The SHAPE crystal-drawing [program] [computer] as an instrument in research

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Crystal drawing has always been the final step crowning a morphological study. Now the laborious, though deeply satisfying, hand drawing has been replaced by computer programs (e.g. Schneer, 1977; Strom, 1979; Mijata et al., 1980; Dowty, 1980, 1989). This communication does not aim to review the previous papers but to relate the author’s experience in using a program available to him for deducing real shapes from drawings, an inverse problem in morphology suited perfectly or the computer.

The traditions of Bulgarian mineralogy in studying morphology as a clue to the understanding of mineralization processes is well known (Kostov, 1977). In particular, the Department of Mineralogy at the Geological Institute of the Bulgarian Academy of Sciences has never neglected crystal shapes in its research and SHAPE of E. Dowty has attracted attention since the publication of its mathematical background (Dowty, 1980). In 1981, I. Bonev at the Department obtained one of the earliest versions and, together with A. Andreev, drew the first crystals; this version needed a large computer.
which prevented them from extending their work (Bonev, 1991, pers. comm.) In 1985, T. Kerestedjian, using the program text of E. Dowty, made a copy for a Pravetz-8 computer (Kerestedjian, 1992, pers. comm.). In 1989, thanks to the efforts of J. Mineva-Stefanova, the program was successfully used for solving a number of practical problems. Finally, in 1991 I. Bonev obtained the SHAPE 1989 IBM-PC Version 3.1 (Dowty, 1989).

During more than a dozen years of work on his program E. Dowty has made a number of important improvements widely extending its capabilities and speed. Although this communication does not aim to discuss the program's power in solving direct problems, i.e. in drawing crystals and aggregates of known (measured) form combinations (e.g. Brock, 1992), it is worth mentioning the ease and speed with which the real shapes are reproduced, including distorted forms and crystals with curved (convex) surfaces. An experienced morphologist can do all this by SHAPE using its main options RUN and RERUN CRYSTAL, TWINS and EPITAXIAL CRYSTALS, supported by ROTATIONS and a number of auxiliary options and suboptions. The interactive and often simple input results in the drawing of crystals becoming an intriguing "play" with the number of forms desired and the distances of their faces from the crystal centre (central distances).

One idea, which naturally suggests itself whilst working with SHAPE, is to approach the inverse morphological problem, i.e. to try and identify real crystal shapes with the aid of drawings. This, and the possible extension of the program to accommodate crystal cross-sections and crystal growth are the subject of this paper in which the points raised will be illustrated with a few well documented examples.

**Identifying the forms of real crystals by SHAPE**

The importance of the morphology of accessory zircon as a genetic criterion is well known and has been discussed by a number of authors, including Caruba, Turco (1971) who were concerned with the need for rapid and unambiguous indexing of the forms on numerous crystals. In the sample being examined zircon usually lies on its prism faces, \{100\} or \{110\}, and its dipyramidal terminal combinations can be identified by measuring the angles between the crystal edges as seen under the microscope. Some twenty years ago the above authors prepared a chart of all edges of the eight most common forms of zircon which rendered measurement unnecessary. Now SHAPE can do the same with the extra possibility of accurately reproducing any face development and habit of the crystal. In a recent study (Arnaudov et al., 1990), SHAPE drawings like those shown in Fig. 1 were used to morphologically characterize numerous crystals extracted from the Rhodope metamorphic rocks. After dividing them in groups of similar face development, the angles between their edges as seen under the microscope were compared by eye with those on the drawings. It required only a little practice to be able to confidently identify the crystal forms present even on crystals with rounded, poorly defined edges. In more difficult cases one may prepare SHAPE drawings on transparent paper and superimpose them onto microphotographs of the crystals to discover the form combination, a procedure similar to that proposed by Caruba, Turco (1971). Another advantage of SHAPE is its SCALING option which enables the size of the drawing to be matched to the size of the photographed crystal; this may be useful for checking shapes in published
works, e.g., zircon photographs in the paper of Puziewicz, Radkowski (1990). It is obvious that SHAPE drawings can be used for the morphological characterization of other mineral species found as well formed crystals in heavy concentrates or similar samples.

The above example is a specialized case of the more difficult problem of identifying crystal forms from photographs showing the crystals in tortuous orientations. This problem arose mainly after the SEM made it possible to obtain good photographs of very small crystals defying direct goniometry; it was solved by procedures commonly used in aerial photogrammetry (Kirov, Gaitandjiev, 1968; Gobarkar, 1977) and involving measurements on stereopairs of SEM photographs which permit the calculation of the interfacial angles and thus the identification of the forms (e.g., Franke et al., 1986). SHAPE now offers a simpler procedure as a result of its ability to rapidly create various combinations, including stereopairs (Dowty, 1980). If the mineral is known, which is generally the case in SEM studies, one can assume the form combination of its crystals, draw it via SHAPE, rotate it as desired and compare the drawing with the photograph. By trial and error, changing the combinations of the forms and their central distances, a complete coincidence between the drawing and the photograph (or their stereopairs) can be quickly obtained, thus deciphering the morphology of the photographed crystal. This approach has been tried by the present author on monohydrocalcite, amongst other minerals, with good results. A unique find of well-formed crystals of that rare mineral had been recently described and illustrated with SEM photographs (Minniev and Stefaanova, Nevolkov, 1990). The largest crystals were kindly given to this author to try refection goniometry. About 0.2 mm in size, they presented a difficult task and partial success was achieved for only two of them. One was identified as a trigonal trapezohedron with rather curved, convex faces, whereas the other had only three, also curved faces obeying the three-fold symmetry, thus offering no indication as to the kind of form they may belong (rhombo-
Fig. 2. SHAPE drawings of monohydrocalcite crystals to be compared with the SEM photographs in the study of Mincheva- Stefanova, Neykov (1990; their Figs 2b, c, d) a — rhombohedron, trigonal prism and dipyramidal; b — trigonal trapezohedron, rhombohedron and trigonal prism; c — the same as b but the trapezohedron is less steep and a minor trigonal dipyramid is present.

Фиг. 2. Чертежи с SHAPE на моноходрокалциеви кристали за сравнение със СЕМ-снимките в статията на Минчева-Стефанова, Нейков (1990; техните фиг. 2б, с, д) a — ромбоедър, тригонална призма и дипирамида тригонална призма; b — тригонален трапецоедър, ромбоедър и тригонална призма; c — като b, но трапецоедърът не е така стръмен и прилича на слабо развита тригонална бипирамида.

It should be noted that drawing distorted crystals with SHAPE is slightly more time-consuming than drawing regular ones but is a great help in a morphological study. An excellent example may be found in the paper of

Fig. 3. SHAPE drawings of distorted combinations on pyrite to verify if the crystal shown in Fig. 9 of the paper of Quezel et al. (1989) is rhombododecahedral or cuboctahedral. The crystal axes are also shown.

Фиг. 3. Чертежи с SHAPE на разтеглени форми на пирит за установяване дали кристалът, показан на фиг. 9 в статията на Quezel et al. (1989), е ромбоодокдекаедричен или кубоктаедричен. Начертани са и осите на кристала:

a — ромбоодокдекаедър, начертан така, че едната му стена да е малко по-голяма от останалите; b — кубоктаедър, на който липсва една кубична стена.
Radulova, Bonev (1993) where the morphology of a chalcopyrite needle is closely reproduced by distorted crystals run through the option EPTAXIAL CRYSTALS. An additional advantage in such cases is that the program optionally shows (option CRYSTAL AXES) the axial cross with its true axial ratio in the given projection. SEM photographs of distorted crystals can be very misleading and SHAPE provides a safeguard against mistakes. In a paper on iron sulphides in coal Quevrol et al. (1989) described rhombododecahedral pyrite (illustrated by two SEM photographs) in addition to the common cuboctahedral one. Since the \{110\} pyrite is a rare occurrence and finding it implies some rather specific conditions of formation, its identification seemed rather doubtful all the more that the SEM photographs suggested that the "rhombododecahedral" pyrites could be simply distorted cuboctahedra. This was easily confirmed by the SHAPE drawings shown in Fig. 3. The two combinations, rotated to coincide with the photographed crystal (Fig. 9 in Quevrol et al., 1989), show conspicuous differences when drawn, and careful comparison with the photograph demonstrated that the latter is actually a cuboctahedron and not the exotic rhombododecahedron.

Drawing crystal sections by SHAPE

Another problem well suited for SHAPE is to deduce crystal forms from cross-sections as observed in polished or thin sections. The solution again consists in drawing and rotating test crystals; in this case, however, coincidence is sought between the outlines of the observed section and those of a plotted crystal cut in two by the plane parallel to the screen (paper). Although SHAPE has no special option for producing crystal sections it supplies all the data needed to perform the task. Firstly we create the desired crystal entering the lowest symmetry 1 in order to be able at a later stage to enter as a crystal face the single plane parallel to the screen (in the same way the faces of distorted crystals are entered one by one instead of symmetry-related groups which reflects the lowering of the real symmetry as the result of distortion). Then, after rotating the plot as desired; we call the option PRINT-OUT, suboption "short printout", to obtain the cartesian coordinates of the ends of the crystal axes in their originally entered lengths as projected on the observer's coordinate system in which $y$ and $z$ lie in the screen and $x$ points at the observer, i.e. the suboption gives the projections of the crystal axes, $A$, $B$, $C$ on $x$, $y$, $z$ for the given orientation in the form of the matrix $x_A y_A z_A / x_B y_B z_B / x_C y_C z_C$. From this the indices of the plane HKL parallel to the screen can be derived as $H:K:L = x_A : x_B : x_C$. In general, the ratios are irrational so that we enter them in option RERUN CRYSTAL as the nearest two-digit integers giving the plane a very small central distance, e.g. 0.01. Plotting the new crystal and rotating it with HKL parallel to screen we get a close approximation of how the crystal would look in the given orientation if cut by half, i.e. we have reproduced a polished section. If we enter $\bar{H} \bar{K} \bar{L}$ in addition to $HKL$ giving it a similar small central distance we will reproduce a thin section. The above procedure is illustrated in Fig. 4 using the pyrite crystals shown in Fig. 3.
Growing crystals by SHAPE

Although the computer simulation of crystal growth was identified as a problem at the start of work on crystal-drawing programs (Schenker, 1977; Dowy, 1980), the author is unaware of any serious attempt at a systematic use of programs for growing crystal shapes. Yet this may be helpful in the study of zoned crystals (i.e. for understanding the internal morphology or anatomy of crystals) where the succession of forms, revealed by the microscope or the microprobe, records important events during the growth of the crystal. SHAPE is capable of plotting such successions with its options DOT-MATRIX/ LASER PLOT and PEN PLOT. An arsenopyrite crystal is produced here to illustrate the point.

Fig. 5. is based on two recent studies of arsenopyrite zoning as a function of composition (Kereskedjian, Minceva-Stepanova, 1988; Vesselino et al., 1990). They used BSE imagery to observe the zoning in an oriented (001) polished section of a crystal termination bounded by {101}, {210} and {010} (orthorhombic approximation). The geometry of 20 zones involving the {210} and {010} growth sectors has provided important clues to the growth history. In Fig. 5 the zones as seen in the polished section are reproduced by SHAPE. Each zone was drawn as a separate crystal, cut in
Fig. 5. SHAPE simulation of the growth of an arsenopyrite crystal bounded by \{101\}, \{210\} and \{010\}. 20 successive shapes (zones) are shown in the (001) cut as seen in the BSE image of a polished section described by Kerestelian, Mincheva-Stefanova (1988) and in Vesselinov et al., (1990). The boundaries between the (010) and (210)/(210) growth sectors are drawn by hand.

Half by the (001) and rotated with the (001) parallel to screen, then plotted on transparent paper to be superimposed onto the BSE-image enlarged photograph and compared with the respective zone. After reaching satisfactory coincidence, the plot was compressed into a window with options DOT-MATRIX or PEN PLOT and sent to the plotter to draw it in the chosen page area along with the other zones. It is clear that the ratios of the \{010\} and \{210\} central distances, used successively to reproduce the zoning, simulate the changing growth-rate ratio of the respective sectors.

The computer also offers the opportunity for graphically testing hypotheses concerning the relative growth rates of the simple forms of a crystal. Using SHAPE, similar to the procedure described above, one can enter numerical values taken from hypothetical growth-rate curves using them as central
distances to see the resulting form successions. This problem was considered during the above-mentioned study on arsenopyrite (Vesselinov et al., 1990), including the intriguing question of following up shape variations during a period of oscillatory zoning as treated in the theory of Allègre et al. (1981). The matter was not pursued however and the problem is only formulated here. One of the reasons for this is that entering so many values, i.e. drawing a growing crystal as a series of separate shapes, is rather time-consuming and tedious. One possible solution is to extend SHAPE in a way that will allow the operator to enter functions as central distances instead of numbers, and then to plot the resulting succession of forms.

Conclusion

The few examples discussed in this paper are an attempt to show how SHAPE can be used to solve, in a new manner, a number of old inverse problems in crystal morphology. The subject, however, is by no means exhausted and the constant improvements in software that the author of SHAPE is making are major contributions in this field. He has recently completed two other programs, QSHAPE and ATOMS. The former has reacted to the latest developments in the science of form and allows the drawing of quasicrystals and related shapes. The latter plots crystal structures, and, in combination with SHAPE, offers exciting opportunities in the study of the relationship between form, structure and growth conditions of crystals.

Note added after the completion of this paper

The author is pleased to relate to the interested readers that he has received an announcement of the newest commercially available versions of SHAPE (Dowty, 1992, pers. comm.) one of which, SHAPE IBM-PC V4.0, has a professional edition allowing to draw crystal forms in section and to model crystal growth. As already discussed in this paper, these are major improvements further extending the field in which SHAPE users may rely on the program as an instrument of research.

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References


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