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SOFTWARE NOTICE

EXCALIBR revisited

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Abstract

EXCALIBR is a FORTRAN computer program that, from extinction data collected on a polarizing microscope equipped with a spindle stage, calculates the orientations of a biaxial crystal's optical directions *X, Y, Z,* two optic axes, and determines $2V$. The program was developed by Bloss and Riess (1973) and refined by Bloss (1978, 1981). Since its development, it has been used extensively by Bloss and co-workers in optical studies of minerals. With the advent of PCs, the program became available to a wider group of scientists who did not have access to a mainframe computer. Several refinements and minor corrections have been made to the original program, which is now available for IBM-PC compatibles, for Macintosh computers, or as an improved mainframe version.

Introduction

Bloss and Riess (1973) discussed the mathematics required to calculate an anisotropic crystal's optical directions and optic axial angle ($2V$). The computer program EXCALIBR (Bloss, 1978, 1981), developed for this work, accepts as input data those microscope stage settings that cause a crystal mounted on a spindle stage to go extinct, under crossed polars, as the spindle stage is set to $S = 0°, 10°, \ldots, 170°$ (see Bloss, 1981, for a complete treatment of spindle-stage methods). Given these data, EXCALIBR determines the orientation, in relationship to the microscope–spindle-stage coordinate system, for *X, Y,* and *Z,* the principal vibration axes of a biaxial mineral. The program also calculates the orientation of the crystal's two optic axes and $2V$. From this information the microscopist can determine the mineral's optic sign with the aid of an accessory plate. The crystal can next be oriented to measure principal refractive indices α, β, and γ—without appreciable error due to misorientation—by use of the double-variation method described in Louisnathan et al. (1978) and Bloss (1981).[1] With aid of the computer programs described in Su et al. (1987), the refractive indices can be quickly determined to within ± 0.0002, or better.[2]

EXCALIBR has been used to solve, and to discover, problems in optical mineralogy. A few examples are Armbruster and Bloss (1982), Gunter and Bloss (1982), Su et al. (1984, 1986a, 1986b, 1986c), Greiner and Bloss (1987). The program, and spindle-stage methods in general, have found use outside of optical mineralogy in such fields as forensics, physics, chemistry, pharmaceuticals, material sciences, and the occurrence of asbestos in the environment, to name a few.

Microscope stage differences

When EXCALIBR was first developed (Bloss and Riess, 1973; Bloss, 1978), most of the rotatable stages of polarizing microscopes were graduated along their circumferences in 1° increments that usually increased from 0° to 359° in a counterclockwise direction (=counterclockwise stage). In newer microscopes, however, the graduations usually increase in a clockwise direction (= clockwise stage). If EXCALIBR in its original version solves extinction data obtained with a clockwise stage, it calculates all S angles correctly, but not the E angles; unfortunately, the calculated E angles actually equal $180° - E$. In consequence, stereographic plots of these data, including the extinction curves themselves, will represent mirror images of the true plots. Nevertheless, the original EXCALIBR program does correctly calculate the microscope stage settings M that orient the three principal vibration axes *X, Y,* and *Z* either E–W or N–S.

The original EXCALIBR program has been modified to calculate correct intermediate E angles for clockwise stages. To distinguish between clockwise stages and counterclockwise stages, the sign of the reference azimuth (LMR) is changed on the control card. For a counterclockwise stage, a positive LMR is entered, as before. For a clockwise stage, the LMR value is entered as negative. This negative value for the LMR sets a flag in the program, which then calculates correct intermediate E angles.

ARCRO and X-ray orientation

A bug was found in ARCRO, a subroutine that provides calculations to aid in X-ray orientation and optical orientation after the optical directions have been determined by EXCALIBR. The problem was remedied by corrections to the program and by modifying the input to the control card. The entries on the control card for LOARC and UPARC (cf. Bloss, 1981, p. 230 et seq.) have been replaced by LO1, LO2, UP1, and UP2. LO and UP refer to lower arc and upper arc settings of an X-ray goniometer head; the number 1 refers to their settings at which extinction data were collected, and 2 refers to the settings to which they are to be rotated. LO1, LO2, UP1, and UP2 values are entered on the control card into columns 36–40, 42–46, 48–52, and 54–58, respectively.

Even without performing the calculations available in ARCRO, the spindle stage proves very useful in optically orienting crystals for X-ray work. For instance, a uniaxial crystal can be mounted on a glass fiber with fingernail polish and placed on a goniometer head, which is in turn mounted on the spindle stage. If the crystal can be oriented so that it remains extinct while the microscope stage is rotated 360°, the optic axis (c axis) has been placed parallel to the microscope axis, and the hexagonal or tetragonal crystal would be correctly oriented with respect to arc settings and dial setting, within 1° or better, for a precession photograph. If an orthorhombic mineral is mounted so that it remains extinct during a full rotation of the spindle stage, where the microscope

[1] The oil cell and heater used in the double-variation method are currently available; contact M. E. Gunter.

[2] These computer programs can be obtained by contacting M. E. Gunter. The oil program has been modified so that it will work with any refractometer.

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stage is set at the reference azimuth, the crystal has a direct crystallographic axis parallel, within 1° or better, of the spindle axis. The crystal axis is thus oriented parallel to the dial axis for a Weissenberg photograph. If the correct orientation cannot be obtained, by using cleavage, pleochroism, or ARCRO, the grain can be removed from the fiber with acetone and remounted in a more favorable orientation.

HARDWARD REQUIREMENTS AND AVAILABILITY

EXCALIBR[3] was originally written in FORTRAN for use on a mainframe computer and is still available in FORTRAN source code. With the advent of PCs, the program was ported down to the MS-DOS–IBM-PC compatible computers, and the necessary modifications made so that the program could be compiled using Microsoft FORTRAN77 version 3.3. The program requires 256k memory and only one disk drive and has been successfully tested on an IBM-PC, IBM-PCXT, IBM-PCAT, IBM Model 20, Leading Edge Model D, DataVue portable, and Columbia portable. For the PC, two different versions are available: one linked with an 8087 math coprocessor, the other not requiring the math chip. Runtime for a one-wavelength data set is 1.25 min with the 8087 and 5.58 min without on a Leading Edge Model D. The program is supplied either on 5.25-in. floppy disks or 3.5-in. floppy disks compatible with the new series of IBM computers.

EXCALIBR has also been ported to the Macintosh series of computers, modified, and compiled using Microsoft FORTRAN77 version 2.2. It has been tested on a 512k, Mac+ and SE. Runtime for a one-wavelength data set on a Mac+ was 1.75 min. The program is supplied on a single-sided 400k disk that will work in either the 512k, Mac+, or SE.

All versions of the program run in batch mode. The input data file is created with an editor or a word processor that creates ASCII files without imbedding any control characters. For the IBM version the output can either be saved to a file, viewed on the screen as the calculations are performed, or printed while the calculations are performed. For the Macintosh version the output is directed to a user-supplied file. At program completion, the result file can be viewed, printed, or discarded.

[3] Any version of the program, along with test data sets and a user's manual is available for $100. Those interested should contact M. E. Gunter.

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REFERENCES CITED

Armbruster, T., and Bloss, F.D. (1982) Orientation and effects of channel H_2O and CO_2 in cordierite. American Mineralogist, 67, 284–291.

Bloss, F.D. (1978) The spindle-stage: A turning point for optical crystallography. American Mineralogist, 63, 433–447.

——— (1981) The spindle stage: Principles and practices, 340 p. Cambridge University Press, Cambridge and New York.

Bloss, F.D., and Riess, D. (1973) Computer determination of $2V$ and indicatrix orientation from extinction data. American Mineralogist, 58, 1052–1061.

Greiner, D.J., and Bloss, F.D. (1987) Amblygonite-montebrasite optics: Response to (OH^-) orientation and rapid estimation of F from $2V$. American Mineralogist, 72, 617–624.

Gunter, M.E., and Bloss, F.D. (1982) Andalusite-kanonaite: Lattice and optical parameters. American Mineralogist, 67, 1068–1087.

Louisnathan, S.J., Bloss, F.D., and Korda, E.J. (1978) Measurement of refractive indices and their dispersion. American Mineralogist, 63, 394–400.

Su, S.C., Bloss, F.D., Ribbe, P.H., and Stewart, D.B. (1984) Optical axial angle, a precise measure of Al,Si ordering in T_1 tetrahedral site of K-rich alkali feldspars. American Mineralogist, 69, 440–448.

Su, S.C., Ribbe, P.H., and Bloss, F.D. (1986a) Alkali feldspars: Structural state determined from composition and optical angle $2V$. American Mineralogist, 71, 1285–1296.

Su, S.C., Ribbe, P.H., Bloss, F.D., and Goldsmith, J.R. (1986b) Optical properties of single crystals in the order-disorder series low albite–high albite. American Mineralogist, 71, 1384–1392.

Su, S.C., Ribbe, P.H., Bloss, F.D., and Warner, J.K. (1986c) Optical properties of a high albite (analbite)–high sanidine solid-solution series. American Mineralogist, 71, 1393–1398.

Su, S.C., Bloss, F.D., and Gunter, M.E. (1987) Procedures and computer programs to refine the double-variation method. American Mineralogist, 72, 1011–1013.

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