

# MILLER INDICES AND SYMMETRY CONTENT: A DEMONSTRATION USING *SHAPE*, A COMPUTER PROGRAM FOR DRAWING CRYSTALS

**Michael A. Velbel**

Department of Geological Sciences  
206 Natural Science Building  
Michigan State University  
East Lansing, MI 48824-1115  
velbel@pilot.msu.edu

The purpose of this exercise is to use *SHAPE*: A COMPUTER PROGRAM FOR DRAWING CRYSTALS to help you visualize the relationship between the morphology of crystals, Miller indices, axial ratios, crystal faces, open and closed forms to the symmetry content of the crystal.

Instructions on how to create and modify crystal drawings, and how to customize the display, are included at the end of this exercise; that part of the handout is referred to as the "general instruction" handout. Use it as a reference for the specifics of how to use *SHAPE* for this lab. These instructions are written for older (MS-DOS) versions of *SHAPE*. The menu structure in Windows versions is similar. If you can't figure out how to enter some command, ask the instructor for help.

**In this exercise, you will generate various crystal drawings, copy them from the screen (using colored pencils), and answer questions about intercepts, Miller indices, symmetry, etc., illustrated by each example. The questions you must answer are printed in bold face. Hand in your drawings, and the answers to the questions, at the end of the lab period, keyed to the filename assigned to each drawing below.**

**A. TETRAGONAL ( $a:c = 1:2$ ) {111}:** First, we will look at how faces with different Miller indices appear in the same crystal class (remember, the crystal class embodies both the coordinate axes and the symmetry content). We will begin with a simple tetragonal crystal. To set this up, go to the general instruction handout, and follow the instructions for creating a new drawing:

1. When prompted for a title, give it any title you want.
2. We will use crystal class 4/m2/m2/m for our first few illustrations. Does *SHAPE* accept this, or does it accept a shorthand form? Check the table in the general instruction handout, or in your text, for any necessary equivalencies.
3. Because you entered a crystal class from the tetragonal group ( $a_1 = a_2 \neq c$ ) in the previous step, *SHAPE* knows that it needs only two more numbers;  $a$  (because  $a_1 = a_2$ ), and  $c$  (which is normally not equal to  $a$ ). When prompted for the  $a:c$  axial ratio, enter 1 2 (for 1:2; be sure to leave a space in between). The unit cell length along the z-direction will be twice that along x & y; that is,  $a:c = 1:2$ .
4. You want to generate {111}. Enter the appropriate numerical values of the Miller index now; finish by entering 1 for the central distance.
5. Continue following the general instructions to finish the calculations and put the display on

the screen.

6. If everything has gone well, a tetragonal dipyramid will now appear on the screen.
7. To see how the axial intercepts for  $\{111\}$  look in  $4/m2/m2/m$ ,  $a:c = 1:2$ , follow the instructions on the general handout for displaying the axes.
8. If you would like to see what the "hidden" faces at the back of the crystal look like, instruct SHAPE to show the back edges.
9. Recalculate and redisplay.
10. **The  $\{111\}$  tetragonal dipyramid should reappear, with axes shown, scaled so that each face intersects each axis at unit length. (IMPORTANT NOTE: The relative lengths of the axes on the screen are proportional to the axial ratio. The unit length  $[c]$  in the  $z$ -direction is in the present case larger than the unit lengths in the  $x$ - or  $y$ -directions  $[a_1]$  &  $[a_2]$ , respectively.) On a piece of paper, carefully draw this display. What are the intercepts of the  $(111)$  face (top right front) on each of the three axes? How are these intercepts related to the Miller index for the face?**
11. Save this file as filename = tetra111.

**B. TETRAGONAL ( $a:c = 1:2$ )  $\{112\}$ :** Next, let's look at what  $\{112\}$  looks like, in the same crystal class and with the same axial ratios as in part A. **Assuming that  $\{112\}$  intersects the  $x$  and  $y$  axes at one unit length, where does it intersect the  $z$  axis? How does this change alter the shape of the resulting crystal?**

1. To generate  $\{112\}$  with the same symmetry and axial ratios, follow the general instructions for modifying an existing drawing. If we just want to change the Miller index of the form we're trying to visualize (in other words, if we want to see a different form), we need only change the Miller index. Do so as in the general instructions for revising the main crystal.
2. **If everything has gone well, an octahedron (actually, an equidimensional tetragonal dipyramid) will now appear on the screen. On a piece of paper, carefully draw this display. What are the intercepts of the  $(112)$  face (top right front) on each of the three axes? How are these intercepts related to the Miller index for the face?**
3. Save this file as filename = tetra112.

**C.I. TETRAGONAL, PSEUDOISOMETRIC ( $a:c = 1:1$ )  $\{111\}$ :** Now, let's see what the same forms  $\{111\}$  look like, in the *same* crystal class (i.e., with the same symmetry), but with *different* axial ratios than in parts A & B. Last time, we used  $a:c = 1:2$ . This time, the unit cell length along the  $z$ -direction will be the same as that along  $x$  &  $y$ ; that is,  $a:c = 1:1$ . We set the axial lengths to be equal in our example for easy visualization only.

1. Make a new crystal from scratch as in part A of this handout (tetragonal  $4/m2/m2/m$ ), repeating all numbered steps as in part I of the general instructions handout, except that, for the  $a:c$  axial ratio, enter 1 (space) 1 (for 1:1). (OR, read existing file tetra111, which you created earlier, and revise the cell parameters.)
2. Observe the axial intercepts. **(IMPORTANT NOTE: The relative lengths of the axes on the screen are proportional to the axial ratio. The unit length  $[c]$  in the  $z$ -direction is now equal to the unit lengths in the  $x$ - or  $y$ -directions  $[a_1]$  &  $[a_2]$ , respectively.) On a piece of paper, carefully draw this display. What are the intercepts of the  $(111)$  face (top right front) on each of the three axes? How are these intercepts related to the Miller**

**index for the face?**

3. Save the file as filename = psiso111.

Note; we have identified the symmetry content, and established the relative lengths of the coordinate axes. You may note that we have entered  $a_1 = a_2 = c$ ; usually in the tetragonal crystal class,  $c$  does not equal  $a$ . Thus, we have set up a situation in which the axial lengths are actually all the same (normally a characteristic of the isometric crystal system), but the symmetry content is lower than that for the isometric crystal system; the symmetry content we have set up is tetragonal ( $4/m2/m2/m$ ). Our example is thus *tetragonal (pseudo-isometric)*. Special cases like this, with special values for some axial length (e.g., length equal to other axes when it is normally not) and/or interaxial angle (e.g., a perpendicular interaxial angle that is normally not, such as beta in the monoclinic system), although not common, do exist among minerals. Again, we have set ours up this way only for ease of visualization.

4. For part C.II. only, we will need to rescale the axes. To do this from the display, see the appropriate part of the general instruction sheet. Try entering 0.67 as the multiplier; the actual value that works for your computer may depend on the graphics card, monitor, &c.

#### **C. II. TETRAGONAL, PSEUDOISOMETRIC ( $a:c = 1:1$ ) {112}:**

1. Maintain the symmetry and axial ratios from part C.I.
2. Change the form from {111} to {112}.
3. **On a piece of paper, carefully draw this display. What are the intercepts of the (112) face (top right front) on each of the three axes? How are these intercepts related to the Miller index for the face?**
4. Save the file as filename = psiso112.
5. **Of the four crystal drawings you just created, which two look identical? Why? Can the same crystal shape result from different axial ratios in the same crystal class? What conditions must be satisfied for this to occur?** (Use the "read crystal" option (B on MAIN MENU) to retrieve and re-examine your earlier drawings).
6. For part D, we must rescale the axes back to 1.0. See the paragraph on "rescaling crystal axes" in the general instruction handout, entering 1.0 as the multiplier in menu [N.6], scale option (2).

**D. ISOMETRIC:** Next, we will investigate how the symmetry content of the crystal class influences the number of faces in a form. We will continue to examine forms {111} and {112}, but this time we will do so in the (true, not pseudo-) isometric crystal class  $4/m\bar{3}2/m$ . **(Does this crystal class have a shorthand form? What is it?)**

1. ISOMETRIC {111}: Make a new crystal, or revise the existing one; enter the appropriate Hermann-Mauguin symbol for  $4/m\bar{3}2/m$ ; generate {111}.
2. **{111} should appear, with axes shown, scaled so that each face intersects each axis at unit length. What are the intercepts of the (111) face (top right front) on each of the three axes? How are these intercepts related to the Miller index for the face?**
3. Save the present example as filename = iso111.
4. **How does this crystal compare with the one you generated in step C.I (filename = psiso111) and in part B (filename = tetra112)?** (Use the "read crystal" option (B on MAIN

MENU) to retrieve and re-examine your earlier drawings).

5. Generate {112}. Examine.
6. **{112} should appear, with axes shown, scaled so that each face intersects each axis at unit length. What are the intercepts of the (112) face (topmost right front) on each of the three axes? How are these intercepts related to the Miller index for the face?**
7. Save as filename = iso112.
8. **Why does form {112} contain a different number of faces in  $4/m\bar{3}2/m$  (filename = iso112) than in  $4/m2/m2/m$  (which you generated in part C.II; filename = psiso112)?** (Hint: See Tables 2.8 [p. 66] & 2.4 [p. 39] in Klein & Hurlbut.)

**E. MONOCLINIC:** In the previous parts of this lab, we generated several crystal drawings in the tetragonal and isometric crystal classes, with form  $\{hkl\}$ . In the classes of such high symmetry, invoking the high symmetry generated as many as eight or more faces in a single form (24 in the case of isometric {112}). Now, we will examine forms in crystal classes of lower symmetry (remember, the crystal class embodies both the coordinate axes and the symmetry content).

We began with simple tetragonal and isometric crystals. Review files psiso112 and iso112. Note how the different symmetry content of the two crystal classes generates different numbers of faces from the same forms. **How many faces are in form {112} in the tetragonal crystal class  $4/m2/m2/m$ ? How many faces are in form {112} in the isometric crystal class  $4/m\bar{3}2/m$ ?**

Many minerals (and many other crystalline substances) are monoclinic. Let's look at some of the various forms in monoclinic  $2/m$ . To set this up, refer to the general instructions .

1. Select crystal class  $2/m$  (enter just as written).
2. Because you entered a crystal class from the monoclinic group ( $a \neq b \neq c$ ,  $\beta \neq 90^\circ$ ) in the previous step, SHAPE knows that it needs numbers for all three axes. For the  $a:b:c$  axial ratio, enter 0.414 1 0.374 (for 0.414:1:0.374; separating them from one another with a space). When prompted, enter 114 degrees for beta. These are the values for gypsum (see your text). SHAPE will now ask if the values stored are the ones you actually want. Check the list. If everything is OK, just press "ENTER".
3. First, try entering just form {111}, as we did in previous exercises.
4. SHAPE will not let you draw the crystal this way. It will tell you that {111} is not a closed form. **What does this mean?** (Review your text.)
5. You want to generate {010}, {001}, and {111}. Add these forms. For each form, enter the appropriate numerical values of the Miller index now.
6. If everything has gone well, a crystal drawing will now appear on the screen.
7. To see how the axial intercepts look, follow the appropriate instructions on the instructions handout. Also, change the back edge mode as needed.
8. **The crystal drawing should reappear, but now the axes are shown. On a piece of paper, carefully draw this display.**

**IMPORTANT NOTE:** The relative lengths of the axes on the screen are proportional to the axial ratio. The unit lengths in all three directions are now different from one another, and the y-axis is no longer perpendicular to the other two. Use the arrow keys to tilt and rotate the drawing; observe the faces and axes.

9. Which faces constitute {111}? Use the "form shading" option in menu [N] to shade {111}.

10. Save this file as filename = monoc11.
11. Compare this case (monoc11) with previous examples. In the tetragonal example (tetra111; p111) previously, {111} was a dipyrmaid; in the isometric case (iso111), it was an octahedron. Both of these are closed forms. **What does this mean?** (Review your text). In 2/m, {111} is an open form; it does not enclose space fully. We need other faces. In this part of this exercise, we have further examined how the number of faces generated in {111} is different in different crystal classes. We have also seen the difference between closed forms and open forms.

Summary: Several textbooks (likely including the one you're using) state that *the number of faces in (that belong to) a form depends on the symmetry of the crystal class*. (Some texts also discuss how this can also be influenced by the orientation of the face in question with respect to symmetry axes and planes, and how the definitions of general and special forms depend upon the crystal system. We have not actually investigated general forms in most parts of this exercise, but some of the same considerations apply nevertheless.) **Write one paragraph describing how the examples you generated in this lab exemplify what the book is talking about; be specific in referring to specific examples.**

**F. STAUROLITE:** Now, we will examine the morphological crystallography of staurolite. We will use SHAPE's tilt-rotate function to inspect the symmetry content of several different crystal drawings involving different symmetry content.

1. For this next exercise, you may wish to turn off the crystal axes (toggle is in the [N.6] menu; see the general instruction handout).
2. Most textbooks state that staurolite is monoclinic; 2/m (pseudo-orthorhombic). **What is it about the crystallographic parameters shown in the book makes it pseudo-orthorhombic?** Is the crystal drawing for staurolite in your text consistent with this? (Your instructor may also provide access to comparable figures from other texts.)
3. (For this question, your instructor may also provide access to Klein & Hurlbut Fig. 13.24, esp. a and b.) **What are the names (e.g., prism, pinacoid) of the forms *m*, *b*, *c*, and *r* present in Klein & Hurlbut Figure 13.24a? (Refer back to your textbook for guidance in naming the forms. Don't use the Klein & Hurlbut chapter 2 text discussion of forms in 2/m, for reasons we'll talk about later) What are the Miller indices of the forms *m*, *b*, *c*, and *r* present in Klein & Hurlbut Figure 13.24a?**
4. Following the general instructions again, generate a crystal drawing for staurolite using the crystallography stated in the text: symmetry; unit cell lengths *a*, *b* & *c* (given in the text); and the forms you identified in the previous question.

When you enter forms (at least in the DOS version), the Miller index is the first three numbers; the fourth number is the distance from the center of the crystal to the face. Remember, the Miller index tells us about the *ratio of intercepts*; two parallel faces on the same side of the crystal will have the same *ratio* of intercepts, but will be different absolute distances from the center. You have probably noticed that we've been entering "1" for the distance all the time up until now. The first time you generate staurolite, use "1" for all distances. Examine the resulting crystal drawing.

5. Next, we will try to better simulate the drawing in Figure 13.24a. To do so, we will adjust the distances of the forms. We do this by editing the entries we've already made; see the general instruction handout for details. Start with form #1 (the first one on your list); select option 2, modify "Central distance" and enter following distances for the forms:  $m = 0.65$ ;  $b = 1.1$ ;  $c = 1.3$ ;  $r = 1.171$ . Alternatively, you could start from scratch, using the same axial ratio & symmetry, and entering the same Miller indices, but changing the last of the four digits (the distance). Use the following distances for the forms:  $m = 0.65$ ;  $b = 1.1$ ;  $c = 1.3$ ;  $r = 1.171$ . The relative overall dimensions of the crystal drawing should now better match Figure 13.24a.
6. Save this file as filename = stauromo.
7. **How does the crystal on the screen now differ from Figure 13.24a? Describe which form(s) and/or face(s) are different, and in what way?** The *size* of each face is not important; by adjusting the central distances, we have made the sizes and shapes of the faces very similar to the drawing; we could make them identical.
8. **What symmetry elements are present in your crystal drawing of staurolite, and how is each symmetry element oriented with respect to the coordinate axes? (You may wish to toggle the crystal axe back on for this) Use the tilt-rotate function (up-down & left-right arrows) to reorient the crystal drawing. (The symmetry elements are, of course, those characteristic of 2/m; review your text to help you properly orient the axes and the drawing.)** Did you save this file as stauromo?
9. Try adjusting the central differences of the different forms in order to reproduce other staurolite crystal drawings.
10. What symmetry elements are present in Figure 13.24a? What point group are these consistent with (see your text)? It may be easier to see this if we reproduce Figure 13.24a in the text on the computer using SHAPE.
11. Let us guess that the reason the figure in the book differs from the one you just created (using the crystallographic data provided in the book) is because they created the drawing using the wrong crystal class. Let's proceed with the assumption that the drawing in Figure 13.24a exhibits orthorhombic symmetry, in crystal class 2/m2/m2/m. The easiest way to do this is to just revise the existing crystal; change the crystal class from 2/m to 2/m2/m2/m (see the table in the general handout, for the "shorthand" form that SHAPE uses). Otherwise, leave everything else the same. What appears on the screen should be essentially identical to Fig. 13.24a.
12. Save this file as filename = stauroor.
13. **What symmetry elements are present in Figure 13.24a? What point group are these consistent with (see your text)? What crystal system does 2/m2/m2/m belong to? Is this what the book says about staurolite? So, in what way are the text and the Figure incompatible; what is the "mistake" in Klein & Hurlbut's treatment of staurolite crystallography? (Actually, there are two, but one is more obvious than the other.)** If it helps, compare files stauromo & stauroor, using the "read file" option from main menu item B.

Although there is little research in morphological crystallography any more, the example you are working on is one where there is a genuine scientific problem, and it is a problem in which morphological crystallography once played an important role.

Staurolite is a metamorphic mineral, that seems to be able to form under several different sets of conditions. This is known in metamorphic petrology as "the staurolite enigma". To correctly

interpret staurolite occurrences the thermodynamic properties of the mineral must be better determined; knowing the chemical energetics (thermodynamics) requires knowing the coordination environment, bonding, etc., of all elements present - in other words, the crystal structure. The earliest X-ray diffraction work on staurolite (in the 1920s) suggested that the mineral is orthorhombic. However, in the 1950s, a student in a mineralogy class at Johns Hopkins University observed that the morphological crystallography of staurolite specimens from Georgia in the teaching collection were inconsistent with orthorhombic symmetry, but were instead consistent with monoclinic. For the last 40 years, researchers have been trying to solve this problem. The most recent research (1993-4) suggests that there are both monoclinic and orthorhombic staurolites, with possibly different properties. Research continues on this petrologically important problem. Careful examination of morphological crystallography provided early major insights into this problem.

For a wonderful historical review of staurolite crystallography (1792-1983), emphasizing morphological crystallography, early X-ray crystallography, and the role of perceptive students in scientific progress, see Donnay, J.D.H., and Donnay, G. (1983), The Staurolite Story, *Tschermaks Mineralogische und Petrographische Mitteilungen*, v. 31, p. 1-15. For a comprehensive discussion of recent progress from X-ray crystallography, see the three-part series of papers by F.C. Hawthorne and his colleagues (1993) in *Canadian Mineralogist*, v. 31, The crystal chemistry of staurolite; part I (p. 551-582), part II (p. 583-595) and part III (p. 597-616).

It is instructive to measure some interfacial angles on real staurolite crystals, and compare them with the data and drawings in the textbooks.

## GENERATING CRYSTAL DRAWINGS USING SHAPE: A COMPUTER PROGRAM FOR DRAWING CRYSTALS

This handout provides general instructions for generating crystal drawings using SHAPE: A COMPUTER PROGRAM FOR DRAWING CRYSTALS. Several lab exercises will use SHAPE to help you visualize the relationship between the morphology of crystals, Miller indices, axial ratios, stereographic projections and face poles, and the relationships of crystal faces and forms to the symmetry content of the crystal.

SHAPE is menu-driven. Hit the RETURN (ENTER) key after each command. Computers already have SHAPE loaded and running. Most benches have a copy of the SHAPE manual. The manual is for reference, and may not leave the computer. If you can't figure out how to enter some command, ask the instructor for help.

These instructions are written for older (MS-DOS) versions of SHAPE. The menu structure in Windows versions is similar.

### I. HOW TO GENERATE A CRYSTAL DRAWING:

#### A. Selecting crystal class and cell parameters.

1. Enter a new crystal (option A on MAIN MENU).
2. When prompted, give it any title you want.
3. Select the crystal class. Use Hermann-Mauguin notation (as summarized in, e.g., Blackburn & Dennen Table 2.4). Note that some of the crystal classes can be written in a "shorthand" form; equivalencies shown here are from Table 2.8 in Dana. Where the "shorthand" form exists, it is the one SHAPE uses.

### EQUIVALENT LONG AND ABBREVIATED FORMS OF SIX CRYSTAL CLASSES

| System       | Long Form        | Short Form   |
|--------------|------------------|--------------|
| Orthorhombic | 2/m2/m2/m        | mmm          |
| Tetragonal   | 4/m2/m2/m        | 4/mmm        |
| Hexagonal    | $\bar{3}2/m$     | $\bar{3}/m$  |
|              | 6/m2/m2/m        | 6/mmm        |
| Isometric    | 2/m $\bar{3}$    | m $\bar{3}$  |
|              | 4/m $\bar{3}2/m$ | m $\bar{3}m$ |

4. Next, SHAPE will prompt you for the axial ratio. Where two or more axes must be equal due to the point group symmetry of the crystal class, SHAPE knows which ones must be equal by definition, so it will only prompt you for what is appropriate (SHAPE will not ask for extraneous information). SHAPE will accept either the axial ratios (available in most older mineralogy texts), or the unit-cell dimensions in Angstroms; SHAPE will calculate the ratio from the dimensions in the latter case. Enter each axial length, separating each by a space.
5. If the crystal class of interest is monoclinic or triclinic, SHAPE will prompt you for the interaxial angle(s), as appropriate. Otherwise, SHAPE will set the angles according to the requirements of the point group symmetry of the crystal class.



6. SHAPE will now ask if the values stored are the ones you actually want. Check the list. If everything is OK, just press "ENTER".

### **B. Entering Miller indices and central distances.**

1. SHAPE will next ask for the Miller index of each form you want to generate, and how far from the center of the crystal you want the faces in that form to be (more on this later). For any arbitrary form  $\{hkl\}$  at a distance of one, enter the numbers for  $h$ ,  $k$ , and  $l$  as follows:

$h$  (space)  $k$  (space)  $l$  (space) 1 (for distance) ENTER.

The first three digits are the Miller index, which define the orientation ("slope") of the face relative to the axes; the fourth tells SHAPE how far out from the center of the crystal you want the face with that "slope" drawn. For each of the form(s) you want to generate, enter the appropriate numerical values of the Miller index now.

2. To let SHAPE know that you are done entering the list of forms, enter:  
99 (space) 0 (space) 0 (space) 0 ENTER.
3. SHAPE will now ask if the list of forms is correct. Check the list; if OK, press "ENTER".
4. Next, you will be given the chance to revise the forms on the list. The first time around, decline this option by "ENTER"ing.
5. **If everything has gone well, an crystal drawing will now appear on the screen.**
6. To return to the MAIN MENU from the display screen, hit the SPACEBAR once.

## **II. SAVING AND READING FILES**

### **A. To save a file:**

From the MAIN MENU:

1. Select the "save" option (B, Read or save crystal file).
2. Then on menu [B], select option 1 "Write file".
3. Save the file by assigning it an 8 character filename.

### **B. To read a file already created:**

From the MAIN MENU:

1. Select the "read" option (B, Read or save crystal file).
2. Then on menu [B], select option 2 "Read file (new format)".
3. Read the file by entering its 8 character filename.

## **III. CUSTOMIZING THE DISPLAY**

### **A. To see how the axial intercepts look, do the following:**

1. Return to the MAIN MENU by hitting the spacebar once.
2. Select "Display modes and options" (N on the MAIN MENU).
3. When the "Display modes and options" menu appears, select "crystal axes" (option 6).
4. In the [N.6] menu, select the on/off toggle (option 1), and toggle "on". When finished, "ENTER" (to leave [N.6] menu).  
We should now be in the [N] menu.
5. "ENTER" again (to leave [N] menu).
6. Upon return to MAIN MENU, select "Replot on screen" (D).

**7. The crystal drawing should reappear, but now the axes are shown, their lengths proportional to the axial ratio you specified, and usually scaled so that each face intersects each axis at unit length.**

8. To return to the MAIN MENU from the display screen, hit the SPACEBAR once.

#### **B. Rescaling the axes.**

For some purposes, we will need to rescale the axes. To do this from the display:

1. Return to the MAIN MENU by hitting the spacebar once.

2. Select "Display modes and options" (N on the MAIN MENU).

3. When the "Display modes and options" menu appears, select "crystal axes" (option 6).

4. When you get to the [N.6] menu (step 11), select the scale option (2).

5. Enter the new multiplier (1.0 leaves the axes the same size; a  $\# > 1$  enlarges them, a  $\# < 1$  makes them smaller).

6. When finished, "ENTER" (to leave [N.6] menu). We should now be in the [N] menu.

7. "ENTER" again (to leave [N] menu).

8. Upon return to MAIN MENU, select "Replot on screen" (D).

**9. The crystal drawing should reappear, but now the axes are shown, their lengths proportional to the axial ratio you specified, and now rescaled as you instructed.**

10. To return to the MAIN MENU from the display screen, hit the SPACEBAR once.

#### **C. To see "hidden" faces:**

As we have set it up so far, SHAPE draws the outlines of crystal faces for the front faces only. If you would like to see what the "hidden" faces at the back of the crystal look like, we must instruct SHAPE to show us the back edges. To do so, we change the back edge mode as follows:

From the MAIN MENU,

1. Select "Display modes and options" (N on the MAIN MENU).

2. When the [N] "Display modes and options" menu appears, select "back edge mode" (option 2).

3. When in menu [N.2], select option 1 (dashed) to draw the back edges as dashed lines (most people will find this easier than trying to sort out front from back if both are plotted as solid lines, especially on monochrome monitors). When finished, press "ENTER" (to leave [N.2] menu).

4. "ENTER" again (to leave [N] menu).

5. Upon return to MAIN MENU, select "Replot on screen" (D).

**6. The crystal drawing should reappear, with back edges shown as you instructed.**

7. Return to the MAIN MENU by hitting the spacebar once.

#### **D. Rotating the crystal.**

The orientation of the crystal drawing on the screen can be modified by using the arrow keys on the keyboard.

**E. Other customizing options** exist, including changing the colors and solid/dashed drawing of front-edge lines, back-edge lines, and axes. These are described in the manual.

## **IV & V: MODIFYING EXISTING CRYSTAL DRAWINGS, AND MAKING MAJOR**

## **CHANGES FROM EXISTING CRYSTAL DRAWINGS**

These instructions show you how to make changes on a crystal that's already been drawn.

1. To return to the MAIN MENU from the display screen, hit the SPACEBAR once.
2. From the MAIN MENU, select (A) Enter or revise main crystal.
3. Then select (0) Revise main crystal. (Starting over would basically take you back to the beginning, as in part I.)
4. The "Revise original crystal" screen should now display choices including (1) Revise title, crystal system, cell parameters, (2) Revise forms, and (3) Remove symmetry - convert faces to forms. This is the jumping-off point for all the following modifications.

## **IV. MODIFYING EXISTING CRYSTAL DRAWINGS: ADDING, DELETING, AND MODIFYING INDIVIDUAL FORMS**

**To add new form(s) or delete or modify existing ones, proceed as follows:**

From the "Revise original crystal" screen:

1. Select (2) Revise forms, by entering 2 at the prompt.  
SHAPE will list the form(s) you've already selected.
2. Press ENTER to continue. A list of revision options will appear below the list of previously selected forms. This is called the "Revise Forms" list.

**A. To add new form(s) or delete existing ones, proceed as follows:**

**Adding new form(s).**

New forms can be added to your crystal using the following procedure.

1. From the "Revise Forms" list, select 4) Add forms, by entering 4 at the "Choice?" prompt.
2. When prompted, enter indices ( $hkl$ ) and central distance for each form you want to add, as in part I.
3. End the list of forms with 99 0 0 0 (as in part I).

**Removing form(s).**

To delete a form,

1. From the "Revise Forms" list, select 3) Delete forms, by entering 3 at the "Choice?" prompt.
2. Select which form number(s) you want to delete from the list; enter the number of the first and the last you want to delete (separated by a space; if you only want to delete one, enter its number twice).
3. Enter 0 0 (separated by a space).

**B. Changing a form to a different form.**

To stop looking at one form and start looking at a different one, with everything else being held constant, you can either simply delete the old one and add the new one, or you can change from one to the other as follows:

1. From the "Revise Forms" list, select 1) "Revise individual form", by entering 1 at the "Choice?" prompt.
2. Select option 1 "Indices".
3. Enter the appropriate integer values for  $\{hkl\}$  (here, you need only enter the three integers for the Miller index; keep the same central distance).

**C. Adjusting the size of faces.**

To change the size of the crystal faces in a form relative to the size of the faces in other forms, change the central distance. The central distance is the shortest distance from the origin (where all the axes intersect) to the crystal face (the shortest distance will be along a line perpendicular to the face). Decreasing the central distance (making the face closer to the origin) makes that face larger relative to the other faces; increasing the central distance (moving the face farther from the origin) makes that face smaller relative to the other faces.

To change the size of the faces in a form:

1. Determine which form from the list of forms you want to change. SHAPE keeps track of them by their place in the list; the first one (listed as form 1) is 1, the next is 2, etc.
2. From the "Revise Forms" list, select 1) , by entering 1 at the "Choice?" prompt.
3. Enter the "Number of form to revise?" (Item number; 1, 2, 3....)
4. From the next menu, modify item 2) Central distance, by entering 2 after the "Number to modify?" prompt.
5. Enter the new multiplier (1.0 leaves the axes the same size; a  $\# > 1$  enlarges them, a  $\# < 1$  makes them smaller).

**V. MAKING MAJOR CHANGES FROM EXISTING CRYSTAL DRAWINGS**

Sometimes we might want to compare the crystal we're working on (with its symmetry,

axial ratio, forms, etc.) with another crystal that differs in only one way from the one we've already made. We could make the new crystal completely from scratch (start completely over, making a new drawing, as in part I of these instructions). However, if we only want a few things to be different, it's usually easier (certainly shorter) to make the new crystal by just changing the thing(s) we want to change, using the one we've already made as our starting point. The following instructions show how to do this.

#### **A. Changing the symmetry.**

1. Select (1) Revise crystal system, by entering 1 at the prompt.
2. From the "Revise title, crystal class, cell parameters" menu, select 2) crystal class.
3. On the "Now select crystal class" screen, select the new crystal class by entering the appropriate code for the class you want from the list.

#### **B. Changing the axial ratio.**

To see what the same form(s) look(s) like, in the *same* crystal class (i.e., with the same symmetry), but with *different* axial ratios:

1. Select (1) Revise crystal system, by entering 1 at the prompt.
2. From the "Revise title, crystal class, cell parameters" menu, select 3), 4) and/or 5)  
CONTINUE.

#### **IV & V: To see the modified drawing:**

1. Check the list of forms and their central distances; if OK, proceed to the next step.
2. From the "Revise Forms" list, select nothing; do this by just hitting ENTER after the "Choice?" prompt. Making no "Choice?" takes you back to the previous ("Revise original crystal") menu.
3. From the "Revise original crystal" list, again select nothing; do this by just hitting ENTER after the prompt.  
SHAPE will then prompt "Recalculate and redisplay (Y/N)?"
4. Enter y (for yes) and the revised crystal will appear.

### **VI. INFORMATION RETRIEVAL USING *SHAPE***

Once you have created or retrieved a crystal drawing, you can instruct SHAPE to highlight an individual face, or all faces in a form.

#### **A. To highlight a face or form:**

1. Return to the MAIN MENU by hitting the spacebar once.
2. Select "Display modes and options" (N on the MAIN MENU).
3. When the [N] "Display modes and options" menu appears, select "fills and shading" (option 4).
4. In the [N.4] menu, select the "Face form or fill" toggle (option 1), and toggle "on".
5. From the [N.4.1] menu, select 2) Individual fills; answer Y to add new one(s).

##### **6a. Highlighting a face.**

Any face can be identified by selecting 0 at the appropriate place in [N.4.1], and entering the desired Miller index. Select a color, and proceed to redisplay.

##### **6b. Highlighting a form.**

All faces in a chosen form can be identified by selecting 1 at the appropriate place in [N.4.1], and entering the desired Miller index. Select a color, and proceed to redisplay.

7. When finished, "ENTER" (to leave [N.4] menu).  
We should now be in the [N] menu.
8. "ENTER" again (to leave [N] menu).
9. Upon return to MAIN MENU, select "Replot on screen" (D).
- 10. The crystal drawing should reappear, but now the face or form you selected is shown in the color you selected.**
11. To return to the MAIN MENU from the display screen, hit the SPACEBAR once.

#### **B. Interfacial angles.**

The interfacial angle between any two faces on your crystal can be calculated (if indices of the two faces are known) by using the INTERFACIAL ANGLE option (select G from the MAIN MENU).

I would like to thank Prof. Ken Brock (Indiana University Northwest; Gary, IN) for inspiring me to assemble these instructions in this format.