Determination of the Optic Angle 2V from the Extinction Curve of a Single Crystal Mounted on a Spindle Stage

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Formulae for determining the optic angle 2V from some angular measurements taken on the stereographic projection of an extinction curve are given. The extinction curve is obtained with a single crystal mounted on a spindle stage. Some properties of the curve are discussed and the practical procedure is outlined. A mathematical appendix is also given.

Introduction

The investigation of the orientation of the optical indicatrix from the extinction curve of a crystal mounted on a one-axis stage goniometer (Joel, 1950; Joel & Garaycochea, 1957) has led to different approaches for determining the optic axial angle 2V. Following Wilcox (1959) we use here for the 'one-axis stage goniometer' the general name of 'spindle stage' (see also Fisher, 1962). The method proposed here is not a method of successive approximations like the one by Wilcox $(1959, 1960, \overline{1962})$ and it requires less graphical constructions than the one by Tocher (1962), as the angle 2V is calculated from measurements made on the extinction curve. In the method recently proposed by Joel (1963) 2V is obtained from measurements made on an equivibration curve derived from the measured extinction positions.

From an extinction curve, as was shown by Joel & Garaycochea (1957), one can determine the orientation of the three axes of the indicatrix. The information contained in an extinction curve, by itself, does not make it possible, however, to distinguish between the X and Z axes; but it is sufficient, on the other hand, for the identification of the Y axis (the optic normal) and for the determination of 2Vreferred to one of the two principal axes in the optic plane. It follows, then, that one can have all the information related to the orientation of the optical indicatrix if, to the extinction curve, one adds the knowledge of the optic sign of the crystal.

In § 1-5 of this paper new equations and properties for the extinction curve are given and some formulae for calculating 2V are derived. These results are used in § 6 where the practical procedure is outlined; examples are given in § 7 and in the Appendix we derive the new form of the equations of the extinction curve starting from the ones given by Joel & Garaycochea (1957). We have kept the notation of this last paper, which is the notation of Wilson's (1943) book Vector Analysis.

1. Equations of the extinction curve

The equation of the extinction curve on a sphere of unit radius can be expressed as follows (see Appendix):

$$(\mathbf{r} \cdot \boldsymbol{\varphi} \cdot \mathbf{r}) (\mathbf{r} \cdot \mathbf{r}_0) = \mathbf{r} \cdot \boldsymbol{\varphi} \cdot \mathbf{r}_0 \tag{1}$$

where the variable unit vectors \mathbf{r} are the vibration directions; \mathbf{r}_0 is a unit vector in the direction of the spindle-stage axis; and $\boldsymbol{\varphi}$ is a uniplanar dyadic, its plane being precisely the optic plane. As is shown in the Appendix, it is possible to express $\boldsymbol{\varphi}$ in two alternative ways, referring it either to the primary optic axes or to the two principal directions of the indicatrix in the optic plane. The first alternative gives:

$$\mathbf{\varphi} = \mathbf{a}_1 \mathbf{a}_2 + \mathbf{a}_2 \mathbf{a}_1 \tag{2}$$

where a_1 and a_2 are unit vectors parallel to the two optic axes; and the second one:

$$\frac{1}{2}\mathbf{\phi} = -\sin^2 V_z \mathbf{i}\mathbf{i} + \cos^2 V_z \mathbf{k}\mathbf{k} \tag{3}$$

where \mathbf{i} and \mathbf{k} are unit vectors parallel to the X and Z axes of the ellipsoid.

Equation (1) with ϕ given by (2) may be expanded in the form:

$$2(\mathbf{r}.\mathbf{a}_{1})(\mathbf{r}.\mathbf{r}_{0}) = (\mathbf{r}.\mathbf{a}_{1})(\mathbf{r}_{0}.\mathbf{a}_{2}) + (\mathbf{r}.\mathbf{a}_{2})(\mathbf{r}_{0}.\mathbf{a}_{1}).$$
(4)

Similarly, equation (1) with φ given by (3) becomes:

$$\sin^2 V_z(\mathbf{r}.\mathbf{i})[(\mathbf{r}_0.\mathbf{i}) - (\mathbf{r}.\mathbf{i})(\mathbf{r}.\mathbf{r}_0)] = \cos^2 V_z(\mathbf{r}.\mathbf{k})[(\mathbf{r}_0.\mathbf{k}) - (\mathbf{r}.\mathbf{k})(\mathbf{r}.\mathbf{r}_0)]. \quad (5)$$

As to the notation, Table 1 relates the points on the stereogram, or on the surface of the reference sphere of unit radius, with the vectors in the formulae. Two capital letters placed side by side express the angular distance between the corresponding points on the stereogram or on the sphere.

Table 1. Notation

Point on the stereogram	Unit vector	Definition in terms of a_1, a_2 and r_0
A_{1}, A_{2}	a ₁ , a ₂	Optic axes
P_0	\mathbf{r}_{0}	Spindle-stage axis
P	r	A point on the extinction curve
G	g	$g\mathbf{g} = \mathbf{\phi} \cdot \mathbf{r}_0; \ g^2 = \mathbf{r}_0 \cdot \mathbf{\phi}^2 \cdot \mathbf{r}_0$
X	i	$2 \sin V_z \mathbf{i} = \mathbf{a_1} - \mathbf{a_2}$
Y	j	$\sin 2V_2 \mathbf{j} = \mathbf{a}_2 \times \mathbf{a}_1$
\boldsymbol{Z}	k	$2\cos V_z \mathbf{k} = \mathbf{a}_1 + \mathbf{a}_2$
$oldsymbol{U}$	u	$\sin P_0 G \mathbf{u} = \mathbf{r}_0 \times \mathbf{g}$
T_{x}	t_x	$\sin P_0 X \mathbf{t}_x = \mathbf{r}_0 - \cos P_0 X \mathbf{i}$
T_y	t_y	$\sin P_0 Y \mathbf{t}_y = \mathbf{r}_0 - \cos P_0 Y \mathbf{j}$
T_z	tz	$\sin P_0 Z \mathbf{t}_z = \mathbf{r}_0 - \cos P_0 Z \mathbf{k}$

2. Some properties of the extinction curves

With equations (1), (4) or (5) one can easily verify the known facts about extinction curves already obtained by means of optical or geometrical arguments. We shall do this here for those properties that are of interest when one deals with an experimental extinction curve.

(a) An extinction curve is centrosymmetric: if \mathbf{r} is a solution of equation (1), so is $-\mathbf{r}$.

(b) The points P_0, X, Y, Z are always on the extinction curve: in fact the vectors \mathbf{r}_0 , i, j, k are solutions of equation (1) or (5).

(c) If a point P is on the curve, the plane PP_0 intersects it at another point P' that is 90° away from P. In fact, if \mathbf{r} is a solution of equation (1), so is \mathbf{r}' defined by:

$$\sin PP_0\mathbf{r}' = \mathbf{r}_0 - \cos PP_0\mathbf{r} \,. \tag{6}$$

In equation (6) \mathbf{r} and \mathbf{r}' are the two vibration directions associated with a given wave front. The statements (a) and (c) together express nothing more than the fact that under orthoscopic observation between crossed polarizers a biaxial crystal extinguishes four times, every 90°, during a 360° rotation around an axis parallel to the microscope axis.

(d) If P_0 is not on a circular section, no point of the circular sections is on the extinction curve, except Y (equation (4)).

We shall agree that P_0 is in a general position when it is neither on a circular section nor on one of the principal planes of the indicatrix. In Fig. 1, P_0 is in the centre of the stereogram but in a general position. In the case shown in this figure, P_0 is in the acute angle formed by the circular sections and the optic sign is negative as the X axis is the acute bisectrix of the optic axial angle. It follows from paragraphs (b) and (c) above that the extinction curve (which is not drawn in Fig. 1) must go through the points P_0 , X, T_x , Y, T_y , Z and T_z . The points T_x , T_y and T_z are 90° away from X, Y and Z across P_0 . In the figure, the loci of the points that are 90° away, across P_0 , from the points of the circular sections are drawn. Certainly these loci go through the poles of the optic axes A_1 and A_2 . By remarks (c) and (d) the extinction curve cannot intersect the circular sections, except at their common point Y; nor the loci just mentioned, except at their common points P_0 and T_y . The branch of the extinction curve that goes through P_0 , T_x , Z and T_y of Fig. 1 is one of the polar curves (the other one is its inverse). And the branch through Y, T_z and X, which runs round the sphere, is the equatorial curve (Joel & Garaycochea, 1957).



Fig. 1. P_0 , on the centre of the stereogram, is in the acute angle of the circular sections CS1 and CS2 for a crystal with $2V_x=70^\circ$. The extinction curve is not drawn, but the polar curve goes through the points P_0, T_y, Z, T_x ; the equatorial curve through Y, T_z, X . The polar and equatorial curves are limited by the circular sections and by the curves $P_0T_yA_2$ and $P_0T_yA_1$ which are the loci of the points that are 90° away — through P_0 — from the points of the circular sections.

In order to draw the extinction curve in Fig. 1 it is sufficient to mark the points on every great circle through P_0 which are half way between the circular sections. The stereogram done with P_0 in the middle of the projection shows the complete polar curve. As Tocher (1962) and Fisher (1962) pointed out, it is very convenient; but certainly it is not a necessity.

It will be noted that if P_0 is changed to the obtuse angle between the circular sections or the crystal has the other optic sign, then the letters X and Z must be interchanged in the description of the polar and equatorial curves.

(e) With P_0 in a general position, each of the principal planes of the indicatrix intersects the

extinction curve at six points: two apices of the triangle XYZ, the point T 90° from the other apex, and the inverse of these three points.

(f) On the equatorial curve there exists a point U, 90° away from P_0 . In fact, a unit vector in the direction of $\mathbf{r}_0 \times (\mathbf{q}, \mathbf{r}_0)$ satisfies equation (1).

Cases where P_0 is not in a general position will be dealt with in § 5.

3. Formulae for calculating 2V

When the equation of the extinction curve is written in the form of equation (5) given above, it becomes clear that it is possible to calculate the angle 2Vusing one point of the extinction curve apart from the points X, Y, Z, P₀. If the scalar products are replaced by the cosines of the corresponding angular distances, formula (5) becomes:

$$tg^2 V_z = \frac{\cos PZ \ (\cos P_0 Z - \cos PZ \ \cos PP_0)}{\cos PX \ (\cos P_0 X - \cos PX \ \cos PP_0)}$$
(7)

which can also be derived directly from the extinction curve equations written in Cartesian coordinates that are given in the paper by Joel & Garaycochea (1957, p. 405, equation (5')).

Thus, if the five angular distances PX, PZ, P_0X , P_0Z and PP_0 are measured with the stereographic net, then 2V can be calculated as shown by (7). Different points P can be selected on the extinction curve and in this way an average can be obtained for 2V. But formula (7) becomes indeterminate (0/0) when P is chosen to coincide with P_0 . X, Y, Z, T_x , T_y or T_z ; and it would seem advisable to avoid choosing Pin the regions around these seven points. The indetermination of (7) when P is equal to P_0 , X, Y or Z is obvious from (5). As to the points T_x , T_y and T_z - which represent the vibration directions with the same wave normal as X, Y and Z respectively substituting in (6) P, r and r' by T_x , t_x and i respectively, and then by scalar multiplication by \mathbf{k} , one obtains:

$$\cos P_0 Z = \cos T_x Z \cos T_x P_0 \tag{8}$$

and a similar relation is obtained by interchanging in (8) Z with X. With P, r and r' replaced by T_y , t_y and **j**, and by successive scalar multiplication by **k** and **i**, relation (6) gives:

$$\cos P_0 Z = \cos T_y Z \cos T_y P_0$$

$$\cos P_0 X = \cos T_y X \cos T_y P_0 . \tag{9}$$

One has a simpler formula than (7) if P is selected to coincide with U, the point on the equatorial curve at 90° from P_0 . In this case (7) takes the form:

$$\operatorname{tg}^{2} V_{z} = \frac{\cos UZ \, \cos P_{0}Z}{\cos UX \, \cos P_{0}X} \tag{10}$$

and four angular distances have to be measured.

They can be reduced to three measurements if one observes the relations (9). From them, one has:

$$\frac{\cos P_0 Z}{\cos P_0 X} = \cot Z T_y \tag{11}$$

so that

$$\operatorname{tg}^{2} V_{z} = \left| \frac{\cos UZ}{\cos UX} \cot ZT_{y} \right| \,. \tag{12}$$

Next we shall see that with the introduction of a new point G, on the plane XZ and 90° from U, the angle 2V can be calculated from only two measurements taken on the stereogram. Introducing the unit vector g, defined by:

$$gg = \varphi . r_0; \ g^2 = r_0 . \varphi^2 . r_0$$
 (13)

the equation (1) for the extinction curve takes the form:

$$(\mathbf{r}.\boldsymbol{\varphi}.\mathbf{r})(\mathbf{r}.\mathbf{r}_0) = g\mathbf{r}.\mathbf{g}. \qquad (14)$$

With (2) and (3) one has respectively:

$$gg = (\mathbf{r}_0 \cdot \mathbf{a}_2)\mathbf{a}_1 + (\mathbf{r}_0 \cdot \mathbf{a}_1)\mathbf{a}_2 \tag{15}$$

$$\frac{1}{2}g\mathbf{g} = -\sin^2 V_z(\mathbf{r}_0.\mathbf{i})\mathbf{i} + \cos^2 V_z(\mathbf{r}_0.\mathbf{k})\mathbf{k}.$$
 (16)

As g is in the optic plane, the point G is on the trace of the plane XZ. Equation (14) is satisfied if r is a unit vector in the direction of $\mathbf{r}_0 \times \mathbf{g}$. This unit vector is **u**. Therefore, G is to be found on the plane XZ, 90° away from U.

Multiplying (16) first by \mathbf{i} and then by \mathbf{k} (scalar products) and dividing the two relations so obtained, one arrives at:

$$\operatorname{tg}^{2} V_{z} = \left| \frac{\cos P_{0} Z}{\cos P_{0} X} \cdot \operatorname{tg} Z G \right|$$
(17)

Combining (17) with (11) it follows that

$$\operatorname{tg}^2 V_z = |\operatorname{tg} ZG \operatorname{cot} ZT_y| . \tag{18}$$

After this, we have the formulae (7), (10), (12), (17) and (18) which give $tg^2 V_z$. In each of them one can interchange Z with X for obtaining $tg^2 V_x$ leading to a value of $2V_x$ that is the supplement of $2V_z$, as it should be. Therefore, once the three principal axes of the indicatrix are located on the extinction curve and the Y axis is identified (see next section), one can obtain the value of the optic angle referred to one of the principal axes on the optic plane, and it does not matter if this one is X or Z: the directions of the optic axes that are obtained will not depend on this choice. Certainly, instead of deriving 2V from $tg^2 V$ one can do it through $\cos 2V$ with the known formula:

$$\cos 2V = \frac{1 - \mathrm{tg}^2 V}{1 + \mathrm{tg}^2 V}.$$
 (19)

Furthermore, combining (18) with (19) one arrives at:

$$\cos 2V_z = \frac{\sin \left(ZT_y - ZG\right)}{\sin \left(ZT_y + ZG\right)}.$$
 (20)

or

Formula (20) is such that if the absolute value of the right hand side turns out to be greater than 1, then its reciprocal value should be taken.

4. The great circles through U

The great circles UP_0 , UX, UY and UZ are tangent to the extinction curve at the points P_0 , X, Y and Zrespectively. As to the great circle UP_0 , this can be shown by substituting in relation (6) \mathbf{r} and P by \mathbf{u} and U; \mathbf{r}' becomes \mathbf{r}_0 and the great circle UP_0 is therefore tangent to the polar curve at the point P_0 . One can check this result by differentiating equation (14):

 $2(d\mathbf{r} \cdot \mathbf{\varphi} \cdot \mathbf{r})(\mathbf{r} \cdot \mathbf{r}_0) + (\mathbf{r} \cdot \mathbf{\varphi} \cdot \mathbf{r})(d\mathbf{r} \cdot \mathbf{r}_0) = g d\mathbf{r} \cdot \mathbf{g} \cdot (21)$

For $\mathbf{r} = \mathbf{r}_0$, and because \mathbf{r} is a unit vector, one has $d\mathbf{r} \cdot \mathbf{r}_0 = 0$ and (21) becomes $d\mathbf{r} \cdot \mathbf{g} = 0$. It thus follows that the tangent vector at the point P_0 has the direction of $\mathbf{r}_0 \times \mathbf{g}$ which is that of \mathbf{u} .

In general, if we are searching for great circles through U that are tangent to the extinction curve, we are looking in fact for the solutions of the equation $d\mathbf{r} \cdot \mathbf{r} \times \mathbf{u} = 0$ which is equivalent to: $d\mathbf{r} \cdot \boldsymbol{\varphi} \cdot \mathbf{r} = 0$ for $\mathbf{r} \neq \mathbf{u}$, as can be shown by making use of the relations (14) and (21). If $\boldsymbol{\varphi}$ is substituted by its expression as given in (3), it becomes obvious that the equation $d\mathbf{r} \cdot \boldsymbol{\varphi} \cdot \mathbf{r} = 0$ is satisfied by $\mathbf{r} = \mathbf{i}, \mathbf{j}, \mathbf{k}$. As to $\mathbf{r} = \mathbf{r}_0$, this equation becomes $d\mathbf{r} \cdot \mathbf{g} = 0$, which is valid as was shown above. Passing through U there are, hence, four great circles tangent to the extinction curve at P_0 , X, Y and Z respectively. The polar curve (Fig. 2)



Fig. 2. A theoretical extinction curve of a crystal with $2V_x = 60^{\circ}$ and the tangent circles UP_0U , UXU, UYU and UZU.

is enclosed by the two tangent circles UP_0U and UZU(or UXU); and the equatorial curve is enclosed by the two tangent circles UYU and UXU (or UZU).

These tangent circles through U can be used quite simply for a first approximate location of the apices X, Y, Z. Furthermore, they provide a convenient means for deciding which of the two apices on the equatorial curve is Y: between the great circles UP_0U and UYU (the acute dihedral angle) there are no points of the extinction curve.

5. Special positions of P_0

Next some special cases will be discussed.

(a) P_0 is on the trace of a circular section, a case that has been illustrated by Fisher (1962, pp. 658 and 663). If one of the points X or Z can be located on the extinction curve, one obtains readily not only the other two apices of the triangle XYZ but also the position of an optic axis and the value of the angle V. In fact, let P_0 be on the trace of the circular section perpendicular to a_1 , that is $\mathbf{r}_0.\mathbf{a}_1=0$. By (15) one has that $\mathbf{g}=\mathbf{a}_1$, so that the point G becomes A_1 . Equation (4) is satisfied in this case by all the points on the circular section where P_0 is. For points other than these, the equation becomes:

$$2(\mathbf{r}.\mathbf{a}_2)(\mathbf{r}.\mathbf{r}_0) = (\mathbf{r}_0.\mathbf{a}_2)$$

$$2\cos PA_2\cos PP_0 = \cos P_0A_2.$$
 (22)

(a') If P_0 is in the intersection of one circular section with the optic plane, (22) can be written:

$$2\cos PA_2\cos PP_0 = \sin 2V_z \,. \tag{23}$$

The curve given by (23) becomes a circumference of radius 45° and centre P_0 when $2V_z=90^{\circ}$. In fact A_2 coincides in this case with P_0 and (23) is equivalent to $1/2 \cos PP_0=1$.

(a'') If P_0 is on both circular sections, that is, P_0 coincides with $Y(\mathbf{r}_0=\mathbf{j})$ equation (4) becomes:

$$(\mathbf{r}.\mathbf{a}_1)(\mathbf{r}.\mathbf{a}_2)(\mathbf{r}.\mathbf{j})=0.$$
 (24)

This equation is satisfied by all the points on the traces of the circular sections and on the trace of the optic plane, altogether three complete great circles. The optic plane however, is not the equatorial curve. In this limiting case, the polar curve consists of one spherical triangle YMN (and its inverse), where M and N are two of the intersections of the optic plane with the circular sections. The rest of the extinction curve is covered by the equatorial curve, and between the latter and the two polar curves there are six common points: Y, M, N and their inverse.

(b) P_0 is on the trace of one of the planes XY or YZ(except the points X, Y, Z). Let P_0 be on the plane YZ. In this case $\mathbf{g} = \mathbf{k}$ (see (16)), hence G and T_y coincide with Z, and U becomes X. The angle 2V can be calculated, by means of four measurements, with formula (7) which can be used in the form:

$$tg^{2} V_{z} = \frac{\cos PZ (\cos PZ \cos PP_{0} - \cos P_{0}Z)}{\cos^{2} PX \cos PP_{0}}.$$
 (25)

(c) P_0 is on the trace of the optic plane (except the points X and Z). In this case the following pairs of points coincide: U and Y, T_y and P_0 , T_z and X, T_x and Z. Hence, it is not possible to locate G by means of the plane whose pole is U. The angle 2V can be calculated with formula (7) taking four measurements, or with three measurements and the formula that follows:

$$\operatorname{tg}^{2} V_{z} = \frac{\cos PZ \, (\sin^{2} PZ - \cos PZ \cos PX \operatorname{tg} P_{0}Z)}{\cos PX \, (\sin^{2} PX \operatorname{tg} P_{0}Z - \cos PZ \cos PX)} \,.$$
(26)

(d) P_0 coincides with Z (or X). In this case the points P_0, Z, T_x, T_y and G (or P_0, X, T_z, T_y and G) coincide. The equatorial curve is a great circle whose pole is P_0 and the polar curve reduces itself to the point P_0 . There is no difference between the curves in this case and in the case of a uniaxial crystal with the spindle-stage axis coinciding with its optic axis (see Appendix).

6. Practical procedure for determining 2V

The results of the previous sections can be summarized in the following procedure for determining 2V.

The extinction readings θ_1 (and $\theta_2 = \theta_1 \pm 90^\circ$) of the microscope stage are plotted on the stereogram for the corresponding settings of the spindle stage. P_0 , the projection of the spindle-stage axis, is chosen in the centre of the stereogram. The polar and equatorial curves are then drawn through the experimental points taking care that any point of the former must be 90° away through P_0 from its corresponding one on the latter. The position of the point U on the equatorial curve, 90° from P_0 , is marked. With P_0 in the centre of the stereogram, U is on the primitive circle at the point where it is intersected by the equatorial curve. One must keep in mind that the great circle that goes through P_0 and U should be tangent to the polar curve at P_0 .

Let us suppose that P_0 is in a general position and that a Wulff net is used. The points at which the great circles through U are tangent to the equatorial and polar curves give us an approximate location of the apices of the right-sided triangle XYZ and this permits a quicker determination of them. If the approximate position of one of these three apices is used, for instance Y, which can be easily identified as explained in the last sentence of §4, one can proceed as follows: the great circle through Y and P_0 determines a point T_y on the polar curve which is 90° away from Y; the great circle through T_y , of which Y is the pole, intersects the extinction curve at two

more points, one on the polar curve and the other one on the equatorial curve. They should be X and Zand should be 90° apart. If they are not 90° apart, then the assumed position for Y is incorrect and one tries another point in the limited region already determined for the point Y. The apices of the triangle are thus obtained.* and as a check of the quality of the stereogram one can use the property given by remark (e) in §2. Then the position of the point Gis determined as the intersection of the plane XZand the great circle at 90° from U. As a check one uses the fact that the point G is also the pole of the great circle that passes through Y and \overline{U} which in turn should be tangent to the curve at Y. As P_0 is in the centre of the stereogram it is advisable to calculate the optic angle referred to the axis on the polar curve. For a moment let us label Z the apex of the triangle on the polar curve. The distances ZG and ZT_y are measured and V_z is calculated with formula (20) or (18). The identification of the axes X and Z can be easily done and then one knows if the apex on the polar curve is really Z or X. But if the sign of the crystal is previously known, the points X and Z are then already identified through the value of the angle just calculated. Alternatively, any of the formulae (17), (12), (10) or (7) might be used if the required angular distances are read off the projection; the choice of the formula may depend on factors such as the accuracy with which some points have been determined, the particular numerical value of the distances to be measured, etc.

As a matter of fact, the errors in the determination of 2V reduce mainly to those of the experimental extinction positions and the attainable precision of these readings depends on the setting of the crystal on the spindle stage. Fairly good extinction readings with a favourable setting are sufficient for the approximate location of the points X, Y, Z, U. Then, one can carefully refine small regions of the extinction curve around any of the relevant points.

When recording the experimental data, it is advisable to look for the setting of the spindle stage for extinction directions θ of 0° or 90° (measured from P_0) and in the neighbourhood of these values, as this helps to locate more accurately the point U, and consequently the point G. To attain accuracy in the determination of the extinction positions, the use of an immersion liquid of adequate refractive index and of monochromatic light are common requirements. Accesories like a Bertrand ocular or others (Johannsen, 1918, pp. 392–398) are useful in certain cases. Valuable suggestions on this topic will be found in the papers by Wilcox (1959), Tocher (1962) and Fisher (1962).

For the evaluation of the errors introduced by the plotting and reading on the stereogram, theoretical

^{*} This procedure is quicker than the one originally proposed by Joel & Garaycochea (1957) and, apart from the use of the circles through U, is similar to the one given by Tocher (1962).

extinction curves were drawn and then some of the formulae given in this paper were used. With a 20 cm Wulff stereographic net, without too much effort, the value of 2V was recuperated with an absolute error of less than 1°. Moreover, the absolute error can be estimated by differentiating formula (18), for instance. Let us call δ , ε and ε' the absolute errors in $2V_z$, ZG and ZT_y respectively. One can obtain:

$$\delta = \sin 2V_z \left[\frac{\varepsilon}{\sin 2ZG} + \frac{\varepsilon'}{\sin 2ZT_y} \right].$$
(27)

7. Examples

The method here described was tried out on several biaxial crystals. Only two examples are given and each of them has a special interest, though none of them represents a precise determination of 2V.

(a) If one wants to identify quickly a single crystal before working in X-ray diffraction, it is not necessary to obtain great accuracy in the value of 2V. A single crystal of brochantite — monoclinic with $2V_x = 77^{\circ} \pm 2^{\circ}$ as given by Palache, Berman & Frondel (1951, p. 542) — has been selected for X-ray diffraction, being mounted on a glass fiber. Before setting the glass fiber on the X-ray goniometer head, it was set on the spindle stage. The extinction positions were obtained with a liquid of refractive index 1.77 (average refractive indices of the crystal) and with



Fig. 3. An extinction curve of brochantite. The stereogram shows: the equatorial curve with the X and Y axes and the point U; the polar curve with the Z axis and the points P_0 and T_y ; the great circle UY tangent to the equatorial curve at Y and its pole G. The point G is the intersection of the great circle XZ and the one whose pole is U.

white light. Special attention was given to the extinction measurements leading to the point U. The setting of the crystal was favourable and the stereogram was drawn with P_0 in the middle (Fig. 3). The optic angle was calculated with formulae (10), (12), (17), (18) and (20) measuring for each of them the required distances. All of them gave values in the range $77^{\circ} 25'$ to $77^{\circ} 45'$. Taking $\varepsilon = \varepsilon' = 30'$, formula (27) gave $\delta = \pm 1^{\circ}$ for the error in 2V.



Fig. 4. The extinction curve of morinite, after the data of Fisher (1962). The stereogram shows: the equatorial curve with the Z and Y axes; the polar curve with P_0 and the X axis; the points U and G.

(b) The extinction curve of morinite is shown in Fig. 4. It was drawn from data given by Fisher (1962, Tables 1 and 2 and considerations in the text). The lack of extinction readings in the neighbourhood of U and P_0 is caused undoubtedly by the fact that P_0 is near the trace of a circular section. Nevertheless, from the great circles tangent to the polar curve at P_0 and X and to the equatorial curve at Y and Z one could determine the limits for the possible positions of the point U, which gave $13^{\circ} \leq XG \leq 15^{\circ}$. With $P_0X = 69^\circ$ and $P_0Z = 45^\circ$, given by Fisher, and with formula (17), the range $37^{\circ} 46' \le 2V_x \le 40^{\circ} 28'$ was obtained. These values are in fair agreement with the values 39° 42' and 40° 07' obtained by Fisher & Runner (1958) and Fisher (1962) from measurements of the principal refractive indices.

APPENDIX

$$\mathbf{r} \cdot \mathbf{\Phi} \cdot \mathbf{r} = 1$$

(1)

represents an ellipsoid if

The equation

(2)

$$\Phi = A\mathbf{i}\mathbf{i} + B\mathbf{j}\mathbf{i} + C\mathbf{k}\mathbf{k}$$

with A, B, C positive numbers and

$$\mathbf{r} = x\mathbf{i} + y\mathbf{j} + z\mathbf{k} \ . \tag{3}$$

If $A = \alpha^{-2}$, $B = \beta^{-2}$, $C = \gamma^{-2}$ where α , β , γ are the principal refractive indices of a crystal, equation (1) represents its optical indicatrix. As usual, we suppose $\alpha < \beta < \gamma$ so that A > B > C > 0.

Let us define two unit vectors a_1 and a_2 by means of the following relations:

$$\begin{aligned} & \sqrt{(A-C)}\mathbf{a}_1 = \sqrt{(A-B)}\mathbf{i} + \sqrt{(B-C)}\mathbf{k} \\ & \sqrt{(A-C)}\mathbf{a}_2 = -\sqrt{(A-B)}\mathbf{i} + \sqrt{(B-C)}\mathbf{k} . \end{aligned} \tag{4}$$

The dyadic Φ of formula (2) can be written now in the form:

$$\Phi = B\mathbf{I} - \frac{1}{2}(A - C)\boldsymbol{\varphi} \tag{5}$$

where the dyadic I is the idemfactor and $\boldsymbol{\phi}$ is the dyadic defined by

$$\varphi = a_1 a_2 + a_2 a_1 . \tag{6}$$

If (5) and (6) are introduced in (1), the equation of the ellipsoid can be written:

$$B\mathbf{r}^{2} - (A - C)(\mathbf{r} \cdot \mathbf{a}_{1})(\mathbf{r} \cdot \mathbf{a}_{2}) = 1$$
. (7)

Now, the equation of the plane normal to a_1 through the origin is

$$\mathbf{r} \cdot \mathbf{a}_1 = 0 \tag{8}$$

and if \mathbf{r} satisfies equations (7) and (8) then it also satisfies

$$B\mathbf{r}^2 = 1 \tag{9}$$

which is a circumference (of radius β) on both the ellipsoid and the plane normal to a_1 . The vectors a_1 and a_2 are therefore normal to the two circular sections of the ellipsoid; that is, they are the optic axes of the indicatrix.

Let us call $2V_z$ the angle formed by the two optic axes (the one which is bisected by the Z axis). From relations (4) it follows easily that

$$a_1 \cdot a_2 = \cos 2V_z = (2B - (A + C))/(A - C)$$
 (10)

$$(\mathbf{a}_1, \mathbf{k})^2 = \cos^2 V_z = (B - C)/(A - C)$$
, (11)

and from (11):

$$tg^2 V_z = (A - B)/(B - C)$$
. (12)

Making use of (4) and (11), (6) becomes

$$\frac{1}{2}\mathbf{\varphi} = -\sin^2 V_z \mathbf{i}\mathbf{i} + \cos^2 V_z \mathbf{k}\mathbf{k} \,. \tag{13}$$

The equations of an extinction curve expressed by means of the dyadic (2) are, as given by Joel & Garaycochea (1957, p. 405, equation (5)) the following:

$$(\mathbf{r} \cdot \boldsymbol{\Phi} \cdot \mathbf{r}) (\mathbf{r} \cdot \mathbf{r}_0) = \mathbf{r} \cdot \boldsymbol{\Phi} \cdot \mathbf{r}_0$$

$$\mathbf{r}^2 = 1 \bullet$$
(14)

By introducing in (14) the expression (5) for Φ the following equations for the extinction curve are obtained:

$$(\mathbf{r} \cdot \boldsymbol{\varphi} \cdot \mathbf{r}) (\mathbf{r} \cdot \mathbf{r}_0) = \mathbf{r} \cdot \boldsymbol{\varphi} \cdot \mathbf{r}_0$$

 $\mathbf{r}^2 = 1$ (15)

which are identical in form with equation (14) but with the dyadic ϕ given by (6) or (13).

The equations of the extinction curve for a uniaxial crystal follow as a particular case of (15). If one has $\mathbf{a}_1 = \mathbf{a}_2 = \mathbf{k}$, or $2V_z = 0$, from (6) or (13) one has that $\frac{1}{2}\mathbf{\phi} = \mathbf{kk}$ and (15) becomes

$$(\mathbf{r}.\mathbf{k})^2(\mathbf{r}.\mathbf{r}_0) = (\mathbf{r}.\mathbf{k})(\mathbf{r}_0.\mathbf{k}); \quad \mathbf{r}^2 = 1.$$
 (16)

Hence, the extinction curve in this case consists of the great circle $\mathbf{r}.\mathbf{k}=0$ and the curve $(\mathbf{r}.\mathbf{k})(\mathbf{r}.\mathbf{r}_0)=\mathbf{r}_0.\mathbf{k}$ which is satisfied by \mathbf{r}_0 and \mathbf{k} .

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Resumen

Con las fórmulas aquí dadas, el ángulo óptico 2V puede calcularse a partir de ciertas medidas angulares realizadas en la proyección estereográfica de una curva de extinción. La curva se obtiene con el monocristal montado en un simple goniómetro de platina. Se discuten algunas propiedades de la curva de extinción y se describe el procedimiento práctico. Se da también un apéndice matemático.

References

- FISHER, D. J. & RUNNER, J. J. (1958). Amer. Min. 43, 585.
- FISHER, D. J. (1962). Amer. Min. 47, 649.
- JOEL, N. (1950). Miner. Mag. 29, 206.
- JOEL, N. (1963). Miner. Mag. In the press.
- JOEL, N. & GARAYCOCHEA, I. (1957). Acta Cryst. 10, 399. JOHANNSEN, A. (1918). Manual of Petrographic Methods. New York: McGraw-Hill.
- PALACHE, C., BERMAN, H. & FRONDEL, C. (1951). Dana's System of Mineralogy, II. New York: Wiley.
- TOCHER, F. E. (1962). Miner. Mag. 33, 52.
- WILCOX, R. E. (1959). Amer. Min. 44, 1272.
- WILCOX, R. E. (1960). Bull. Geol. Soc. Amer. 71, 2003.
- WILCOX, R. E. (1962). Personal communication.
- WILSON, E. B. (1943). Vector Analysis. New Haven: Yale University Press.