Using Shape to Make Crystal Drawings

July 13, 2005
C:\a-StudioClassroom\minex24.rtf

(This exercise has a number of questions that you have to answer-the answers won't fit on this handout - use separate pages. And, you have to print out some crystal drawings to staple to your answers. Do it all neatly and clearly so that I can figure things out!)

Starting the program: Start the program SHAPE by clicking on the appropriate icon. The main screen appears. It consists of several options on the bar at the top as well as a number of buttons. (Before going further, on the top bar, click on "modes" then "display" and select "standard." if it is not already selected.)

To draw a crystal from scratch: Click on "*File*"; then "*New*", and then "*Yes*" when it asks you if you want to enter all the data and use default display options.

Title and axes: This gets you to the "*Title/Axes*" screen. If you wish, you may click on the "*Title*" box and enter a title. You must choose a crystal system, so click on the arrow on the right side of the *"Crystal system*" box, and scroll down to click on "*cubic*." (You could choose any system, but for our first try we are using "*cubic*", which is called "*isometric*" in some books.) Note that "*a: 1*" appears on the screen; this means that the program is assuming that the unit cell dimension of your crystal is equal to 1. (It really doesn't matter what value *a* is for cubic minerals because everything looks the same shape regardless of the value of *a.*) Click on "*OK*."

Point Group: You should now be at the "*Symmetry - Point Group or Crystal Class*" screen. This screen allows you to select the symmetry of the crystal you are drawing. .

1. How many different symmetry choices are there to choose from? How many should there be (what did I tell you)? (There are a few more than there should be because of redundant ones listed in the Trigonal and Hexagonal systems.)

The easiest thing would have been if the program wrote out the (conventional) complete Hermann-Mauguin symmetry symbol, but for some reason the programmer decided not to do that. The symmetries are given in two notations: to the left of the hyphen is a *international short hand notation for the Hermann-Mauguin symbol*; to the right of the dash is the corresponding *Schoenflies notation*. Here's a table relating short hand symbols to Hermann-Mauguin symbols:

abbrev.	H-M	abbrev.	H-M	abbrev.	H-M
1	1	3m	3m	6/m	6/m
B1	1	B3m	32m	622	622
2	2	4	4	6mm	6mm
m	m	B4	4	B6m2	6m2
2/m	2/m	4/m	4/m	6/mmm	6/m2/m2/m
mm2	mm2	422	422	23	23

222	222	4mm	4mm	mB3	2/m3
mmm	2/m2/m2/m	B42m	42m	B43m	43m
3	3	4/mmm	4/m2/m2/m	432	432
B3	3	6	6	m3m	4/m32/m
32	32	B6	6		

2. . How many of the point groups listed belong to the cubic system?

You chose the "*cubic*" system and now you have to choose a cubic point group. Click on *m3m*, and then on "*OK*." (You could choose any of the cubic point groups, but for this exercise we will start with the highest symmetry possible.)

3. What is the conventional *Hermann-Mauguin symbol* that corresponds to *m3m*?

Forms: (If it asks you if you want to use the Donnay-Harker forms - click on "*no*.") You should now be at the *Forms List* Screen. This is where you tell the program which crystal faces are to be on your drawing. You do this by entering *Miller Indices* (*h*,*k* and *l*) and *Central Distances* (*CD*). (Recall that Miller Indices describe the orientation of a face. The central distance tells how far a face is from the center of the crystsl.) Click on "*Add Forms*" to get to the "*Add/Revise Forms*" screen.

Drawing a Cube: Click on the appropriate boxes and type numbers and enter to input a value of 1 for *h* and a value of 1 for *CD* (central distance). Leave *k* and *l* set to zero. (Ignore color options for now, unless you want to get creative and explore what this program can do--it is way cool!) Now click on "*OK*" to get back to *Forms List* Screen. There should be one form listed with *Miller Index* 100 and *CD* = 1. Click on "*OK*." The program asks you whether to "*calculate now*?" Click on "*yes*" and you should soon have a cube. (Before going further, on the top bar, click on "*modes*" then "*display*" and try various selection – but be sure to leave it on "*standard*" when you go on to the next part of this lab.)

What do you see? You can see three *faces* of a cube. They all belong to the same *form* (which means they are identical in shape and related by the *point group symmetry*), but have different *Miller Indices*. (Check to make sure that "*identify faces*" is selected on the right hand side of the screen.) To see the different *Miller Indices*, point the cursor at each of the three faces and click. The program will tell you all sorts of stuff, including *miller indices of the face* (*hkl*) and of the *form* {*hkl*}.

4. What is the Miller Index of each of the three faces that are visible? They all belong to the same form. What is the Miller Index of the form?

Color: Click on "*Input1*" on the bar at the top of the screen and then click on "*Shading*".

Click in the "*Shading on*" box and then click on "*OK*." You should now see your cube with shading. Click on "*Input1*" agan, click on "*Shading*" and "*Select color*." Choose your favorite color. Hit "*OK*" twice to change the color of the cube. Finally, to turn on the color option (if it is not already on), click on "*Display*" on the bar at the top of the screen and then on "*Color*." Your cube is now shaded in different colors depending on face orientation.

Hidden Faces: Click on "*Input2*" on the bar at the top of the screen and then click on "*Line attributes.*" Select "*dashed*" for back edges and then click on "*OK*." You should now be able to see the hidden edges (and faces) on the back of your cube. If the lines are not a good color, click on "*Input2*" on the bar at the top of the screen and then click on "*Line color*" and then select colors as you wish.

Try the (111) Form: Click on *Input1* on the bar at the top of the screen and then click on "*Forms*". Click on "*Revise Form*" and change the *Miller Indices* to (111) instead of (100). Click on "*OK*" to get to the *Forms List* screen, and then click on "*OK*" again. Now click on "*Calculate*" on the left hand side of the screen and you should see a different shape that has the same symmetry as the cube you were just looking at.

5. How many faces does your new crystal have? What is this shape called? (You could look up the name in a book, but you don't need to if you are a clever student who has been listening to your instructor!)

Determine Miller Indices of the faces: To determine the Miller indices (*hkl*) of a face, point at it with the mouse and click the left mouse button.

6. Make a list of the Miller Indices of all the visible faces. Now figure out (or guess if you have to) the Miller indices of the hidden faces and list them.

Try the (110) Form: Click on *Input1* on the bar at the top of the screen and then click on "*Forms*". Click on "*Revise Form*" and change the *Miller Indices* to (110) instead of (111). Click on "*OK*" to get to the *Forms List* screen, and then click on "*OK*" again. Now click on "*Calculate*" on the left hand side of the screen and you should see a different shape that has the same symmetry as the last two crystals.

7. How many faces does this crystal have? What are the *Miller Indices* of all the faces? This form is called a *dodecahedron*--why? What common mineral has this form?

Try the general form: The three forms you just looked at are called *special forms*. Special forms are forms that have some Miller Indices that are equal to each other or to

zero. Special forms do not have the maximum number of faces possible. So, now go back through *Input1*==>"*Forms*"==> "*Revise Form*" and change the indices so that *h*, *k* and *l* are all different and not equal to zero. (Use small integer values to avoid making things messy.) Then click on "*OK*", "*OK*", and "*Calculate*" to get the general form. To make it less messy, click on "*Input2*", then "*Line attributes*", set *back edges* to "*none*", and click on "*OK*." The *hidden edges* (dashed lines) should now disappear.

8. If all has gone well, you are looking at the general form in the m3m class. It is called a *hexoctahedron*--why is that? How many faces does it have?

Symmetry of the general form: You should be able to see all sorts of symmetry elements in your drawing. 4-fold axes, 3-fold axes, 2-fold axes and mirror planes are all present in this drawing just as they were in the other forms you generated. To help see all this, let's print out a few drawings.

Turn off color and shading: Important: you must turn off the color and shading now so that you can print without errors. To turn off the color, click on "*Display*" and "*Color*." To turn off the shading, click on "*Input1*", "*Shading*", uncheck "*Shading on*", and "*OK*".

Printing: Now, click on "*Print*" on the left side of the screen, and then on "*OK*."

Rotate the crystal to see symmetry: To rotate the drawing, you use the six buttons near the top of the left hand edge of the screen. You click on one of the six buttons and then on "*replot*" to get the new drawing. Rotation is by steps--the amount of each rotation is the number of degrees displayed in the box just below the buttons. Double click on this box and set it equal to 5° for now and then try rotating the crystal to different orientations in order to see the different symmetry (rotation axes and mirror planes).

9. Print out several different drawings that have the crystal oriented so you are looking down the various rotation axes and mirror planes. Label the axes and mirrors.

Change the symmetry/Select a different *Point Group*: Click on "*Input1*"==>"*Symmetry*", select point group *23*, and then click on "*OK*." Click on "Calculate" and the drawing will change to one with less symmetry. This crystal still belongs to the cubic system, but only 2-fold and 3-fold axes of symmetry are present. There are no mirror planes! It has the least amount of symmetry that any crystal in the cubic system can have. I think it is kind of ugly.

10. Rotate the drawing and print out several views that show the 2-fold and 3-fold axes of symmetry. Label the symmetry elements on the drawings. What common mineral has this symmetry?

Drawing crystals with multiple forms: cubo-octahedron: Start over and redraw a cube. To do this, click on "*File*"==>"*New*." Then answer "*NO*" when (if) it asks you whether to save what you have. Answer "*Yes*" when it asks you whether to read display default values. Follow the same steps as you did above to create a cube with one form (100) at a *CD* of 1.0. Now add an octahedron by clicking on "*Input1*"==>"*Forms*"==>"*Add Forms*." Enter *Miller Indices* (111) and *CD*=1.7, and click on "*OK*," "*OK*," and then "*Calculate*." The computer will draw your crystal. The octahedron faces appear as tiny triangles at each corner of the cube. Note that the 1.7 CD for {111} was almost too great; if {111} had been spaced farther away, say 1.8, the octahedron faces would not have been present at all.

What are the angles between the faces of the two forms? Click on one of the small {111} faces--you will get to the "*Face at Cursor*" screen; click on "*OK*." Now click on one of the {100} faces adjacent to the face you last clicked on. You will get the "*Face at Cursor*" screen; on that screen the "*Angle with last face*" is given.

11. What is the angle between the two faces you just clicked on? Check and see if all {100} and {111} faces intersect at the same angle. Do they? Why or why not? Print a copy of this crystal drawing.

Change the CD for the {111} form and recheck the angles between faces: Click on one of the {111} faces to get to the "*Form at Cursor*" screen. Now change the *CD* to 0.61, click on "*OK*," and then click on "*Calculate*."

12. Check the angles between faces on your crystal drawing. Are they the same as in question 11? Print a copy of this crystal drawing and compare it with the one printed in question 11. Note that all the faces are at the same orientations, but the relative sizes are different. The *Miller indices* depend only on orientation, so the faces have the same *Miller indices* in the two drawings. Label all the faces with correct (*hkl*) indices. You may wish to click on the faces to figure out what the indices are.

Now let's add one more form: First click on one of the {111} faces and change the *CD* to 0.9; click on "*OK*" and then on "*Calculate*." All faces should now be about the same size. Now click on "*Input1*"==>"*Forms*"==>"*Add Forms*" and enter {*hkl*} values of {011} with a *CD* of 0.95. Cick "OK" a couple of times and then "Calculate." You now have a crystal with three forms: *cube*, *octahedron* and one other.

Now let's find the symmetry axes: Rotate the crystal until you are looking down a *2-fold axis*, the rotate it again until you are looking down a *3-fold axis*, and finally do the same for a *4-fold axis*.

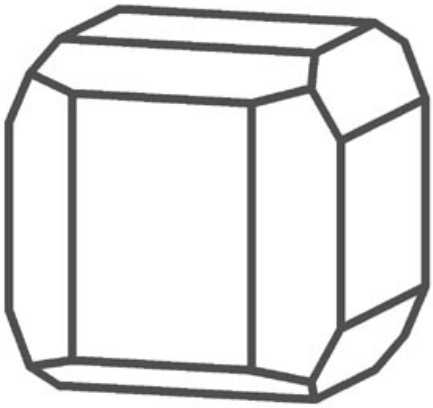
13. What are the *Miller Indices* of the faces perpendicular to each axis?

14. You have a *cube* and an *octahedron* and something else. What is the third form called? (To answer this, you may wish to delete the other forms. To do this, click on "*Input1*"==>"*Forms*"==>the {111} form==>"*Delete form*"==>"*Yes*"==>"*OK*"==>"*Calculate*" to get rid of the {111} form. You can get rid of the {100} form in the same way. You may now be able to recognize the single remaining form as one you have seen before.)

Now lets make a pyritohedron: Click on "*File*"==>"*New*." Then answer "*No*" when it asks you whether to save what you have. Answer "*Yes*" when it asks you whether to read display default values. Select the "*Cubic*" crystal system if it is not already there, and then "*OK*." On the "*Symmetry-Point Group or Crystal Class*" screen, choose symmetry *mB3* and click on "*OK*."

15. What is the *Hermann-Mauguin* point group that is abbreviated *mB3*?

Now click on "*Add Forms*" to get to the "*Add/Revise Forms*" screen. Enter the form {102} with *CD*=1.0. Then click on "*OK*"==>"*OK*" and then "*Yes*" when it asks if you are ready to calculate. You now have a *pyritohedron*. This is what an ideal pyrite crystal looks like!



Now add cube faces: You figure out how to do it so that you get the drawing shown at right. (This is actually what many pyrite crystals look like.)

16. After you figure out how to get the above, print it out. What are the Miller Indices and CD for your cube faces? Why aren't they square like on a normal cube?

We changed symmetry from *m3m* to *mB3* a couple of steps ago. That means that our crystal does not have the same symmetry as the first few we played with. It does have a cubic form (in addition to the pyritohedron); cubic forms exist in more than one point

group.

17. Does this new crystal have mirror planes of symmetry? 4-fold axes of symmetry? 3-fold axis of symmetry? 2-fold axes of symmetry?

18. We have just seen that the cubic form exists in both *m3m* and *mB3* point groups. The pyritohedron does not--it does not exist in the *m3m* point group. Why?

Let's take a look at quartz: Start over with "*File*"==>"*New*"==>"*No*"==>"*Yes*" to get to the "*Title/Axes*" screen. Select "*Trigonal-hexagonal*" as the crystal system and enter the values *a*=4.9 and *c*=5.4. These are the unit cell dimensions for quartz. Click on "*OK*" and select point group *321* (equivalent to *32*, the point group of quartz). Click on "*Add Forms*". Enter the following faces and *CD* values:

(100) 1.0
(101) 1.0
(011) 1.0

Click on "*OK*", etc. and then "*Calculate*" or "*Yes*" to get the crystal drawing. You now have a hexagonal prism terminated by two pyramids (a hexagonal dipyramid). This is not typical of quartz, but does occur. If you rotate the drawing, you will see that it has true 6-fold symmetry (looking down its long direction). Click on some faces and you will find that one of the forms is not showing (because the *CD* value is inappropriate).

Now let's adjust the CD values to get a more common quartz crystal: Click on "*Input1*"==>"*Forms*" and then change the CD for the {011} form. Change the *CD* to 1.7, click on "*OK*" and then on "*Calculate*." You now have a strange looking crystal that has symmetry 32 but looks nothing like quartz crystals. Find a face that belongs to {101}, change the *CD* value to 1.5, click on "*OK*" and then on "*Calculate*." Now you have a quartz crystal.

19. Print out your drawing, and then label every face with the correct *Miller Indices*. Rotate the drawing so you are looking down the long dimension and print a copy. Is there still a 6-fold axis of symmetry?