Determination of the optic axes and 2V: electronic computation from extinction data

By N. Joel

Instituto de Física y Matemáticas, Universidad de Chile, Casilla 2777, Santiago, Chile[1]

Summary. Extinction readings are taken, on a polarizing microscope, for several wave-fronts in a biaxial crystal (more than four wave-fronts are required). With these extinction data, the machine then calculates the directions of the two optic axes and of the three principal axes of the indicatrix, as well as the value of the optic axial angle 2V, using a least-squares successive approximation technique. The programme was written for an IBM 1620 computer.

IN a recent paper (Joel, 1964) a graphical procedure was developed for determining the directions of each of the two optic axes of a biaxial crystal—hence also the value of 2V—using as data the vibration directions of a few (four or more) wave-fronts in the crystal. The problem was, at that time, solved graphically because a numerical solution of the equations involved would only be practicable with an electronic computer. Such a numerical solution has now been attempted and has turned out to be quite simple. The experimental procedure is also very simple and fast: all that is required is to get a few extinction readings and feed these into the computer. The latter then calculates the directions of each of the two optic axes (A_1 and A_2) and the three principal axes (B_1, B_2, and β) of the indicatrix,[2] as well as the value of the optic axial angle 2V.

A brief presentation of the method will be given here for those who may wish to use the programme. Details of the mathematics of the problem will be published separately.

Experimental procedure

General case: any wave-normals. After having determined a vibration direction P, in any given wave-front, usually by rotation to extinction

---

[1] Present address: Dept. of Natural Sciences, UNESCO, Place de Fontenon, Paris 7e, France.

[2] With these extinction data only, the computer will not be able to decide which of the two bisectrices (B_1 and B_2) is α, and which is γ. If this differentiation were required, some of the usual observations with retardation plates or with refractive index liquids could be made.

about the microscope axis (A_5), two arbitrary points Q and Q' are chosen and plotted in the stereographic projection of the wave-front, one on each side of P, and such that $QP = PQ'$ (fig. 1). This relationship ensures, for any pair of points Q and Q', that they both belong to the same equivibration curve (Joel, 1963a; 1963b).
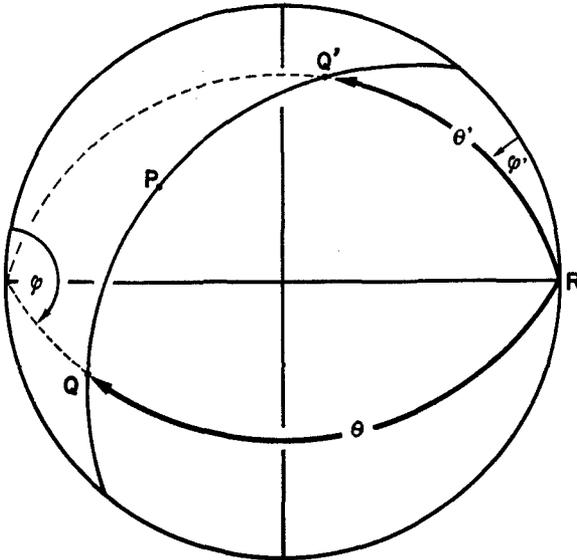
FIG. 1. P, one of the vibration directions in the wave-front shown. Q and Q', pair of points on the same wave-front such that $QP = PQ'$. For each wave-front, the data to be supplied to the computer are the values of ϕ, θ, ϕ', and θ' relative to the zero meridian and the polar axis R.

For each wave-front, the data to be supplied to the computer are the polar co-ordinates of Q (ϕ, θ) and Q' (ϕ', θ') with respect to a conveniently chosen zero meridian and a polar axis contained in it. When using the Federov stage, these could be the plane of the thin section and a direction R contained in it, as in fig. 1.

Wave-fronts in any orientation with respect to each other may be used provided that their correct relative orientations are preserved in the stereogram (see, for instance, Joel and Muir, 1958a; Joel and Tocher, 1964) and that for all the wave-fronts the polar co-ordinates of Q and Q' are referred to the same zero meridian and the same polar axis R.

Special case: coplanar wave-normals. A convenient simplification of the above general procedure arises if the wave-fronts to be observed are

limited to those that can be obtained by rotating the crystal around
a fixed axis set perpendicular to the microscope axis. This can be
achieved by means of a spindle stage (one-axis instrument), or with
a Federov stage using rotations around A_4 only. The wave-normals are
now all coplanar, and the experimental procedure is greatly simplified.
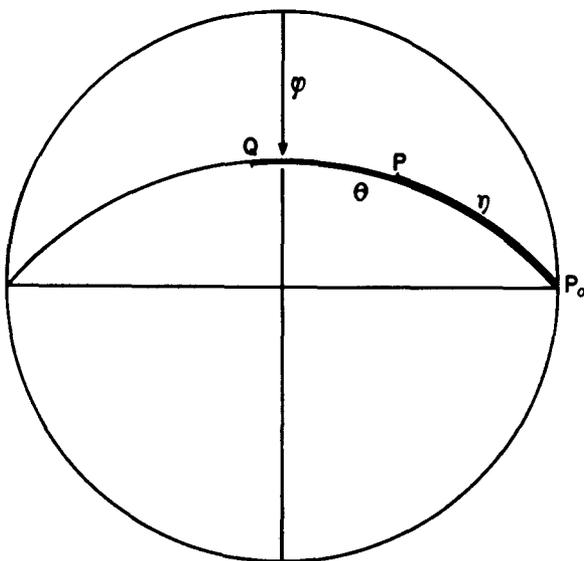
FIG. 2. P_0, projection of the spindle-stage axis. A rotation ϕ on the spindle stage
brings into observation a wave-front of which P is one of the vibration directions.
η, extinction angle relative to P_0. $P_0P = PQ$. $\theta = 2\,\eta$. For each wave-front the
data to be supplied to the computer are the values of ϕ and θ, relative to the zero
meridian and the polar axis P_0.

All the observed wave-fronts are parallel to the single rotation axis
of the instrument; and this axis can be chosen as the polar axis R from
which the polar angles of Q and Q' are measured in each wave-front.
Following established usage (Joel and Garaycochea, 1957), R may thus
be referred to as P_0 (fig. 2).

The point Q' can now be chosen, for all the observed wave-fronts, to
coincide with P_0; Q is then located so that $QP = PP_0$. In this way, for
all the wave-fronts, $\phi' = \theta' = 0$. Furthermore, P_0 and the points Q
of all the wave-fronts belong to the same equivibration curve, namely
the one that goes through P_0, that is, the n_0 curve (Joel, 1963a).

No stereographic projection is necessary for determining the polar

co-ordinates of Q and Q'. For Q' (P_0), $\phi' = \theta' = 0$ for all wave-fronts. And for Q, ϕ is read directly on the spindle stage or on the A_4 drum of the Federov stage, while $\theta = 2\eta$, where η is the extinction angle P_0P as measured by rotation about the microscope axis (fig. 2).

The simplifications introduced by the use of coplanar wave-normals (with a spindle stage, or with a Federov stage rotating around A_4 only), make the rapid routine determination of 2V possible for a large number of specimens. In fact, if only the value of 2V is required, but not the directions of the two optic axes within each specimen, then no stereographic projection is necessary and no system of reference has to be recorded for each specimen. All that has to be done is to read the angles ϕ and η ($\theta = 2\eta$), as explained above, for a few wave-fronts (more than four). These are all the experimental data required for the computation.

Basic ideas of the computation

The equations which the computer solves are of the form:[1]

$$(\mathbf{q}.\mathbf{a}_1)\,(\mathbf{q}.\mathbf{a}_2) = (\mathbf{q}'.\mathbf{a}_1)\,(\mathbf{q}'.\mathbf{a}_2)$$

where $\mathbf{a}_1$ and $\mathbf{a}_2$ are two unit vectors parallel to the optic axes A_1 and A_2 of the crystal, and $\mathbf{q}$ and $\mathbf{q}'$ are unit vectors pointing towards the points Q and Q' of each wave-front (Q and P_0 in the special case of coplanar wave-normals described in the preceding section). There are thus as many equations as wave-fronts have been measured. Four are mathematically sufficient for determining $\mathbf{a}_1$ and $\mathbf{a}_2$ from the experimental data, but this set of equations cannot be solved algebraically. Therefore a successive approximation method was used, based on the following ideas:

If one of the vectors—$\mathbf{a}_1$ or $\mathbf{a}_2$—is accurately known, it is easy to calculate the other one. Two equations only are required; they are linear and can thus be solved algebraically. This is the numerical equivalent of the graphical procedure developed by Joel and Muir (1958b).

If one of the two vectors—$\mathbf{a}_1$ or $\mathbf{a}_2$—is known, but only approximately, it would still be possible to calculate an approximate solution for the other one. This can be done better by using more than four equations (hence using data from more than four wave-fronts) and minimizing the sum of the squares of the errors.

Then if, with a postulated initial vector $\mathbf{a}_1$, an approximate solution

---

[1] These are equivalent to equation (1) in Joel (1964).

for a_2 is computed, it is possible, using the computed vector a_2 as a basis, to recompute a_1, obtaining for the latter a better approximation than the initial one. This cycle of operations can then be repeated several times until the directions of a_1 and a_2 are refined either to the extent desired by the operator or to that permitted by the experimental data. The number of cycles required to reach the desired degree of refinement is also partly dictated by the accuracy of the initial postulated direction of a_1: an arbitrary hoice or even a deliberately bad choice, say close to β, has the effect of increasing the number of cycles; but the computation will still converge to the best possible solution compatible with the experimental data.

It is necessary to have a criterion for stopping the computation when the solutions are sufficiently approximate. This can be done in several ways. In the present programme it was decided to programme the computer to stop as soon as the change between the last two cycles, in both a_1 and a_2, became less than a pre-specified angle, say $0 \cdot 1°$, or any other angle δ pre-selected by the user of the programme.

It is interesting to note that successive approximation procedures have also been used in some new graphical methods recently developed by Tocher (1964a, 1964b, 1964c, 1965), the last of which is the graphical equivalent of the numerical method outlined above.

Data and results

The computer is supplied with the following data:

n (> 4) sets of values of ϕ, θ, ϕ', and θ' (in degrees, with decimal fractions if desired), as follows from the earlier section on experimental procedure. When the wave-normals are all coplanar it is possible to have $Q' = P_0$ for all wave-fronts, that is, $\phi' = \theta' = 0$. As to the number n, good results have been obtained with n between 8 and 15. The programme, however, allows for up to 50 wave-fronts.

The angles ϕ_0 and θ_0 (also in degrees) defining the initial postulated direction of any one of the optic axes. This initial direction can be arbitrary, but a good approximation for it may save a few computing cycles.

The angle δ that tells the computer to stop when between the last two cycles both a_1 and a_2 have varied by less than δ. (It was found more convenient in practice to use a parameter ϵ, where $\epsilon = \sin^2\delta$; values of ϵ of 10^{-6} and 10^{-7} have been used.)

The maximum number of cycles to be computed. This is a safeguard in case the condition imposed by δ is too demanding for the experimental

data available. The computer will stop as soon as either condition is fulfilled.

With the above data the computer will produce and print the optic axial angle 2V (or its supplement), together with two sets of co-ordinates (the three Cartesian components, and the polar angles ϕ and θ) for each of the five vectors: $\mathbf{a_1}$, $\mathbf{a_2}$, $\mathbf{b_1}$, $\mathbf{b_2}$, and $\boldsymbol{\beta}$. In this way the directions of the two optic axes and of the three principal axes of the indicatrix are known relative to the setting chosen for the measurements, that is, relative to the zero meridian and the polar axis R (or P_0). This part of the results is not required in those cases where only the value of 2V is wanted.

The number of cycles actually performed is also printed, and some indication of the accuracy of the results.

More details on the mathematics involved in the present method will be given in a separate publication. It is also hoped to make the programme (IBM 1620) available as soon as possible to anyone interested in it, together with the necessary description and instructions.

References

JOEL (N.), 1963*a*. Min. Mag., vol. 33, pp. 679–692.
—— 1963*b*. Bull. Soc. franç. Min. Crist., vol. 86, pp. 405–408.
—— 1964. Min. Mag., vol. 33, pp. 769–779.
—— and GARAYCOCHEA (I.), 1957. Acta Cryst., vol. 10, pp. 399–406.
—— and MUIR (I. D.), 1958*a*. Min. Mag., vol. 31, pp. 860–877.
—— —— 1958*b*. *Ibid.*, pp. 878–882.
—— and TOCHER (F. E.), 1964. *Ibid.*, vol. 33, pp. 853–867.
TOCHER (F. E.), 1964*a*. *Ibid.*, pp. 780–789.
—— 1964*b*. *Ibid.*, pp. 1038–1054.
—— 1964*c*. Amer. Min., vol. 49, pp. 1622–1630.
—— 1965. The universal stage and 2V: a new extinction technique of high accuracy (in preparation).