronic calculators also have built-in complex arithmetic functions and can be programmed, so there is a natural extension of the matrix method to deal with opaque minerals. All the examples in this paper have been calculated initially with a Hewlett Packard HP15c calculator, although for a hard copy a Pascal program was written for an Apricot microcomputer.

Matrix methods for the calculations of reflectivities have been made by Cervelle et al. (1970) for hexagonal pyrrhotite with experimental evidence to confirm the calculation method. The principle was also used by Rath and Ansorge (1983) in a paper on the complex indicatrix. A pictorial approach to the complex indicatrix was attempted in Galopin and Henry (1972) and they also used the Poincaré sphere for a graphical representation of the polarization state of reflected waves.

The theory of tensors and their use in crystallography has been given by Nye (1985). Readers unfamiliar with matrices and complex numbers are referred in the first instance to the Appendices.

This article has been written in the form of a series of worked examples, starting with a relatively easy problem and introducing additional aspects of theory as they become necessary. The four principal examples are olivine, to deal with an orthorhombic transparent mineral; diopside to deal with a monoclinic mineral and to show how extinction angles are calculated; covelline and then stibnite are used to show how reflectivities and the polarization states of reflected light are calculated. Optical activity is not specifically dealt with since few minerals—quartz and cinnabar being notable exceptions—have sufficient optical activity to affect their more dominant anisotropy.

## Example 1: Olivine

We will consider firstly the orthorhombic, transparent and not optically active mineral olivine. The relative dielectric tensor is $T$. The elements of this tensor at optical frequencies are the squares of the refractive indices, $\alpha$, $\beta$, $\gamma$. The tensor we require in optical mineralogy is the inverse of this tensor, called the relative impermeability tensor $T^{-1}$ (Nye, 1985, p. 237). In olivine, the principal crystal axes are orthogonal and the relationships between the axes of the dielectric tensor and the axes of the crystal are such that:

$\alpha$ is parallel to [010], with RI = 1.635;
$\beta$ is parallel to [001], with RI = 1.651;
$\gamma$ is parallel to [100], with RI = 1.670.

Data are from Deer *et al.*, 1962.

Hence the relative dielectric tensor, written as a matrix with the columns representing respectively the [100], [010], and [001] crystal axes, is

$$T = \begin{bmatrix} 2.789 & 0 & 0 \\ 0 & 2.673 & 0 \\ 0 & 0 & 2.726 \end{bmatrix}$$

and the inverse $T^{-1} = \text{diag}\{0.3586, 0.3741, 0.3668\}$. The unit cell constants of olivine are $a = 4.76$, $b = 10.2$, $c = 5.98$ Å (Deer *et al.*, 1962).

We consider plane polarized light perpendicularly incident on the (111) section. A stereogram to illustrate this problem is given in Fig. 1 with the complete Biot–Fresnel solution. We can specify the location of the pole of the section by the vector $\mathbf{p}$ which has the direction cosines $[p_1\, p_2\, p_3]$ where $p_1$ etc. are the cosines of the angles between the normal to the section and the three principal crystal axes [100], [010], [001] respectively. These are calculated from the axial constants and are in the proportions $1/a$, $1/b$, $1/c$ and found to be [0.7352, 0.3430, 0.5846]. Such a vector is normalized, i.e. the sum of the squares of the elements equals 1. The data in this and all subsequent examples are displayed to three or four significant figures, but it is important in the manipulation of matrices to avoid rounding error, and so the data are stored to more places.

We wish to locate the vibration directions of the two plane polarized waves which travel through the olivine section and their refractive indices.

The first calculation is to generate a matrix $R1$ which has as its third row, the direction cosines of the pole of the section, $\mathbf{p}$. The first and second rows of the matrix are guesses as to the position of the vibration directions $\mathbf{u}$ and $\mathbf{v}$. Such directions are necessarily orthogonal to the incident direction of light. One first guess for the vector $\mathbf{u}$ is the direction [−0.423, 0.906, 0.0] which plots at the end of the trace of the section in Fig. 1. The values of these
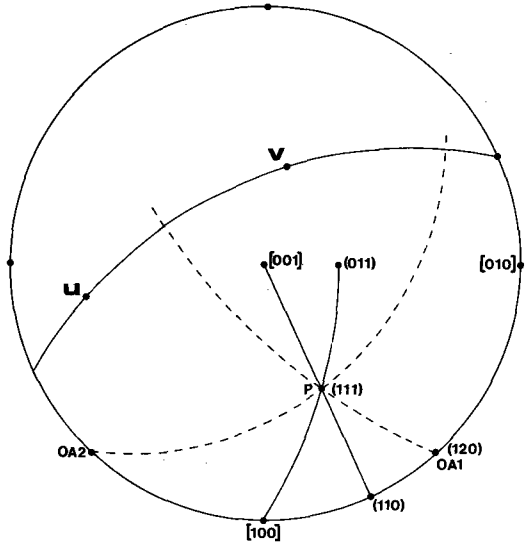


FIG. 1. Stereogram of olivine to show the Biot–Fresnel construction for the (111) section. The positions of the two vibration directions $\mathbf{u}$ and $\mathbf{v}$ are also calculated in the text using the matrix method.

direction cosines are simply the normalized values of the direction $[-p_2\, p_1\, 0]$. The second vibration direction $\mathbf{v}$ is necessarily orthogonal to the incident light direction and the vector $\mathbf{u}$ and this is determined from the vector cross product $\mathbf{p} \wedge \mathbf{u}$, $[p_2 u_3 - p_3 u_2, p_3 u_1 - p_1 u_3, p_1 u_2 - p_2 u_1]$ which in this case is $[-0.530, -0.247, 0.811]$.

The three rows of the matrix $R1$ are thus the direction cosines of a new X′, U′, Z′-orthogonal axial system. We use the matrix $R1$ as a rotation matrix and transform the relative impermeability tensor from the crystal axes to the new axial system which has its Z′-axis lying along the line of incident light, and with its X′- and Y′-axes lying along the quessed vibration directions. The matrix transformation for tensors is (Nye, 1985, Chapter 9) $R1\, T^{-1} R1^t = M$. The results of this calculation yields a new tensor $M$ which has the numerical values

$$M = \begin{bmatrix} 0.3713 & -0.0035 & 0.0048 \\ -0.0035 & 0.3650 & 0.0026 \\ 0.0048 & 0.0026 & 0.3632 \end{bmatrix}.$$

In this case, it is observed that the element $m_{21}$ is not zero. This means that the first guess as to the vibration directions was incorrect.

We must, therefore, make a further rotation $R2$ of the tensor $M$ about the new Z′-axis by an angle such that $R2\, M\, R2^t = N$, where the elements $n_{21} = n_{12} = 0$. This rotation matrix $R2$ is discovered by determining the eigenvalues and eigenvectors of the

$2 \times 2$ matrix that forms the upper left part of the matrix $M$ (Appendix B). These eigenvectors form the upper left part of the matrix $R2^t$, and hence the matrix $R2$ is determined and found in this case to be

$$R2 = \begin{bmatrix} -0.9147 & -0.4041 & 0.0000 \\ 0.4041 & -0.9147 & 0.0000 \\ 0.0000 & 0.0000 & 1.0000 \end{bmatrix}.$$

The two rotations can be multiplied in the order $R2\,R1$ to yield a single rotation matrix $R3$ which in this case is

$$R3 = \begin{bmatrix} 0.1726 & -0.9288 & 0.3279 \\ 0.6555 & -0.1401 & -0.7421 \\ 0.7352 & 0.3430 & 0.5846 \end{bmatrix}$$

and the matrix $N$ has the values

$$N = \begin{bmatrix} 0.3728 & 0.0000 & -0.0034 \\ 0.0000 & 0.3634 & -0.0043 \\ -0.0034 & -0.0043 & 0.3632 \end{bmatrix}.$$

The first row of the matrix $R3$ has the direction cosines of the $\mathbf{u}$ vibration direction, the second row has the vibration direction $\mathbf{v}$ and the third row has not changed and is still the direction of incident light. The reader can verify the location of these vibration directions in Fig. 1 with the points from the Biot–Fresnel construction.

But the matrix method yields an important extra factor. The refractive indices for these two waves are given from the first two diagonal elements of the matrix $N$, which are also the eigenvalues $\lambda_1$ and $\lambda_2$ determined earlier. These eigenvalues are the reciprocals of the square-roots of the refractive indices and hence for this section, the refractive indices are 1.638 and 1.659 for $\mathbf{u}$ and $\mathbf{v}$ respectively.

If the exercise is repeated but with light perpendicularly incident on the (120) section, the reader will find that the elements of the diagonal of matrix $N$ are almost exactly equal and the refractive indices are near to $\beta$. This means that the pole to the section (120) is close to an optic axis and the section is almost isotropic, a feature shown on the stereogram Fig. 1 by the locations of the optic axes.

### Example 2: Diopside

The principal axes of a dielectric tensor are necessarily orthogonal but most crystals belong to systems with non-orthogonal axial systems. A well-known procedure is available, most recently described by Boisen and Gibbs (1985), which shows how to transform data from any axial system to a Cartesian axial system, i.e. having orthogonal equal axes.

Diopside is monoclinic with axial constants of $a = 9.73$, $b = 8.91$, $c = 5.25$ Å, and $\beta = 105.83°$ (Deer et al., 1962). The covariant metric tensor, $G$, is the tensor whose elements are

$$G = \begin{bmatrix} \mathbf{a.a} & \mathbf{a.b} & \mathbf{a.c} \\ \mathbf{b.a} & \mathbf{b.b} & \mathbf{b.c} \\ \mathbf{c.a} & \mathbf{c.b} & \mathbf{c.c} \end{bmatrix}$$

$$G = \begin{bmatrix} a^2 & ab\cos\gamma & ac\cos\beta \\ ab\cos\gamma & b^2 & bc\cos\alpha \\ ac\cos\beta & bc\cos\alpha & c^2 \end{bmatrix}.$$

Boisen and Gibbs (1985) refer to this as the metrical matrix. The determinant of $G$, det $G$ is $V^2$, the square of the volume of the unit cell. From the metric tensor, the contravariant metric tensor, $G^*$, can be found by inversion or otherwise and is

$$G^* = \begin{bmatrix} a^{*2} & a^*b^*\cos\gamma^* & a^*c^*\cos\beta^* \\ a^*b^*\cos\gamma^* & b^* & b^*c^*\cos\alpha^* \\ a^*c^*\cos\beta^* & b^*c^*\cos\alpha^* & c^{*2} \end{bmatrix}.$$

The terms $a^*$, etc., are the reciprocal lattice constants. Two matrices are derived from the direct and reciprocal lattice constants, called Matrix $A$ and Matrix $B$ by Boisen and Gibbs (1985)

$$A = \begin{bmatrix} a\sin\beta & -b\sin\alpha\cos\gamma^* & 0 \\ 0 & b\sin\alpha\sin\gamma^* & 0 \\ a\cos\beta & b\cos\alpha & c \end{bmatrix}$$

$$B = (A^{-1})^t = \begin{bmatrix} a^*\sin\gamma^* & 0 & -c^*\cos\beta\sin\alpha^* \\ a^*\cos\gamma^* & b^* & c^*\cos\alpha^* \\ 0 & 0 & c^*\sin\alpha^*\sin\beta \end{bmatrix}.$$

These matrices are used to transform data from the crystal axial system to a Cartesian axial system. Matrix $A$ is used to convert zone axes and direction cosines. Matrix $B$ is used to convert the Miller Indices of crystal faces or cleavage planes. The Cartesian Z-axis is parallel to the [001] axis of the crystal, and the Cartesian Y-axis is parallel to the $b^*$-axis of the crystal. For our diopside example, the covariant and contravariant tensors are

$$G = \begin{bmatrix} 94.67 & 0.00 & -13.94 \\ 0.00 & 79.39 & 0.00 \\ -13.94 & 0.00 & 27.56 \end{bmatrix}$$

$$G^* = \begin{bmatrix} 0.0114 & 0.0000 & 0.0058 \\ 0.0000 & 0.0126 & 0.0000 \\ 0.0058 & 0.0000 & 0.0392 \end{bmatrix}$$

and hence

$$A = \begin{bmatrix} 9.3609 & 0.0000 & 0.0000 \\ 0.0000 & 8.9100 & 0.0000 \\ -2.6547 & 0.0000 & 0.0392 \end{bmatrix}$$

$$B = \begin{bmatrix} 0.1068 & 0.0000 & 0.0540 \\ 0.0000 & 0.1122 & 0.0000 \\ 0.0000 & 0.0000 & 0.1905 \end{bmatrix}.$$

The stereogram in Fig. 2 shows the poles of the

faces (100), (011), (110) and (111) which are located using Matrix B. For example, the location of the face (111) is in the direction B.(111) = [0.1608, 0.1122, 0.1905] and the direction cosines are this vector normalized, i.e. [0.5883, 0.4105, 0.6967]. By similar multiplication using matrix $A$, the plotting points [001], [100] and [010] are shown. The result is the conventional orientation of stereograms for monoclinic crystals.



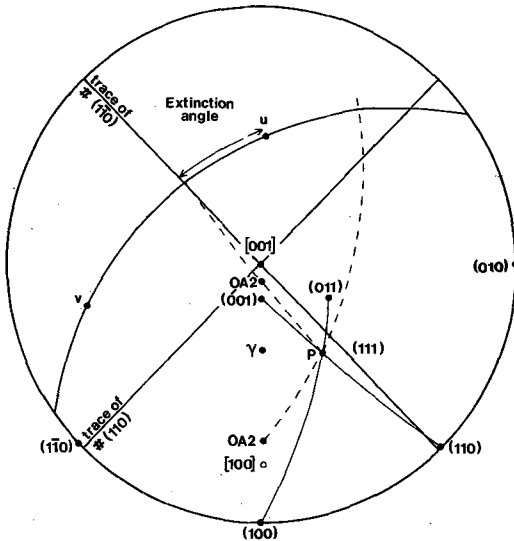FIG. 2. Stereogram of diopside to show the Biot–Fresnel construction for the (111) section. The positions of the two vibration directions **u** and **v**, the position of the trace of the (1 $\bar{1}$ 0) cleavage on the section, and the extinction angle are also calculated in the text using the matrix method.

The dielectric tensor for a monoclinic crystal is required to have one of its principal axes parallel to the direction [010] of the crystal. The directions of the other two orthogonal tensor axes have to be determined by measurement and specified by direction cosines from the Cartesian axial system. The optical data (Deer *et al.*, 1962) show that for diopside, the vibration $\gamma$ is situated in obtuse $\beta$ with the angle $\gamma$: [001] of 38.5°. The direction cosines of the $\gamma$ vibration in the Cartesian axis system are therefore [cos 51.5°, cos 90°, cos 38.5°] = [0.6225, 0.0, 0.7826]. Similar calculations for the other two vibration directions yield the columns of an orientation matrix $Q$ for the transformation of the dielectric tensor to the Cartesian axial system

$$Q = \begin{bmatrix} 0.7826 & 0.0000 & 0.6225 \\ 0.0000 & 1.0000 & 0.0000 \\ -0.6225 & 0.0000 & 0.7826 \end{bmatrix}.$$

The refractive indices lead to the tensor $T = \text{diag}$ {2.7689, 2.7939, 2.8696}. The relative impermeability tensor on the Cartesian axial system is

$$S = QT^{-1}Q^t = \begin{bmatrix} 0.3562 & 0.0000 & -0.0062 \\ 0.0000 & 0.3579 & 0.0000 \\ -0.0062 & 0.0000 & 0.3534 \end{bmatrix}.$$

For light perpendicularly incident on a (111) section of diopside, the vibration directions are given by exactly the same procedure outlined in the olivine example. The direction cosines of the incident light are [0.5883, 0.4105, 0.6967], which leads to the first rotation matrix $R1$ being

$$R1 = \begin{bmatrix} -0.5722 & 0.8201 & 0.0000 \\ -0.5713 & -0.3986 & 0.7174 \\ 0.5883 & 0.4105 & 0.6967 \end{bmatrix}.$$

The rotation of the re-oriented relative impermeability tensor $S$ to the new axial system leads to a new tensor $M$

$$M = R1\,S\,R1^t = \begin{bmatrix} 0.3574 & 0.0020 & 0.0030 \\ 0.0020 & 0.3610 & -0.0018 \\ 0.0030 & -0.0018 & 0.3501 \end{bmatrix}.$$

This does not have the element $m_{21}$ equal to zero and so a second rotation $R2$ is needed using the eigenvalues and eigenvectors of the upper left $2 \times 2$ sub-matrix. This leads to

$$R2 = \begin{bmatrix} 0.4654 & 0.8851 & 0.0000 \\ -0.8851 & 0.4654 & 0.0000 \\ 0.0000 & 0.0000 & 1.0000 \end{bmatrix}$$

and hence the overall double rotation,

$$R3 = R2\,R1 = \begin{bmatrix} -0.7720 & 0.0288 & 0.6349 \\ 0.2405 & -0.9114 & 0.3339 \\ 0.5883 & 0.4105 & 0.6967 \end{bmatrix}.$$

The direction cosines of the two vibrations **u** and **v** are the first two rows of the matrix $R3$. The eigenvalues are respectively 0.3611 and 0.3563 and so the refractive indices are 1.664 and 1.675. The stereogram in Fig. 2 confirms the orientation of these vibration directions using the Biot–Fresnel construction.

It is frequently necessary to relate vibration directions to cleavages visible in sections. In the case of diopside, there are two cleavages {110}. The poles of these cleavages and the traces of the cleavages are given in Fig. 2. A cleavage is only clearly visible in a section if it intersects the section at a high angle. In other words, the angle between the pole of the section and the pole of a cleavage plane must be greater than, say, 70°. The angle between two vectors **p** and **q** is given by the dot product **p**.**q** which is in any axial system $pq \cos \theta$. For Cartesian axes, all vectors which are direction

cosines have the same unit length, so the angle between the pole of the section (111) and the pole of the cleavage (110), which has the direction cosines [0.689, 0.724, 0], is given by $\cos\theta = p_1 q_1 + p_2 q_2 + p_3 q_3 = 0.703$, and hence $\theta = 45°$ for this example. The cleavage (110) would therefore not be seen clearly in the (111) section. However, the (1$\bar{1}$0) cleavage is clearly visible because the corresponding angle $\theta$ is 84°. The trace of the cleavage (1$\bar{1}$0) in the plane of the section is a direction given by the vector cross product $\mathbf{p} \wedge \mathbf{q}$. In this case, the direction cosines of the trace of the cleavage (1$\bar{1}$0) on the plane (111) are $[-0.508, -0.483, 0.713]$. The angle between the vibration direction $\mathbf{u}$ and this cleavage trace is then the dot product of the direction cosines for $\mathbf{u}$ and the just calculated cleavage trace, which is 33.8°.

## Example 3: Covelline

The mineral covelline, CuS, is hexagonal with axial constants of $a = 3.8$, $c = 16.36$ Å (Vaughan and Craig, 1978). Covelline is opaque and the elements of its relative dielectric tensor $\mathbf{T}$ are complex numbers, which carry information concerning the refractive index and the absorption of light. The tensor elements are the squares of the complex refractive indices $(n+ik)$, where $n$ still represents the refractive index (although in opaque minerals it can be less than 1) and $k$ is an absorption coefficient. The tensor in red light (650 nm) is

$$T = \begin{bmatrix} 0.674+0.975i & 0 & \\ 0 & 0.674+0.975i & \\ 0 & 0 & \\ & & 0 \\ & & 0 \\ & & 6.327+3.679i \end{bmatrix}.$$

Two axes are identical, and the third axis is for light vibrating parallel to the hexad axis. These values were calculated from the reflectivity data in the IMA/COM Quantitative Data File (Henry, 1977), using the equations in Galopin and Henry (1972) p. 265. The relative impermeability tensor is thus diag$\{0.4797-0.6940i, 0.4797-0.6940i, 0.1181-0.0687i\}$.

We will consider red light perpendicularly incident on the (10$\bar{1}$1) section. The procedure is the same as in the previous examples, although the arithmetic requires manipulation of complex numbers (Appendix D). The orientation matrices $A$ and $B$ for the hexagonal crystal data to the Cartesian axial system are

$$A = \begin{bmatrix} 3.8000 & -1.9000 & 0.0000 \\ 0.0000 & 3.2909 & 0.0000 \\ 0.0000 & 0.0000 & 0.0037 \end{bmatrix}$$

$$B = \begin{bmatrix} 0.2632 & 0.0000 & 0.0000 \\ 0.1519 & 0.3039 & 0.0000 \\ 0.0000 & 0.0000 & 0.0611 \end{bmatrix}.$$

From these the direction cosines for the face normal (10$\bar{1}$1) are calculated as [0.8490, 0.4902, 0.1972].

The orientation matrix $Q$ for the relative impermeability tensor to the Cartesian axis system is the identity matrix. Uniaxial minerals have two tensor axes orthogonal to the unique axis which are not in otherwise defined directions unlike orthorhombic minerals. It is a matter simply of computing convenience to set these axes parallel to two directions such as [2$\bar{1}$$\bar{1}$0] and [01$\bar{1}$0] at right angles to the unique axis.

The first rotation matrix $R1$ for the section (10$\bar{1}$1) is

$$R1 = \begin{bmatrix} -0.5000 & 0.8660 & 0.0000 \\ -0.1708 & -0.0986 & 0.9804 \\ 0.8490 & 0.4902 & 0.1972 \end{bmatrix}$$

and when the matrix multiplications $R1\,T^{-1}R1^t$ are made, the tensor after this rotation is

$$M = \begin{bmatrix} 0.4797-0.6940i & 0 & 0 \\ 0 & 0.1322-0.0930i & -0.0699+0.1209i \\ 0 & -0.0699+0.1209i & 0.4657-0.6697i \end{bmatrix}.$$

It is seen that the element $m_{21}$ is zero so the vibration directions, $\mathbf{u}$ and $\mathbf{v}$, are the first two rows of matrix $R1$ respectively. The complex refractive indices for these vibrations are derived from the diagonal elements $m_{11}$ and $m_{22}$ as before and hence the refractive indices $n_u$, $n_v$ and absorption coefficients $k_u$, $k_v$ can be determined. In this case

Vibration $\mathbf{u}$, direction cosines $[-0.500, 0.866, 0.000]$
Complex relative impermeability = $0.4797 - 0.6940i$,
Complex refractive indices, $n_u = 0.9642$,
$k_u = 0.5056$
Vibration $\mathbf{v}$, direction cosines $[-0.1708, -0.0986, 0.9804]$
Complex relative impermeability = $0.1322 - 0.0930i$,
Complex refractive indices, $n_v = 2.372$,
$k_v = 0.7507$.

The mineral has such high absorption, that there is effectively no transmitted wave, but instead we can study the reflected waves. The Fresnel equation states that the reflectivity of an opaque mineral with complex refractive index $N = (n+ik)$ and for light perpendicularly incident is given by

$$(N-1)(N^*-1)/(N+1)(N^*+1) = (n-1)^2 + k^2/(n+1)^2 + k^2.$$

For this section, viewed in (EW) plane polarized light, when the vibration direction **u** is parallel to the EW axis of the microscope, the reflectivity is 0.063, i.e. 6.3%, and when the section is turned through 90°, the reflectivity is 0.205 or 20.5%. The amplitudes of the reflected waves are the square roots of these values, i.e. 0.250 and 0.453 respectively and relative to a unit value for input light intensity. In addition to suffering a loss of amplitude upon reflection, the incident light also suffers a phase lag $\delta$ at the surface of the mineral, and this lag is given by the expression $\tan \delta = -2k/(n^2 + k^2 - 1)$ (Ditchburn, 1952, p. 433). For these two waves, the phase lags are $-1.390$ and $-0.282$ radians respectively. The information of the amplitude and phase lag of these waves may be written in complex polar form as $A_u \exp(i\delta_u)$ and $A_v \exp(i\delta_v)$ respectively, or more conveniently converted into complex rectangular form for use in subsequent calculations.
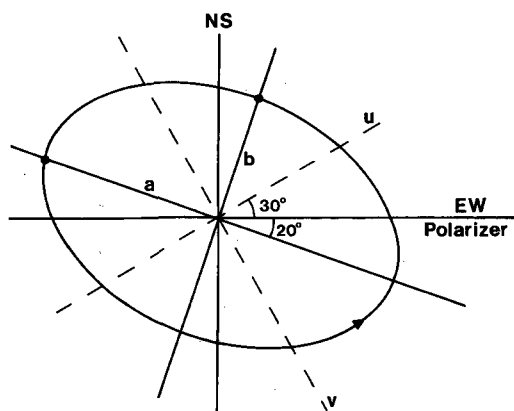


FIG. 3. Covelline (10$\bar{1}$1) section to show the ellipticity of the reflected red light for the section oriented in the 30° position. The principal axis of the ellipse is inclined at $-20°$ to the incident EW polarized light.

The (10$\bar{1}$1) section thus shows bireflectance, analogous to the birefringence seen in thin sections of transparent minerals. In the two extinction positions, the reflected wave is plane polarized. However, in intermediate positions the reflected light wave is elliptically polarized. We can explain this by modelling the behaviour of the section as if there were two reflected light waves with their orientations in the directions of the permitted vibrations of the admittedly absent transmitted waves. These two model waves are orthogonal and plane polarized, but they are out of phase with each other because of the differential phase lags that occurred when the light was reflected. The reader is

referred to the excellent diagrams which illustrate elliptically polarized light in texts such as Bloss (1961). Fig. 3 shows the ellipticity (ratio of minor to major axis) and the inclination angle $\omega$ of the principal axis of the ellipse wave and these depend on the angle $\theta$ that the section has been rotated from an extinction position. These parameters may now be calculated. In fig. 4 the section of covelline has been rotated by an angle = 30° with the direction of original **u** vibration now in the NE quadrant. The amplitudes of the two model waves are reduced to $A_u \exp(i\delta_u) \cos \theta$ and $A_v \exp(i\delta_v) \sin \theta$ due to the rotation of the section. The two model waves can each be written as if they were formed by the linear combination of two orthogonal waves each parallel to the crosswires NS and EW. The corresponding NS components of each wave can therefore be added, and similarly the EW components. The rotation matrix performs this decomposition and addition, with the minus sign of the **v** wave arising from the geometry of fig. 4.

$$\begin{bmatrix} E_x \\ E_y \end{bmatrix} = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}$$
$$\begin{bmatrix} H2 \end{bmatrix} \begin{bmatrix} A_u \exp(i\delta_u) \cos \theta \\ -A_v \exp(i\delta_v) \sin \theta \end{bmatrix}.$$

The equation is derived from ideas in Azzam and Bashara (1977). Like other minerals with a unique axis, covelline has the matrix $H2$ in this equation as the identity matrix; its use as a Hermitian matrix becomes apparent in the next example. The Jones vector, $[E_x, E_y]$, shows the polarization state of the reflected light wave. The numerical values calculated for the covelline example written in polar form are $0.259 \exp(-0.988i)$, $0.1767 \exp(-2.844i)$.

It is more useful to describe the reflected light wave by means of the four Stokes parameters, a four element vector. These parameters are calculated by the four matrix multiplications of the type

$$[E_x^*, E_y^*] \begin{bmatrix} Pn \end{bmatrix} \begin{bmatrix} E_x \\ E_y \end{bmatrix}$$

where the matrices $Pn$ are the four Pauli spin matrices (Gerrard and Burch, 1975),

$$P0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad P1 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$
$$P2 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad P3 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

and $E_x^*$ is the complex conjugate of $E_x$ etc. The four Stokes parameters [S0, S1, S2, S3] for this covelline example with $\theta = 30°$, are [0.0981, 0.0357, $-0.0257$, $-0.0877$]. The interpretation of these parameters is that S0 is the intensity of the reflected

wave, which in this case is 9.8%, the ellipticity is given by $\tan(\frac{1}{2}\arcsin(S3/S0)) = -0.617$, with the negative sign indicating that the ellipse is left-handed. The inclination $\omega$ of the principal axis to the EW axis is given by $\frac{1}{2}\arctan(S2/S1) = -17.9°$, and the negative sign indicates that the axis is in the south-east quadrant, as shown in Fig. 4.

The data of Cervelle *et al.* (1970) for oriented sections of hexagonal pyrrhotite have been processed through this procedure. The results for the complex refractive indices are identical to those obtained by Cervelle *et al.* and by Rath and Ansorge (1983) who used the same data as a justification of their matrix methods.
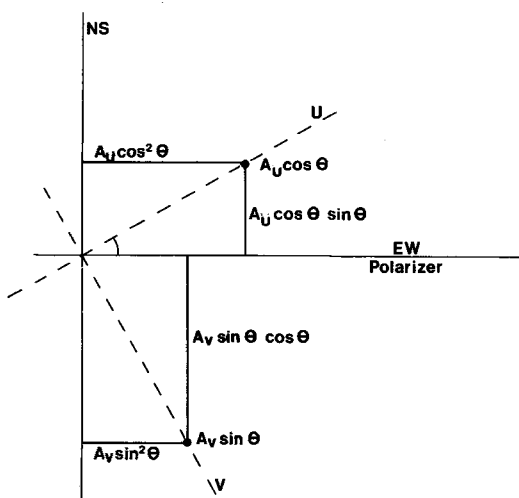
FIG. 4. Covelline (10$\bar{1}$1) section to show the directions of the permitted vibration directions **u** and **v** for the section in the 30° position. The NS and EW components of the reflected waves are shown, to justify the rotation matrix $R$ in the text. The relative amplitudes have been drawn to scale for red light.

## Example 4: Stibnite

Stibnite is orthorhombic and opaque. Its axial constants are $a = 11.20$, $b = 11.28$, $c = 3.83$ Å. The relative dielectric tensor $T$ referred to the crystal axes is, for green light 520 nm, $T = \text{diag}\{8.485 - 14.69i, \quad 10.714 - 5.120i, \quad 3.002 - 18.286i\}$. The direction cosines for the (111) section are [0.3081, 0.3059, 0.9009] and the vibration directions are calculated in the same manner as in previous examples. The first rotation matrix is

$$R1 = \begin{bmatrix} -0.7046 & 0.7096 & 0.0000 \\ -0.6393 & -0.6347 & 0.4341 \\ 0.3081 & 0.3059 & 0.9009 \end{bmatrix}.$$

The relative impermeability tensor on this axial system is

$$M = \begin{bmatrix} 0.0529 - 0.0436i \\ -0.0209 - 0.0066i \\ 0.0101 + 0.0032i \end{bmatrix}$$

$$\begin{bmatrix} -0.0209 - 0.0066i & 0.0101 + 0.0032i \\ 0.0443 - 0.0455i & -0.0171 - 0.0037i \\ -0.0171 - 0.0037i & 0.0170 - 0.0515i \end{bmatrix}.$$

The element $m_{21}$ is not zero, so as in the pyroxene case of Example 2, the upper left $2 \times 2$ matrix is solved for its eigenvalues and eigenvectors. The results are

$$N = \begin{bmatrix} -0.7732 + 0.0054i & -0.6342 - 0.0066i & 0 \\ 0.6342 + 0.0066i & -0.7732 + 0.0054i & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

In this case, the eigenvectors are complex numbers. They are thus not immediately interpretable as a rotation matrix. The transpose of the complex matrix $N$ is further decomposed into two matrices, $H$ and $R2$ where $H$ is a Hermitian matrix and $R2$ is a pure real matrix which is a rotation matrix.

$$N^t = H R2.$$

The method is outlined in Appendix C. The results are

$$H = \begin{bmatrix} 1.00004 + 0i & 0 - 0.0086i & 0 \\ 0 + 0.0086i & 1.00004 + 0i & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$R2 = \begin{bmatrix} -0.7732 & 0.6342 & 0 \\ -0.6342 & -0.7732 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

The Hermitian matrix has equal diagonal elements which are pure real numbers and the off-diagonal elements are pure imaginary numbers. The interpretation of this matrix is that the light waves transmitted and reflected from the surface of the section are elliptically polarized. The ellipticity, $\tan \varepsilon$, is the ratio of the imaginary and real components. Both waves have the same ellipticity and the same handedness. According to Galopin and Henry (1972), it is possible to find sections of opaque minerals which have an ellipticity of 1, in which case the reflected (and transmitted) waves are circularly polarized.

If the stibnite (111) section is viewed in monochromatic light, there is no exact extinction position, only a very dark minimum. When the permitted vibration directions are exactly parallel to the polarizer, the reflected wave has both an EW and a small NS component. Even under perfectly crossed polars, the section will fail to extinguish. This is why ilmenite is recommended by Galopin and Henry (1972) for the correct setting of the microscope analyser. Ilmenite is hexagonal, and so

like the covelline example above, all sections have permitted vibrations which are plane polarized. In *hkl* sections of lower symmetry crystals, the permitted vibrations are elliptically polarized.

The matrix calculations shown in Example 3 for the study of the polarization state of sections not in extinction are still valid, but require the additional matrix $H2$. The elliptically polarized wave reflected from the surface of the mineral has its ellipticity formed by a combination of the ellipticity produced from the differential phase lags of the two surface waves and their own ellipticities. The Hermitian matrix $H2$ is obtained from the ellipticity, $\varepsilon$ (Azzam and Bashara, 1977), and is

$$H2 = \begin{bmatrix} \cos\varepsilon & -i\sin\varepsilon \\ i\sin\varepsilon & \cos\varepsilon \end{bmatrix}.$$

The ellipticity of the light reflected from the (111) surface of stibnite is 0.0086 for the section at angle $\theta = 0°$ and increases to 0.063 for the section at approximately $\theta = 40°$.

## Summary

This paper has shown that a series of matrix manipulations can be applied to the relative dielectric tensor of a mineral to enable the permitted vibrations directions, refractive indices, reflectivities and the polarization state of reflected light to be determined. The method has advantages over analytical geometric techniques: it can be performed with calculators and is readily amenable to computer programming. The required data are the relative dielectric tensor, its orientation with respect to crystal axes, the axial constants of the mineral and the specification of the direction of incident light. For minerals of low symmetry, the data are most conveniently referenced to a Cartesian axial system, rather than the crystal axial system.

The summarized matrix calculations are

    1. $\Lambda = H\,R3\,Q\,T^{-1}\,Q^t\,R3^t\,H^t$

where $T$  is the relative dielectric tensor,

     $Q$  rotates the tensor to a Cartesian axial system,

     $R3$  rotates the tensor so that the third row of $R3$ is along the direction of the incident light, and the first and second rows are in the directions of the permitted vibration directions,

     $H$  is a Hermitian matrix which shows the ellipticity of the refracted and reflected waves.

     $\Lambda$  is a tensor with the first two off-diagonal elements zero.

2. The first two diagonal elements of the tensor yield the refractive indices of the two permitted vibrations. In opaque minerals, these values are complex numbers and yield the complex refractive indices. Using the Fresnel equation the amplitudes and phase lags of each permitted reflected wave can be calculated.

3. For opaque minerals, the polarization state of the reflected light can be calculated by the matrix operations

$$J = R\,H2\,A$$
$$S = J^* P\,J$$

where $A$  is the vector of amplitudes and phase lags of the two permitted waves,

    $H2$ is a Hermitian matrix derived from the ellipticity calculated from Hermitian matrix $H$.

    $R$  is a rotation matrix for the angle between the permitted vibration directions and the EW polarizer,

    $J$  is the Jones vector $[E_x, E_y]$, and $J^*$ is its complex conjugate,

    $P$  represents the four Pauli spin matrices,

    $S$  represents the four element Stokes vector.

From $S$, the values of the reflectivity, ellipticity and the inclination of the principal axis of the elliptically polarized reflected light wave can be calculated.

## Appendices

A. *Vector and matrix manipulations.* There are many texts which deal with matrix algebra more than adequate to the needs of this paper. A suitable text is Boas (1983), and Boisen and Gibbs (1985) give some mineralogical examples. A few modern electronic calculators will perform matrix manipulations, and an example is the Hewlett Packard HP15c. The matrix operations required are multiplication, transpose, determinant and inversion with matrices $2 \times 2$ and $3 \times 3$ in size.

B. *Eigenvalues and eigenvectors.* We need only consider $2 \times 2$ matrices and so the eigenvalues and eigenvectors are quickly determined, even when the elements of the matrix are complex numbers. The eigenvalues of a $2 \times 2$ matrix $M$ are the two values $\lambda$ where $\det |M - \lambda I| = 0$, where $I$ is the identity matrix and $\Lambda$ is the diagonal matrix

$$I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad \Lambda = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}.$$

If the matrix $M$ is written as

$$M = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

then    $\det \begin{bmatrix} a-\lambda & b \\ c & d-\lambda \end{bmatrix} = 0$

which, upon expansion gives $(a-\lambda)(d-\lambda)-bc = 0$ and hence $\lambda^2 - (a+d)\lambda + (ad-bc) = 0$. This is a quadratic equation with $\lambda = \frac{1}{2}[(a+d) + \sqrt{\{(a+d)^2 - 4(ad-bc)\}}]$ having the two solutions $\lambda_1$ and $\lambda_2$. Examples are given in the text for cases where the matrices are pure real and complex.

The two eigenvectors of the matrix $M$ are given by the two values of $(\lambda-d)/c = p/q$. The eigenvectors form the columns of a matrix

$$N = \begin{bmatrix} p & -q \\ q & p \end{bmatrix}.$$

In our matrices, the matrix $N$ is required to have a determinant of 1, and so the vectors are normalized, i.e. $p^2 + q^2 = 1$. The procedure is correct even where the elements of the matrix $M$ are complex numbers. If the elements $b$ and $c$ are zero, the eigenvalues are $a$ and $d$, and the eigenvector matrix $N$ is the identity matrix $I$. The eigenvalues and eigenvectors are related such that $N \Lambda N^t = M$. The matrix $N$ has a determinant of $+1$, and the matrix $\Lambda$ is a diagonal matrix. The matrix $M$ is therefore diagonalized by the matrix transformation $N^t M N = \Lambda$. Some examples are given in the main text with both real and complex cases. For these examples, the $2 \times 2$ matrix of eigenvectors is expanded to a $3 \times 3$ matrix by replacing the upper left part of a $3 \times 3$ identity matrix by $N$.

C. *Complex eigenvectors.* The transpose of the matrix of eigenvectors, $N^t$, produced for opaque minerals may be complex. Such a matrix can be decomposed into the product of two matrices $H$ and $R$, i.e. $N^t = H R$. $R$ is a matrix whose elements are the elements of a rotation matrix with an angle of rotation $\alpha$, i.e.

$$R = \begin{bmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{bmatrix}.$$

The matrix $H$ is a Hermitian matrix which in this case has diagonal elements which are equal and purely real, and the off-diagonal elements which are skew symmetric and purely imaginary, i.e.

$$H = \begin{bmatrix} \Phi + 0i & 0 + \rho i \\ 0 - \rho i & \Phi + 0i \end{bmatrix}$$

where the element $h_{11} = \Phi$ which is equal to $\sqrt{(1+\rho^2)}$. Both matrices have determinants of $+1$. If the element $n_{11}$ is written as $a + ib$ and $n_{12}$ is $c + id$ then $\rho^2 = (b^2 + d^2)$ and

hence $\Phi$ is calculated. The element $r_{11}$ is $a/\Phi$ and $r_{12} = c/\Phi$ and hence the elements of $R$ are calculated. The matrix $H$ is calculated by the back-substitution matrix calculation $N^t R^t = H$ in order to ensure the correct signs for $\rho$. One example is given in the main text for stibnite.

D. *Complex numbers.* The arithmetic of complex numbers is described in many standard mathematics texts such as Boas (1983). Calculators such as the Hewlett Packard HP15c (and HP41c with its Maths module) perform all the operations required in this paper.

## References

Azzam, R. M. A., and Bashara, N. M. (1977) *Ellipsometry and polarized light.* North-Holland Publ. Co., Amsterdam.

Berek, M. (1937) *Fortschr. Mineral. Kristallogr. Petrogr.* **22**, 1–103.

Bloss, F. D. (1961) *An introduction to the methods of optical crystallography.* Holt, Reinhart & Winston.

Boas, M. L. (1983) *Mathematical methods in the physical sciences.* 2nd Ed. Wiley.

Boisen, M. B., and Gibbs, G. V. (1985) *Reviews in Mineralogy* **15**, Mineral. Soc. Am.

Cervelle, B. D., Caye, R., and Billard, J. (1970) *Bull. Soc. fr. Mineral. Cristallogr.* **93**, 72–82.

Deer, W. A., Howie, R. A., and Zussman, J. (1962) *Rock-forming minerals.* Longmans.

Ditchburn, R. W. (1952) *Light.* Blackie and Son.

Galopin, R., and Henry, N. F. M. (1972) *Microscopic study of opaque minerals.* Published since 1975 by McCrone Research Associates Ltd. London.

Gerrard, A., and Burch, J. M. (1975) *Introduction to Matrix Methods in Optics.* J. Wiley & Sons.

Henry, N. F. M., ed. (1977) *Commission on Ore Microscopy: IMA/COM Quantitative Data File (First Issue).* Applied Mineralogy Group, Mineralogical Society, London.

Nye, J. F. (1985) *Physical properties of crystals.* 2nd Ed. Clarendon.

Phemister, T. C. (1954) *Am. Mineral.* **39**, 172–92.

Rath, R., and Ansorge, R. (1983) *Neues Jahrb. Mineral. Abh.* **147**, 160–8.

Vaughan, D. J., and Craig, J. R. (1978) *Mineral chemistry of metal sulphides.* Cambridge Univ. Press.