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OrientXplot: a program to analyse and display relative crystal orientations

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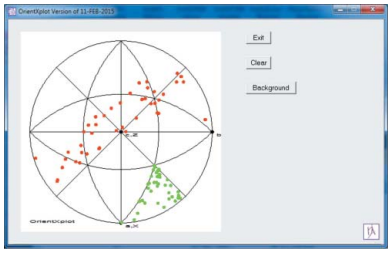
Orientations of single crystals are usually determined by diffraction experiments. Indexing of a diffraction pattern from one crystal leads to the determination of its 'orientation matrix', which defines the orientation of its crystallographic axes relative to a set of reference axes associated with the diffractometer. Crystal orientations can also be described in terms of Euler angles, especially from electron backscattered diffraction measurements. *OrientXplot* is a Windows program that reads all common types of orientation matrices, as well as orientation data such as Euler angles. The program calculates and displays the relative orientations of pairs of crystals, such as twins or inclusion crystals trapped inside host crystals. *OrientXplot* can manipulate (under user control) the orientation matrices to allow for ambiguities in indexing that arise from crystal symmetries. Orientation data can be displayed on a stereogram or output in numerical form for plotting in external programs.

1. Introduction

The relative orientations of inclusion crystals within a second host crystal provide one of the few pieces of evidence about growth conditions in natural materials such as rocks, for which the pressures, temperatures and mechanisms of crystal growth are either completely unknown or poorly constrained and can never be reproduced experimentally on a laboratory time-scale. Claims of the occurrence of preferred orientation of olivine inclusions trapped within diamonds during their growth deep within the Earth, for example, have been used as evidence for the simultaneous growth of diamonds and their entrapped inclusions [*e.g.* see reviews in the book by Hazen *et al.* (2013)]. If true, geochemical analysis of the inclusions would then yield constraints on the chemical conditions at the time of diamond growth, and isotopic dating of inclusions would reveal the ages of the diamonds. If not, as suggested by Nestola *et al.* (2014), then results obtained from inclusions would not provide constraints on the formation conditions of the diamonds, but only on the formation of the original inclusion minerals that were later entrapped by diamonds during growth. Similar arguments have been applied to the multiphase inclusions found trapped inside minerals in rocks originally formed as fluid inclusions at ultra-high pressures. The crystallographic preferred orientation of some inclusion minerals with respect to others allows the crystallization sequence of the inclusion to be deduced and thus further constraints to be placed upon the pressure–temperature history of the rock as a whole (Malaspina *et al.*, 2015).

To properly answer such geological questions, both a systematic and comprehensive study of inclusion orientations and the tools for handling such orientation data are required.



Many software tools certainly exist for 'polycrystalline' materials consisting of many grains, aimed variously at determining the statistics of grain orientations, known as crystallographic texture analysis (*e.g.* Matthies *et al.*, 1988), or the correlations between the orientations of adjacent grains for the purpose of understanding grain-boundary structure. Software tools for determining the orientations of thin films on substrates, or the limited number of domain orientations that arise in ferroic materials as a result of transitions from the *para* state, are also widespread and often directly incorporated into the software that controls measurement instruments such as texture goniometers. These are all tools that operate primarily on data from one measurement of one specimen. In a review of the literature we were unable to find software capable of handling observations from large numbers of independent samples, from different types of measurements (*e.g.* X-ray single-crystal diffraction and electron backscattered diffraction, EBSD), with each 'observation' consisting of a measurement of the orientations of a small number of individual crystals. This paper briefly describes the methodology needed to handle such data and its implementation in a new Windows program called *OrientXplot* that we have developed and made freely available. Although the program was originally written to analyse the orientations of single-crystal inclusions trapped by diamonds at the time of their growth, it can generally be applied to analyse and display in stereograms the relative orientations of limited sets of single crystals, including those deposited on substrates, twinned crystals and domains arising from structural phase transitions. As such, we hope that the program also has utility as a pedagogic tool.

The description of the *OrientXplot* program in this paper is written in terms of 'host' and 'guest' crystals. The host crystal is the one to which the orientations of the guest crystals are referenced. In the case of single-crystal inclusions in a host crystal, the guest crystals are the inclusions. For thin films deposited on a substrate, one can treat the substrate as the host and the film as the guest. If systems such as twinned crystals are studied, one should equate the host crystal with the parent crystal and the guests with the twinned orientations. Of course, the choice of which of a pair of crystals is the host and which is the guest does not change their relative crystallographic orientation. The 'host–guest' terminology is used solely to simplify the description of the *OrientXplot* program and to make user interaction with the program much simpler by restricting each guest crystal to have only one host crystal; any host crystal can contain, or be related to, many guest crystals.

2. Methods

In this section we first (§§2.1–2.3) describe the steps necessary to proceed from the measurement and indexing of diffraction patterns of host and guest crystals to the determination of their relative orientations and how we implement these procedures in the *OrientXplot* program. Subsequently we discuss how *OrientXplot* manipulates the orientation relationships to remove the ambiguities in these orientations that arise from the symmetries of the two crystals (§2.4).

2.1. Orientations from single-crystal diffraction

In a traditional single-crystal diffractometer measurement the orientations of the host crystal and the guest crystal or crystals on their sample mount are determined by collecting diffraction patterns from the whole sample simultaneously. The positions of the diffraction peaks from the host and the guest (or guests) are indexed and used to determine their 'orientation matrices', which specify the orientation of each crystal (host and guests) relative to the mount holding the sample on the instrument. The orientation matrices are composed of the components of the reciprocal lattice vectors of the crystal with respect to the φ axis coordinate system of the diffractometer (Busing & Levy, 1967). The definitions of the φ axis system and the values in the orientation matrix differ from one diffractometer system to another. *OrientXplot* assumes that the data for each host–guest system come from one measurement, and therefore the orientation matrices for any host crystal and all of its guest crystals are of the same type from the same software. The orientation matrices from all major commercial single-crystal diffractometers (*e.g.* Oxford Diffraction, Rigaku, Bruker, Stoe) are read and interpreted correctly by *OrientXplot*, which calculates the unit-cell parameters directly from the input orientation matrices by the method of Busing & Levy (1967). Owing to experimental uncertainties, the resulting cell parameters do not normally exactly match those required by the symmetry of the crystal system (*e.g.* angles that should be 90° are not usually exactly this value). No 'idealization' of the unit-cell parameters is performed on the data; only the unit-cell parameters used as the basis of the plotting of the stereographic projections of the data are idealized to symmetry-constrained values.

The φ axis coordinate system (Busing & Levy, 1967) is an orthonormal coordinate system, and the angles between the reciprocal-lattice axes of two different crystals that have been measured in the same data collection can therefore be simply obtained by taking the scalar products of their reciprocal lattice vectors described on this φ axis system. Although the definition of the φ axis system differs between diffractometers, no conversion of the φ axis system is performed within *OrientXplot*, because only the relative orientations of guest crystals with respect to their hosts are calculated. Users are often interested in the orientation of the real-space axes, which are not all parallel to the reciprocal axes for the triclinic, monoclinic, trigonal and hexagonal crystal systems. On input, *OrientXplot* therefore calculates the directions of the real-space crystal axes on the φ axis system by taking vector products between pairs of the reciprocal-lattice axes and stores this information in terms of unit vectors (whose components are thus direction cosines of the real-space lattice vectors with respect to the φ axis system), which form a 3×3 matrix we call $\boldsymbol{U}^{\rm r}$.

2.2. Orientations by other methods

Other methods of orientation (*e.g.* by electron diffraction or optical goniometric measurements) will not yield orientation matrices of the Busing & Levy (1967) type. For these cases the orientations of the host and guest crystals can be input to *OrientXplot* as Cartesian rotation matrices that describe the orientation of the real-space crystallographic axes of each crystal relative to a common external reference frame. These are therefore $\boldsymbol{U}^{\rm r}$ matrices and they are not converted on input by *OrientXplot*, except that they are normalized to ensure that the matrix elements are equivalent to direction cosines. Alternatively, the program can read the Euler angles that describe the crystal orientations with respect to the instrument, as widely used for EBSD and other measurements on polycrystalline specimens, and convert them to $\boldsymbol{U}^{\rm r}$ matrices allowing for appropriate conventions of definition (*e.g.* Bunge, 1969; Matthies *et al.*, 1988). In both of these cases the unit-cell parameters of the host and guest crystals have to be specified in addition to the orientation data, in order to allow the plotting of crystallographic directions other than the crystallographic axes.

2.3. Absolute orientations

The cosines of the angles between the crystallographic axes of the host and the guest can be simply calculated as the elements of the matrix product $\boldsymbol{U}^{\rm r}_{\rm hg} = (\boldsymbol{U}^{\rm r}_{\rm host})^{-1}\boldsymbol{U}^{\rm r}_{\rm guest}$. These angles can be used to plot the directions of the guest lattice vectors on a stereogram whose orientation is that of the host lattice. For more general directions $[UVW]$ of the guest, the lattice vector is first converted to a unit vector in the orthonormal cell and then to a vector on the host cell by multiplication by $\boldsymbol{U}^{\rm r}_{\rm hg}$. An equivalent calculation in reciprocal space allows plane normals (hkl) to be calculated and plotted.

When there is more than one guest crystal associated with a host, these diagrams also clearly show the orientation relationship between the different guest crystals, as they are oriented with respect to a common host reference orientation. We term these orientations determined directly from the input matrices (and therefore the original orientation determination) 'absolute orientations'. Fig. 1(*a*) shows the absolute orientations of five olivine inclusions measured inside three different diamond crystals (three in one diamond, one each in the other two) which are a subset of the data reported by Nestola *et al.* (2014).

2.4. Relative orientations

For a comparison between the orientations of guest crystals in different hosts, it is necessary to take into account the ambiguity in indexing the diffraction patterns that arises from the symmetry of both the guest and the host crystals. Failure to allow for this ambiguity can lead to errors in interpretation of orientation data, or failure to recognize systematics in the relative orientations of two phases. In principle, the symmetry could be allowed for in the diffractometer software by re-indexing of the diffraction patterns in each of the symmetrically equivalent orientations, but such an approach would be time consuming and tedious. Instead, the 're-indexing' is performed in *OrientXplot* by applying the symmetry directly to the transformation matrix $\boldsymbol{U}^{\rm r}_{\rm hg}$ that describes the relative orientations of the host and guest crystals.

We continue to use olivine inclusions in diamonds as an example of a host–guest pair of crystals. Olivine has orthorhombic symmetry, which makes the $[100]$ direction equivalent to $[\bar{1}00]$, and $[010]$ equivalent to $[0\bar{1}0]$, *etc*. Therefore it is impossible by diffraction or any other physical measurement method to determine any difference between the $[100]$ direction and $[\bar{1}00]$. Thus an olivine described as having its '*a* axis' or $[100]$ vertically upwards could equally well be described as having this direction as '$-a$' or $[\bar{1}00]$. We therefore have to take into account this symmetry-allowed ambi-

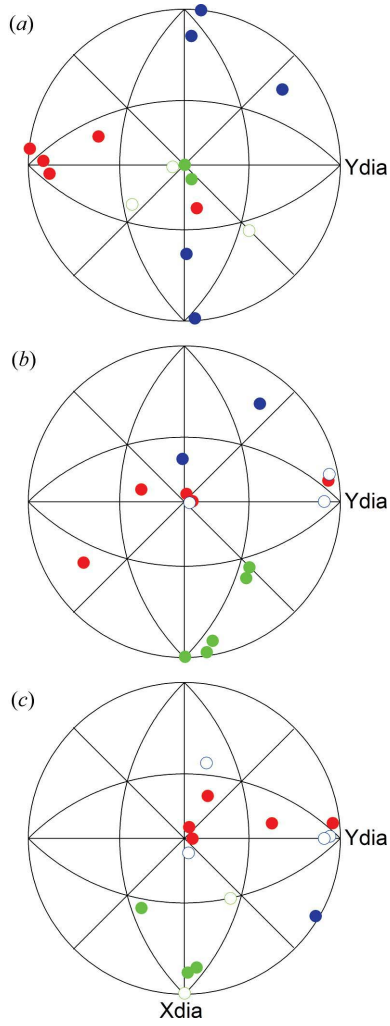


Figure 1
Differences in types of orientation choices for five natural olivine single-crystal inclusions in three diamond host crystals [a subset of the data of Nestola *et al.* (2014)]. (*a*) The absolute orientations of the olivines relative to their diamond host crystals, as determined directly from the measured orientation matrices. (*b*) The relative orientations chosen with the *b* axis of the inclusion in the asymmetric unit of the host and the *a* axis in the upper hemisphere. (*c*) The relative orientations chosen with the *b* axis of the inclusion closest to the *a* axis of the host, with the inclusion *a* axis in the upper hemisphere. Colour coding is red/green/blue for the *a*, *b* and *c* axes of the olivines.

guity. Although the crystallographic point symmetry of olivine that defines these equivalent orientations is *mmm*, the indexing of a diffraction pattern should always result in a right-handed description of the unit-cell axes of the crystal. This handedness has to be maintained, so the ambiguity in the indexing is described instead by the subgroup of *mmm* that does not include any inversion symmetry (including mirrors), that is point group 222. For any one olivine on its own, this point group indicates that there are four indistinguishable orientations of a right-handed unit cell, related to one another by 180° rotations of the unit cell around the lattice vectors. A similar ambiguity is present in the orientation of diamond. However, its crystallographic point group symmetry is *m*3*m*. The operators that describe symmetrically equivalent orientations without inverting the handedness of the lattice vectors thus correspond to the point group 432.

To determine the orientations of all olivines relative to their host diamonds, we eliminate the ambiguity in indexing due to symmetry by the following process. We first rotate the relative orientation matrix of each olivine inclusion, $\boldsymbol{U}^{\rm r}_{\rm hg}$, by the elements of point group 432 oriented to coincide with the unit-cell axes of the diamond host. This produces 24 possible orientations of the olivine with respect to its host, all of which are symmetrically equivalent and physically indistinguishable by any method. From each of these 24 relative orientations, each described by a $\boldsymbol{U}^{\rm r}_{\rm hg}$ matrix, we generate the four orientations that are symmetrically equivalent orientations of the olivine because of its symmetry. This generates a possible 24 × 4 = 96 symmetrically equivalent descriptions of the orientation relationship between the orthorhombic olivine inclusion and its cubic host. The separate effects of the host and inclusion (guest) symmetry can be visualized in *OrientXplot* by specific commands that allow the user to apply the symmetry of the host or guest crystal alone to the relative orientation data. The number of equivalent orientation descriptions of course depends on the point or Laue symmetries of the two crystals.

Now we have to choose one of these symmetrically equivalent descriptions of the orientation relationship between the host and inclusion. *OrientXplot* provides two ways of selecting one characteristic orientation for each host–guest pair. The first is to select the orientation that puts a specific guest direction, termed the primary axis, within the asymmetric unit of the host with a specific secondary axis of the guest crystal closest to the *z* axis of the stereogram (which is, except for monoclinic hosts, the *c* axis of the host). For our example of olivine inclusions in diamond this option clearly demonstrates (Fig. 1*b*) that there is no special preferred orientation of these olivine guests in multiple diamonds (Nestola *et al.*, 2014). The second possibility is to select the orientation that places the primary axis of the inclusion closest to a selected direction of the host (Fig. 1*c*). If more than one orientation has the same angle between the primary axis of the inclusion and the selected host direction, the orientation with its secondary inclusion axis closest to another user-specified host direction is selected. Fig. 1(*c*) shows the same olivine data also plotted in this way. Such criteria always define one, no more and no less, of the possible equivalent orientations. Other orientation choices are also possible, provided that they are 'symmetrically reasonable and consistent'; that means that they must always yield one unique orientation out of the possible symmetry-equivalent descriptions of the relative orientation. It is important to note that, because the possible descriptions of the relative orientation of the guest and the host crystals are symmetrically equivalent, the choice of which one to display (provided it is valid) does not affect the conclusions that are drawn from the resulting stereographic projections. If one choice indicates a strong orientation relationship, then all choices will do so. If, as shown in Fig. 1, there is no preferred orientation, then this will be evident in all plots of all valid choices of orientation pairs.

3. *OrientXplot* program

The *OrientXplot* program is written in standard Fortran95 using the open-source Crystallographic Fortran Modules Library CrysFML (Rodriguez-Carvajal & Gonzalez-Platas, 2003) for data and symmetry manipulation and the GINO graphics library from Bradley Associates (http://www.gino-graphics.com) for the graphical user interface.

The program is a command-line console program with an integrated graphics window composed of three elements (Fig. 2): a graphics window in which stereograms are plotted, a

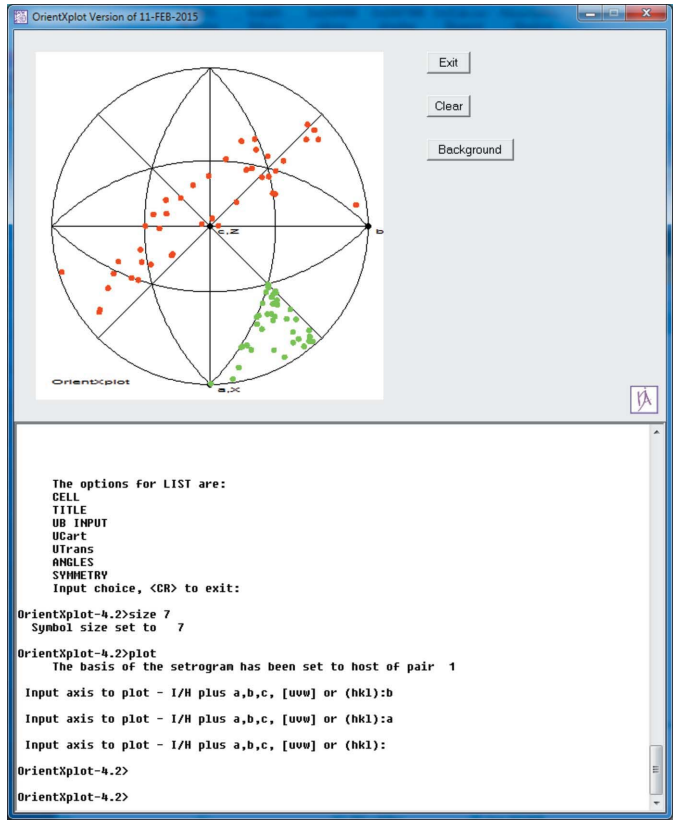


Figure 2
A screenshot of the user interface of *OrientXplot*, showing the plotting window (top) and the integrated command-line console (bottom). The data are the relative orientations of olivines in diamonds (Nestola *et al.*, 2014), chosen with the *b* axis of the inclusion in the asymmetric unit, with the inclusion *a* axis in the upper hemisphere.

limited number of buttons for direct control of the graphics window, and a console window where commands can be typed in and where non-graphical output from the program is displayed. The command line interface is structured in the same way as the *EosFit7c* program (Angel *et al.*, 2014) with commands grouped by function:

(*a*) General commands (*e.g.* Exit, Help) and some advanced commands that allow commands and input to be logged and subsequently rerun as a macro.

(*b*) Data handling commands, including the reading of data files and listing of their contents and quantities derived from their contents such as relative orientations. There are several commands that allow subsets of the data to be used, so that data files do not have to be edited once they have been created. We find this reduces the numbers of cut-and-paste errors that would normally occur during data analysis.

(*c*) Graphics commands (*e.g.* Plot, Clear). The Plot command allows any real or reciprocal direction of the host or guest crystals to be plotted on the stereogram, relative to the corresponding host.

(*d*) Calculations including the reorientation by symmetry.

All of the console input and output can be logged to a text file, so that numerical results can be used as input to external graphics programs that can produce publication-quality graphics. The stereograms in Fig. 1 were produced in this way.

OrientXplot does not allow orientation data to be typed in directly at the console, as this is tedious and liable to result in errors. Instead a data file must be created that contains the orientation data, symmetry information and sometimes ancillary data necessary for the correct interpretation of the orientation data. The data file must be a text file and can be created with any simple editor. The data file is read in 'free format' and contains keywords to define the meaning of entries and values. Keywords can appear in any order, but they affect the interpretation of all of the data following them in the data file. Orientation data can be entered as orientation matrices copied directly from the software supplied with all major modern single-crystal diffractometer systems or can be supplied as Cartesian rotation matrices or as Euler angles. Details of the datafile format, and the conventions associated with the interpretation of orientation information, are documented fully in the users' manual of the program.

4. Availability

OrientXplot runs under most modern versions of the Windows operating system. The program is available free from http://www.rossangel.net. The distribution package includes full documentation in a users' manual and some example files. No commercial licenses are needed to install and run the program.

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