

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

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В е с е л и н о в, И. 1994. Компютърната програма за чертане на кристали SHAPE като изследователско средство. — *Геохим., минерал. и петрол.*, 29, 97—105.

Компютърното чертане на кристали, заместило трудното ръчно чертане, разширява много възможностите за решаване на обратни морфоложки задачи. С програмата SHAPE на E. Dowty са дадени примери на нови решения на някои стари задачи и се предлагат други, разширяващи приложението на програмата в изследователската работа. С чертежи с SHAPE бързо и точно се характеризира морфологията на добре остенени микроскопични кристали (пример циркон); идентифицират се формите на кристали в произволни ориентации върху СЕМ снимки (пример монохидрокалцит), като при трудни случаи може да се използват стереодвойки; избягва се погрешно идентифициране при разтеглени кристали (пример пирит). Възпроизвеждат се случайни прерези в аншлифи и дюншлифи (пример пирит). Възможно е и симулиране на кристален растеж, илюстрирано с един зонален арсенопиритов кристал. В съчетание с програмата за чертане на кристални структури ATOMS от същия автор SHAPE разкрива богати възможности в изучаването на връзката между форма, структура и условия на растеж при кристалите.

Ключови думи: кристали, компютърно чертане, циркон, монохидрокалцит, пирит, арсенопирит

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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 Now the laborious, though deeply satisfying, hand drawing has been replaced by computer programs (e. g. S c h n e e r, 1977; S t r o m, 1979; M i y a t a et al., 1980; D o w t y, 1980, 1989).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 (K o s t o v, 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 (D o w t y, 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 (B o n e v, 1991, pers. comm.) In 1985, T. Kerestedjian, using the program text of E. Dowty, made a copy for a Pravetz-8 computer (K e r e s t e d j i a n, 1992, pers. comm.). In 1989, thanks to the efforts of J. Minčeva-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 (D o w t y, 1989).

During more than 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. B r o c k, 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 accomodate 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 C a r u b a, T u r c o (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 dipyrimal 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 (A r n a u d o v 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 C a r u b a, T u r c o (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, Radkowska (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 fortuitous 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; Ghobarkar, 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 (Minčeva-Stefanova, Neykov, 1990). The largest crystals were kindly given to this author to try reflection 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-

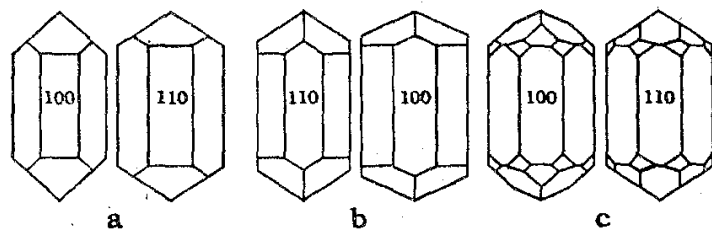


Fig. 1. SHAPE drawings of zircon crystals used to morphologically characterize specimens from the Rhodope metamorphic rocks (Arnauđov et al., 1990). Indexing follows the structural setting, $c_0/a_0=0.905$. Three pairs of combinations are shown in alternative orientations to demonstrate the differences in the crystal terminals which permit rapid and unambiguous identification of forms on natural crystals (cf. with the procedure proposed by Caruba, Turco, 1971)

a — the combination $\{100\}$, $\{110\}$, $\{101\}$ lying on a $\{100\}$ face compared to $\{100\}$, $\{110\}$, $\{112\}$ lying on a $\{110\}$ face; *b* — a $\{100\}$, $\{110\}$, $\{101\}$ crystal lying on a $\{110\}$ face compared to $\{100\}$, $\{110\}$, $\{112\}$ one lying on a $\{100\}$ face; *c* — $\{100\}$, $\{110\}$, $\{101\}$, $\{112\}$, $\{211\}$ lying on a $\{100\}$ face compared to the same combination lying on a $\{110\}$ face

Фиг. 1. Чертежи с SHAPE на цирконови кристали, използвани за морфоложко характеризирани за морфоложко характеризирани на циркони от метаморфните скали в Родопите (Arnauđov et al., 1990). Индексирането е по структурната ориентировка, $c_{00}/a_0=0.905$. Показани са три комбинации в две ориентировки, за да се видят разликите в терминалните ръбове, които позволяват бързо и еднозначно идентифициране на формите върху природни кристали (срв. с метода, предложен от Сагуба, Турсо, 1971)

a — комбинацията $\{100\}$, $\{110\}$, $\{101\}$, легнала върху $\{100\}$, сравнена с $\{100\}$, $\{110\}$, $\{112\}$, легнала върху $\{110\}$; *b* — кристал с $\{100\}$, $\{110\}$, $\{101\}$ върху стена на $\{110\}$, сравнен с комбинацията $\{100\}$, $\{110\}$, $\{112\}$ върху стена на $\{100\}$; *c* — $\{100\}$, $\{110\}$, $\{101\}$, $\{112\}$, $\{211\}$ върху стена на $\{100\}$, сравнена със същата комбинация, но върху стена на $\{110\}$

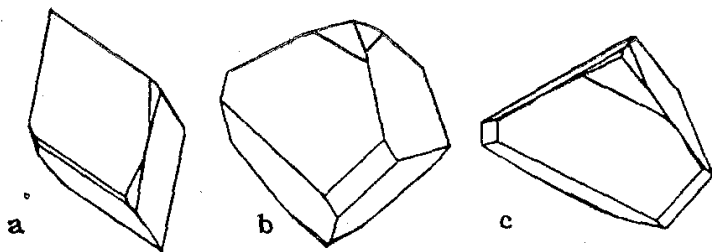


Fig. 2. SHAPE drawings of monohydrocalcite crystals to be compared with the SEM photographs in the study of Minčeva-Stefanova, Neykov (1990; their Figs 2b, c, d) *a* — rhombohedron, trigonal prism and ditrigonal prism; *b* — trigonal trapezohedron, rhombohedron and trigonal prism; *c* — the same as *b* but the trapezohedron is less steep and a minor trigonal dipyrmaid is present

Фиг. 2. Чертежи с SHAPE на монохидрокалцитови кристали за сравняване със СЕМ-снимките в статията на Минчева-Стефанова, Нейков (1990; техните фиг. 2b, c, d)

a — ромбодедър, тригонална призма и дитригонална призма; *b* — тригонален трапецодедър, ромбодедър и тригонална призма; *c* — като *b*, но трапецодедърът не е така стръмен и присъствува и слабо развита тригонална бипирамида

hedron, trigonal dipyrmaid or trigonal trapezohedron). This scanty information was used to draw test crystals of monohydrocalcite (Fig. 2) until they coincided with the photographs in the original paper (Minčeva-Stefanova, Neykov, 1990). The readers are invited to compare the latter with the drawings in Fig. 2 to convince themselves that the coincidence is satisfactory. If SEM stereopairs were available, they could have been compared with SHAPE stereopairs which is actually the correct way of using the procedure; if needed, it permits comparison between measured interfacial angles (e. g. by the method of Ghobarkar, 1977) and those in the drawing which SHAPE will produce via its INTERFACIAL ANGLES option.

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

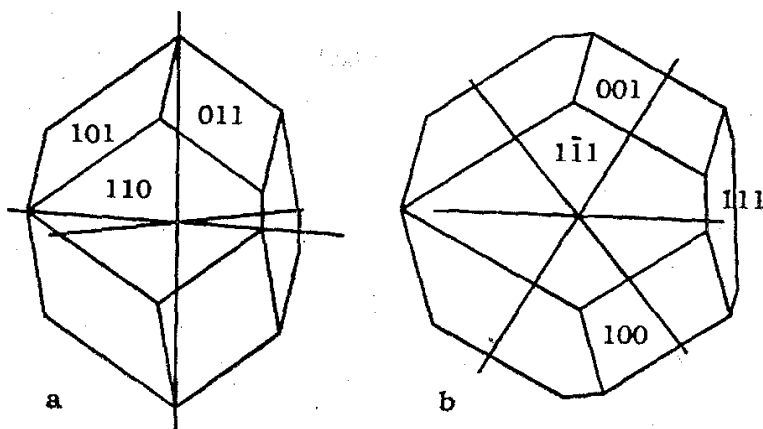


Fig. 3. SHAPE drawings of distorted combinations on pyrite to verify if the crystal shown in Fig. 9 of the paper of Querol et al. (1989) is rhombododecahedral or cuboctahedral. The crystal axes are also shown

a — a rhombododecahedron with one face slightly larger than the others; *b* — a cuboctahedron lacking one cube face

Фиг. 3. Чертежи с SHAPE на разтеглени форми на пирит за установяване дали кристалът, показан на фиг. 9 в статията на Querol et al. (1989), е ромбододедкаедричен или кубооктаедричен. Начертани са и осните кръстове

a — ромбододедкаедър, начертан така, че едната му стена да е малко по-голяма от останалите; *b* — кубооктаедър, на който липсва една кубична стена

Радлова, Бонев (1993) where the morphology of a chalcopyrite needle is closely reproduced by distorted crystals run through the option EPI-TAXIAL 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 Querol 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 Querol 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.

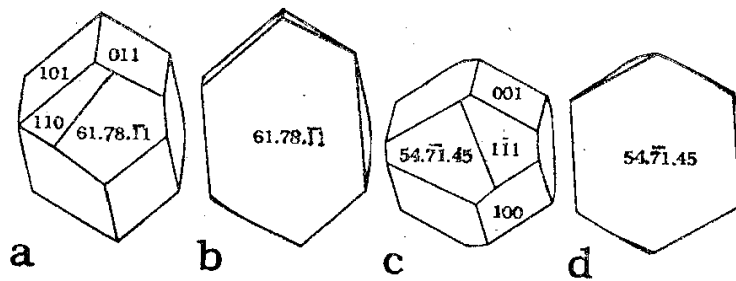


Fig. 4. SHAPE simulation of polished and thin sections. The two pyrite crystals shown in Fig. 3 in random orientations are cut by the plane approximately parallel to the screen (paper) entered as a face of rational indices. The procedure simulates random cuts as seen in polished sections. If the cutting plane is doubled by entering a second one parallel to it the drawing will reproduce a thin section

a — the crystal in Fig. 3a with the cutting plane shown relative to the normal faces; *b* — the same as *a* but the cutting plane is given a very small central distance to cut the crystal in half; *c* and *d* — the two stages of halving the crystal in Fig. 3b

Фиг. 4. Чертане с SHAPE на кристални прерези. Двама пиритови кристала, показани на фиг. 3 в случайна ориентация, са пресечени с равнината, приблизително успоредна на екрана (хартията), която е въведена като стена с рационални индекси. Така могат да се възпроизведат случайни прерези, наблюдавани в аншлифи. Прерези в дюншлифи могат да се възпроизведат, като чертежът се пресече с още една равнина, успоредна на първата

a — чертежът от фиг. 3a, но със секущата равнина, показана спрямо нормалните стени; *b* — като *a*, но на секущата равнина е зададено много малко централно разстояние, за да разполови кристала; *c* и *d* — същите два етапа на разполовяване на кристала от фиг. 3b.

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 (S c h n e e r, 1977; D o w t y, 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 (K e r e s t e d j i a n, M i n č e v a - S t e f a n o v a, 1988; V e s s e l i n o v e t a l., 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

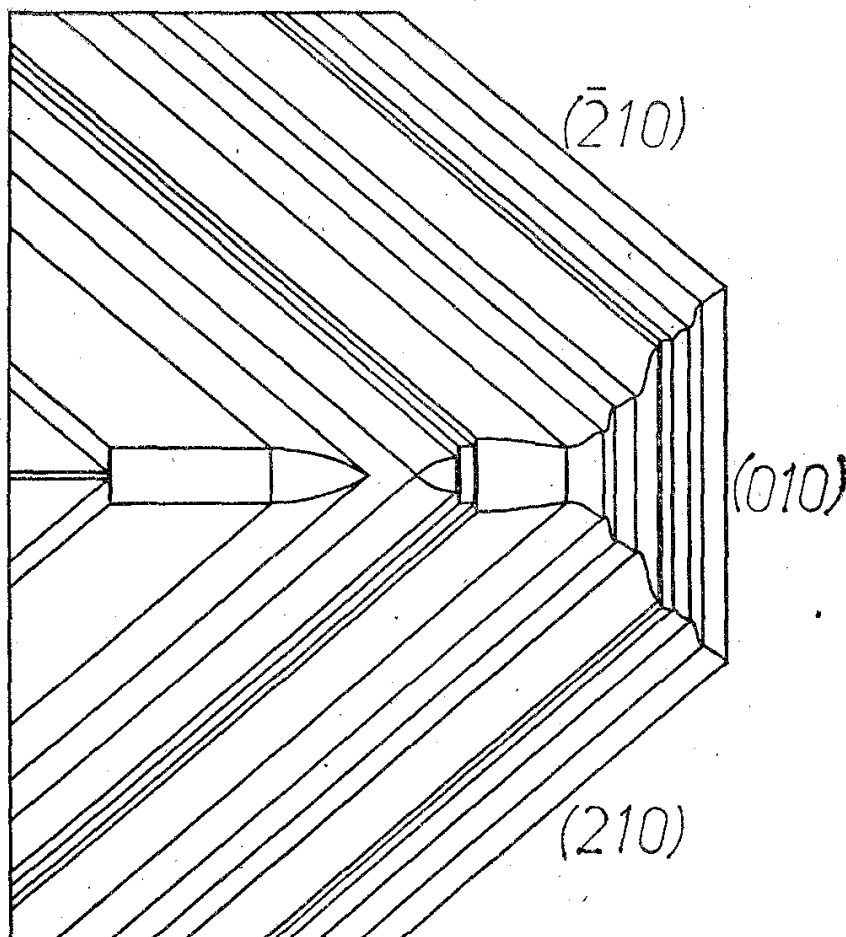


Fig. 5. SHAPE simulation of the growth of an arsenopyrite crystal bounded by $\{101\}$, $\{210\}$ and $\{010\}$. 20 successive shapes (zones) are shown in the (001) cut as seen in the BSE image of a polished section described by Kerestedjian, Minčeva-Stefanova (1988) and in Vesselinov et al., (1990). The boundaries between the (010) and (210)/ $\bar{2}10$ growth sectors are drawn by hand

Фиг. 5. Възпроизвеждане с SHAPE на растежа на един арсенопиритов кристал, остенен от $\{101\}$, $\{210\}$ и $\{010\}$. Показани са 20 последователни форми (зони) в сечението (001) така, както се виждат на снимката в обратни електрони в работата на Kerestedjian, Minčeva-Stefanova, (1988), както и на Vesselinov et al. (1990). Границите между секторите на растеж на (010) и на (210)/ $\bar{2}10$ са изчертани на ръка

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 Allégre 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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