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Matrix calculation of optical indicatrix parameters from central cross sections through the index ellipsoid

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Abstract

A minimum of three arbitrarily oriented, but independent, central sections through a crystal's optic ellipsoid are used for a calculation of the principal indices and the orientation of the index ellipsoid. The crystal is rotated about the x axis of the spindle, limiting the choice of cuts to those containing the x axis. The matrix for this ellipsoid is calculated. Finally the matrix is diagonalized to find the eigenvectors and eigenvalues that in turn give the principal indices and orientation. To illustrate the method, data were generated from a known albite crystal in an arbitrary orientation of the ellipsoid with respect to the spindle axes. In the example, four cuts are used; thus individual matrix elements can be calculated using different algebraic expressions.

Introduction

In a biaxial crystal, the angle ($2V$) between the two optic axes is constant at a given temperature and for a given wavelength (Bloss, 1961; Julian and Bloss, 1982). The technique of measurement of the angle involves rotation of the crystal about an axis parallel to the microscope stage and analysis by the Bloss-Riess-Rohrer program EXCALIBR (Bloss and Riess, 1973). If a crystal happens to be mounted about a principal axis, then the program EXCALIBR cannot be used because the crystal remains extinguished for all settings. In addition, for cases where a crystal exhibits strong absorption for X, Y, or Z, this crystal's refractive index for light vibrating parallel to that particular direction may not be measurable even though solution by EXCALIBR gives coordinates for this strongly absorbing vibration direction. This paper represents a general method for the location of the index ellipsoid of an arbitrarily mounted crystal on a spindle-stage microscope.

Experimental data

A crystal mounted on a spindle stage (Bloss, 1981, p. 11) rotates about the x axis of the standard orthogonal set x, y, z. Following Leitz (1972), the z axis is perpendicular to the microscope stage and is along the direction the light travels, the x axis is due east, and the y axis is due north (see Fig. 1). The angle S represents a rotation of the crystal about the x axis with $S = 0°$ lying along the y axis. When the refractive index of the crystal matches the refractive index of the oil surrounding the crystal for monochromatic light, the refracted wave normal travels in the crystal along z. The wave front for this wave normal is parallel to the x-y plane and passes through the center of the optical indicatrix. This wave front intersects the indicatrix in an ellipse with a major semiaxis m_S and a minor semiaxis n_S. These two semiaxes define two mutually perpendicular vectors, $\mathbf{m}_S$ and $\mathbf{n}_S$; the directions of these vectors indicate the direction the light vibrates, and the corresponding lengths are the refractive indices m_S and n_S. Note that if m_S equals n_S, then the ellipse becomes a circle, and there are three possible cases: first, if the crystal is biaxial, then the light is traveling parallel to the optic axis; second, if the crystal is uniaxial, then the light is traveling along the unique axis; and finally, if the crystal is isotropic, the orientation is irrelevant.

Let $S = 0°$ represent the initial reading of the spindle. Similarly let $\mathbf{m}_0$ and $\mathbf{n}_0$ represent the two vectors defined by the ellipse of intersection between an anisotropic crystal's optical indicatrix and the wave front (=x-y plane). Let E_0 represent the angle between the spindle axis x and vector $\mathbf{m}_0$. If the spindle is now rotated 50° ($S = 50°$), the crystal's optical indicatrix has rotated correspondingly so that the wave front (=x-y plane) now intersects it in another ellipse that defines two new vectors, $\mathbf{m}_{50}$ and $\mathbf{n}_{50}$, with $\mathbf{m}_{50}$ being at an angle E_{50} to spindle axis x (see Fig. 1). Similarly, the spindle can be rotated to $S = 90°$ and thus obtain $\mathbf{m}_{90}$, $\mathbf{n}_{90}$, and E_{90}, etc.

In general, if the spindle is rotated by angle S, angle E represents the angle between the spindle axis and the major semiaxis of the intersected optical index ellipse. The index of refraction at angles E and S is ρ (see Fig. 2). The transformation between x, y, z and ρ, S, E is

$$x = \rho \cos(E)$$
$$y = \rho \sin(E)\cos(S)$$
$$z = \rho \sin(E)\sin(S).$$

Three S settings provide three sections through a crystal's optical index ellipsoid. In this paper we show that if, for each of three independent setting $S = a, b, c$ degrees, we determine experimentally the refractive indices of the pairs of privileged directions $\mathbf{m}_a$, $\mathbf{n}_a$; $\mathbf{m}_b$, $\mathbf{n}_b$; and $\mathbf{m}_c$, $\mathbf{n}_c$ and the angles E_a, E_b, and E_c, we can determine

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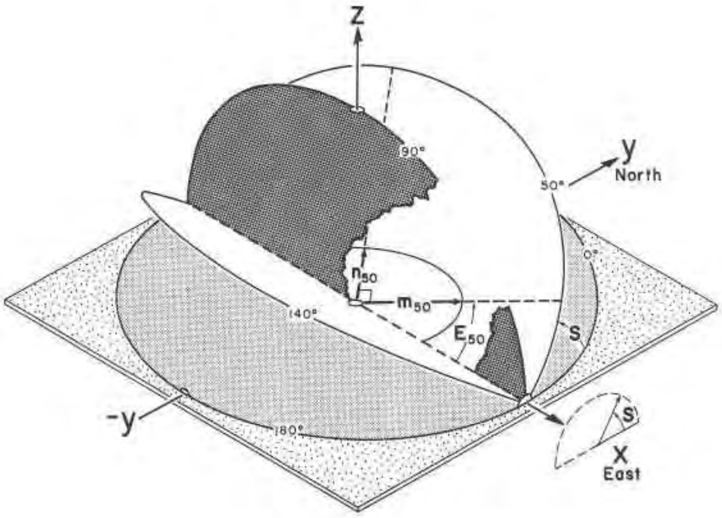

Fig. 1. S planes at 0°, 50°, 90°, 140°, and 180°. For the $S = 50°$ cut, the two privileged directions for which the crystal exhibits the refractive indices are $\mathbf{m}_{50}$ and $\mathbf{n}_{50}$. E_{50} represents the angle between the spindle axis and the $\mathbf{m}_{50}$ vibration axis.

the crystal's principal refractive indices (α, β, and γ). If the crystal is biaxial, we can also determine the directions of α, β, and γ relative to the original arbitrary axes along which the crystal was mounted.

In the example below, the principal axes have been overdetermined by measuring four sections. The general method is to devise a way to calculate the matrix associated with the index ellipsoid with respect to the spindle axes. Then the eigenvectors and eigenvalues of this matrix permit calculation of the orientation of the ellipsoid and its principal axes. By measurements of four sections, the individual matrix elements can be calculated by using different algebraic expressions and compared.

Construction of the ellipsoid

The general algebraic equation of an ellipsoid with its center at the origin can be written as

$$a_{11}x^2 + a_{22}y^2 + a_{33}z^2 + 2a_{12}xy + 2a_{13}xz + 2a_{23}yz = 1.$$

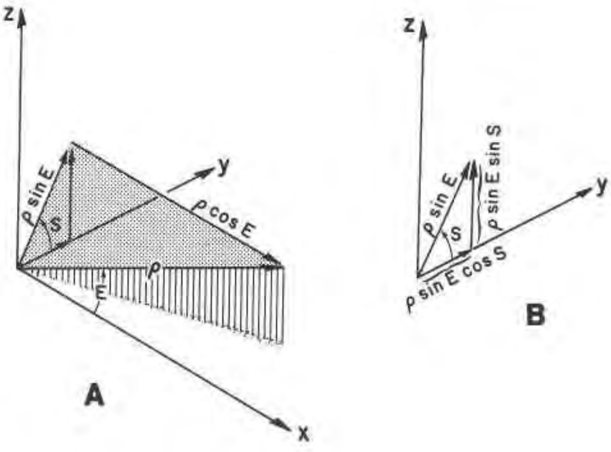

Fig. 2. (A) Transformation between x, y, z and ρ, S, E. (B) Isolation of y-z plane with components of $\rho \sin E$ identified.

This form, with the coefficient 2 included explicitly in the cross term, can be readily taken over into the matrix form. If the ellipsoid were oriented with its principal axes X, Y, Z along the x, y, z axes, each cross-term coefficient (a_{12}, a_{13}, a_{23}) would equal zero, and the above equation would take on the form

$$x^2/\alpha^2 + y^2/\beta^2 + z^2/\gamma^2 = 1,$$

where $a_{11} = \alpha^{-2}$, $a_{22} = \beta^{-2}$, and $a_{33} = \gamma^{-2}$.

In matrix notation, with $a_{ij} = a_{ji}$, the quadratic form can immediately be taken into the matrix form, $\mathbf{A} = (a_{ij})$. Note that $\mathbf{A}$ is a symmetric matrix. If $\mathbf{x}$ is the column vector with elements x, y, z and $\mathbf{x}^T$ is the transpose of the vector $\mathbf{x}$, then an ellipsoid may be represented as:

$$\mathbf{x}^T\mathbf{A}\mathbf{x} = 1.$$

The eigenvectors of the matrix $\mathbf{A}$ are the principal directions of the refractive index ellipsoid. The eigenvalues of this ellipsoid are the squares of the reciprocals of the principal indices α, β, and γ. The problem is to write down the matrix for the ellipsoid at an arbitrary orientation determined by the experiment. The matrix is diagonalized in order to find the eigenvectors and eigenvalues, which in turn give the directions of the principal axes and the values of the principal indices α, β, and γ. One complication is that, owing to the experimental design, the cuts are all parallel to the x axis, and so the yz cross term must be calculated indirectly.

First, the data for $S = 0°$ give the x-y cut and three out of the six independent matrix elements of $\mathbf{A}$, namely a_{11}, a_{12}, and a_{22}. The data for $S = 90°$ give the x-z cut and the matrix elements a_{11}, a_{13}, and a_{33}. Note that the a_{11} term is calculated twice because both cuts are parallel to the x axis. These two values for a_{11} are averaged before being entered into the matrix. These two cuts have now given us five of the six matrix elements needed. We are unable to calculate the a_{23} term because we do not have information about the y-z cut.

In order to find the a_{23} cross term, consider a rotation about the x axis to obtain data for the orthogonal pair of sections at $S = 50°$ and $S = 140°$. Let us call this new matrix $\mathbf{A}_{50}^{\exp}$ because it is rotated 50° from the original matrix **A** and represents the experimental data. Here we have rotated y into y_{50} and z into z_{50}. Note that the x axis remains unchanged. Again five out of the six matrix elements can be calculated with the a_{11} being calculated twice. Note that we now have calculated four values for a_{11}, and so they can be averaged.

In order to find the a_{23} cross term, we calculate the elements of **A** after a rotation of 50° about the x axis. Call this matrix $\mathbf{A}_{50}^{\mathrm{cal}}$. Since $\mathbf{A}_{50}^{\mathrm{cal}}$ equals $\mathbf{A}_{50}^{\exp}$, then the elements of these two matrices $\mathbf{A}_{50}^{\mathrm{cal}}$ and $\mathbf{A}_{50}^{\exp}$ can be compared term by term. Two independent algebraic expressions for the a_{23} cross term are derived. That is, if only three sections had been collected, there would still be enough information to calculate the complete matrix **A**.

All 3 by 3 similar matrices have three dyadic invariants: namely, the trace, the sum of the principal minors, and the determinant (Hollingsworth, 1967, p. 122). Of these the trace (or sum of the diagonal elements: $a_{11} + a_{22} + a_{33}$) is the most useful at this point because it is independent of the off-diagonal elements. The trace provides a convenient parameter for evaluating the quality of the data. The second dyadic invariant is defined as $a_{11}a_{22} + a_{22}a_{33} + a_{11}a_{33} - (a_{12})^2 - (a_{13})^2 - (a_{23})^2$. The third dyadic invariant is the determinant. These invariants provide a means to check the consistency of the data after the entire matrix has been calculated.

Once all the elements of the matrix are known, the eigenvectors and eigenvalues can be calculated by standard procedures (see Irving and Mullineux, 1959, p. 280) or by use of standard programs such as SAS (1982, p. 499) or MINITAB (1985, p. 179).

The eigenvectors of the matrix give the principal directions of the index ellipsoid. The eigenvalues are the reciprocals of the square roots of the principal refractive indices α, β, and γ. In a later paper we will consider a least-squares minimization of data for many sections, the errors involved, and complications due to refraction of the wave normal.

Detailed example for an albite crystal

First, for a constant value of S, 2 by 2 matrices are constructed. Let $\mathbf{m}_S$ be the direction of the major axis of the cut, $\mathbf{n}_S$ be the direction of the minor axis, and y_S be the direction perpendicular to x in the cut determined by S. Since the rotation is about x, x is common to all cuts and needs no subscript. We wish to calculate the matrix elements in terms of the x and y_S axes as $\mathbf{m}_S$ is rotated by $-E_S$ into x and n_S into y_S (see Goldstein, 1959, p. 99). The eigenvalues of this matrix are $L_m = \mathrm{m}_S^{-2}$ and $L_n = \mathrm{n}_S^{-2}$. Thus the matrix is

$$\begin{bmatrix} \cos E_S & -\sin E_S \\ \sin E_S & \cos E_S \end{bmatrix} \begin{bmatrix} L_m & 0 \\ 0 & L_n \end{bmatrix} \begin{bmatrix} \cos E_S & \sin E_S \\ -\sin E_S & \cos E_S \end{bmatrix}.$$

After performing the matrix multiplication, we have

$$\begin{bmatrix} L_m\cos^2E_S + L_n\sin^2E_S & (L_m - L_n)\sin E_S\cos E_S \\ (L_m - L_n)\sin E_S\cos E_S & L_m\sin^2E_S + L_n\cos^2E_S \end{bmatrix}.$$

For a rotation S and ellipsoid coordinates a_{ij}, the above matrix can also be written as

$$\begin{bmatrix} a_{11} & a_{12}\cos S + a_{13}\sin S \\ a_{12}\cos S + a_{13}\sin S & a_{22}\cos^2S + a_{33}\sin^2S \\ & \quad + 2a_{23}\cos S\sin S \end{bmatrix}.$$

TABLE 1. Generated optical data for albite crystal

S (°)	E_S (°)	m_S	n_S
0	37.701	1.53917	1.52893
50	38.489	1.53816	1.53084
90	11.606	1.53541	1.53291
140	147.481	1.53754	1.52987

Note: See text for description of symbols and orientation of ellipsoid.

For illustrative purposes, the data for Table 1 was generated assuming that $\alpha = 1.528\,90$, $\beta = 1.532\,91$, and $\gamma = 1.539\,29$ from Su et al. (1986) and that X, Y, and Z, the principal axes for the albite, have coordinates $S_x = 174.39°$, $E_x = 52.81°$, and $E_y = 99.02°$. From these three assumed values of the orientation of the ellipsoid, the other parameters were calculated, namely, $S_y = 91.3080°$, $S_z = 12.7601°$, and $E_z = 38.6427°$. The ellipsoid was parameterized in terms of E, S, and ρ. The parameter ρ is the optical index of refraction for a given, but arbitrary, angle E and angle S.

At $S = 0°$, $E_0 = 37.7014°$, $m_0 = 1.539\,17$ and $n_0 = 1.528\,93$. The calculated values of this 2 by 2 matrix are

$$\begin{bmatrix} 0.424\,235 & -0.002\,746 \\ -0.002\,746 & 0.425\,665 \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{bmatrix}.$$

Repeating a similar calculation for $S = 90°$,

$$\begin{bmatrix} 0.424\,235 & -0.000\,274 \\ -0.000\,274 & 0.425\,512 \end{bmatrix} = \begin{bmatrix} a_{11} & a_{13} \\ a_{13} & a_{33} \end{bmatrix}.$$

Note that two values have been calculated in different ways for a_{11}. The values are identical because the data are generated data and therefore essentially without error.

Collect this information together in one matrix **A**:

$$\begin{bmatrix} 0.424\,235 & -0.002\,746 & -0.000\,274 \\ -0.002\,746 & 0.425\,665 & a_{23} \\ -0.000\,274 & a_{23} & 0.425\,512 \end{bmatrix}$$

$$= \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{33} \end{bmatrix}.$$

The same calculations are repeated for $S = 50°$ (and $S = 140°$). Two more values of a_{11} are obtained again in different ways. Except for the a_{11} term, all the rest of the elements from this rotated matrix $\mathbf{A}_{50}^{\text{exp}}$ are different from **A**. The matrix $\mathbf{A}_{50}^{\text{exp}}$ becomes

$$\begin{bmatrix} -0.424\,235 & -0.001\,975 & 0.001\,927 \\ -0.001\,975 & 0.425\,148 & a_{23}^{\text{exp}} \\ 0.001\,927 & a_{23}^{\text{exp}} & 0.426\,029 \end{bmatrix}.$$

Proceed with the calculation of the cross term a_{23}. First rotate **A** through 50° about x. This new matrix is called $\mathbf{A}_{50}^{\text{cal}}$ because we have calculated what the matrix **A** would be if it were rotated by 50°. The calculations necessary to get $\mathbf{A}_{50}^{\text{cal}}$ are

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos 50 & \sin 50 \\ 0 & -\sin 50 & \cos 50 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{33} \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos 50 & -\sin 50 \\ 0 & \sin 50 & \cos 50 \end{bmatrix}.$$

After performing the multiplication, we get the following expression for the 3 by 3 matrix $\mathbf{A}_{50}^{\text{cal}}$:

$$\begin{bmatrix} a_{11} & a_{12}\cos 50 + a_{13}\sin 50 & -a_{12}\sin 50 + a_{13}\cos 50 \\ a_{12}\cos 50 + a_{13}\sin 50 & a_{22}\cos^2 50 + a_{33}\sin^2 50 + 2a_{23}\cos 50 \sin 50 & a_{23}(1 - 2\sin^2 50) + (-a_{22} + a_{33})\cdot\cos 50 \sin 50 \\ -a_{12}\sin 50 + a_{13}\cos 50 & a_{23}(1 - 2\sin^2 50) + (-a_{22} + a_{33})\cdot\cos 50 \sin 50 & a_{22}\sin^2 50 + a_{33}\cos^2 50 - 2a_{23}\cos 50 \sin 50 \end{bmatrix}$$

The only unknown, a_{23}, in the above expression for the $\mathbf{A}_{50}^{\text{cal}}$ matrix appears in three distinct terms. To calculate a_{23}, we must compare $\mathbf{A}_{50}^{\text{cal}}$ with $\mathbf{A}_{50}^{\text{exp}}$ term by term. Since the off-diagonal term in $\mathbf{A}_{50}^{\text{exp}}$, i.e., a_{23}^{exp}, is also unknown, only two diagonal terms are useful for calculating a_{23}. Specifically we have

$$0.425\,148 = a_{22}\cos^2 50 + a_{33}\sin^2 50 + 2a_{23}\cos 50 \sin 50.$$

(Note that the a_{22} is measured at $S = 0°$, the a_{33} term comes from the $S = 90°$ ellipse, and the 0.425 167 matrix element comes from the 2,2 matrix element of the $S = 50°$ section. Thus the entire **A** matrix can be calculated from three cuts.) Substituting and solving for a_{23} gives

$$a_{23} = -0.000\,434.$$

Likewise, using the data from the $S = 140°$ cut, we have

$$0.426\,029 = a_{22}\sin^2 50 + a_{33}\cos^2 50 - 2a_{23}\cos 50 \sin 50.$$

Again, solving for a_{23} gives

$$a_{23} = -0.000\,434.$$

Note these two identical results for $a_{23} = -0.000\,434$. This value is substituted into matrix **A**.

The matrix **A** is now complete. In this case, the program MINITAB (1985, p. 179) was used to find the eigenvalues and the eigenvectors of **A**. The eigenvalues are

$$L_x = 0.427\,801$$
$$L_y = 0.425\,566$$
$$L_z = 0.422\,045.$$

From the eigenvalues, the principal indices can be calculated:

$$\alpha = L_x^{-1/2} = 1.528\,90$$
$$\beta = L_y^{-1/2} = 1.532\,91$$
$$\gamma = L_z^{-1/2} = 1.539\,31.$$

These values agree with the original values from Su et al. (1986).

The eigenvectors of **A** are the column vectors in the following matrix:

$$\begin{bmatrix} 0.604\,46 & -0.156\,78 & 0.781\,06 \\ -0.792\,82 & -0.022\,58 & 0.609\,04 \\ 0.077\,88 & 0.987\,38 & 0.137\,93 \end{bmatrix}.$$

Thus $X = 0.604\,46x - 0.792\,82y + 0.077\,88z$. In terms of E and S coordinates, with $\rho = 1$,

$$0.604\,46 = \cos E_x$$
$$-0.792\,82 = \sin E_x \cos S_x$$
$$0.077\,88 = \sin E_x \sin S_x.$$

Thus $E_x = 52.81°$ and $S_x = 174.39°$, which agree with the original assumed data. Similar agreement is found for Y and Z.

Another check of the consistency of the calculations is to compare the matrix invariants. Note, however, that to calculate the data for the $\mathbf{A}_{50}^{\text{exp}}$ matrix, we equate the off-diagonal terms in $\mathbf{A}_{50}^{\text{cal}}$ with $\mathbf{A}_{50}^{\text{exp}}$ and find that $a_{23}^{\text{exp}} = -0.000\,023\,9$. The trace is particularly valuable because it does not contain any cross terms. Thus, it can be used to compare the consistency of the $S = 0°$ and $S = 90°$ data with the $S = 50°$ and $S = 140°$ data. Because calculated data are used, these invariants are identical for **A**, $\mathbf{A}_{50}^{\text{cal}}$, and the diagonalized matrix. Specifically, the trace is 1.275 41, the second dyadic is 0.542 217, and the determinant is 0.076 384. Note also that the programs for these calculations carried more figures than is reported for the intermediate steps, which is why the invariants agreed to six places.

Conclusions

Light incident along a general direction has refractive indices given by the ellipse formed by the intersection of the optical ellipsoid and the plane through the origin of the ellipsoid and perpendicular to the general direction. The major and minor axes of any three independent ellipses are used to reconstruct the original optical index ellipsoid. The albite example is a severe test because its optical ellipsoid is nearly a sphere. Even in this case, α,

β, and γ and the orientations of the principal axes of albite could be recovered with data measured to the hundredths place. Note that although these data were collected at S = 0°, 50°, 90°, and 140°, this method is not limited to these values.

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