

# COMPUTER GENERATED CRYSTALS USING *SHAPE*

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The software package known as SHAPE (Shape Software 521 Hidden Valley Road, Kingsport, TN 37663) provides an excellent method for accurately drawing crystals. The following three boxes describe the basic steps involved in using SHAPE. Refer to these instructions when completing the exercises.

## GETTING STARTED

The program will be loaded into the computer for you. You may have to activate the program by clicking twice on the crystal icon entitled SHAPE 4.2. When everything is ready a screen headed by

◇>CRYSTALLOGRAPHIC DATA FOR CRYSTAL 1<◇

will appear on the screen. You are now ready to begin.

## ENTERING THE CRYSTALLOGRAPHIC DATA

### Selecting Crystal Class and Cell Parameters

All 32 crystal classes are listed (by crystal system) on this first screen. The computer automatically selects  $m\bar{3}m$  (short for  $4/m\bar{3}2/m$ ) under the ISOMETRIC heading.

If you choose any isometric class, and activate the OK button, the computer will automatically enter unit cell dimensions (all 1.0) and inter-axial angles (all  $90.0^\circ$ ) and display a new screen.

If you choose any non-isometric class the computer will request the necessary "parameters" (unit cell dimensions and inter-axial angles) in boxes at the screen bottom. Note that SHAPE automatically adds fixed dimensions or angles for you. After the appropriate parameters are entered activate the OK button. A new screen will appear headed:

◇>FORMS 1 TO 20 FOR CRYSTAL 1<◇

### Entering Miller Indices and Central Distances

This second screen allows you to enter the Miller indices of each form you choose to draw on the crystal. Three indices must be entered (one each for H, K, & L) for each form. In addition, the central distance (relative distance from crystal's center to face) must be entered for each form on the drawing. Enter each index in the appropriate box provided, i.e. 1 0 0. The fourth box (headed "Dist") is for the central distance (CD).

Note, SHAPE automatically enters  $CD = 1$  for each form; if some other value is desired it must replace the one. After all four numbers are entered, press the "return" key. You will immediately see a prompt asking for indices and CD of the second form. You may enter as many additional forms (up to 20) as you desire. After all the forms and CD's are entered, select the "DONE" button to exit the form entry cycle. SHAPE will then draw the crystal.

## MODIFYING CRYSTAL DRAWINGS

### Adjusting the Size of Faces

This option allows you to increase or decrease the relative size of a form on the crystal. It is activated by selecting the ADJUST FACE SIZE option under the EDIT menu. After the ADJUST FACE SIZE option has been activated select the desired face by placing the cursor on it and clicking the mouse. Face size is adjusted by modifying the CD. This is accomplished with the ↑ and ↓ keys.

↓ increases CD, decreases face size

↑ decreases CD, increases face size

Faster CD adjustments are made by depressing the Option key (fairly fast) or Shift key (very fast), while using the arrow keys. After adjustments are complete redraw the crystal by selecting "Recalculate Crystal" under the "ADJUST FACE SIZE" menu.

### Adding New Form

New forms can be added to your crystal using the following procedure. Select the MODIFY FORM LIST option from the EDIT menu. At the bottom of the screen select NEW FORM, then enter the desired Miller indices and CD. Activate the ACCEPT button to add the new form to your list (you will see the new form added to the bottom of your form list). Click the DONE button to redraw the crystal with the new form.

### Removing a Form

To delete a form select MODIFY FORM LIST from the EDIT menu. Select the form you want to remove by clicking the circle in front of the indices. These indices will then appear in the boxes at the screen bottom. Click the REMOVE option then the ACCEPT button and the deletion is complete (indices of the deleted form will disappear from the form list). Click the DONE button to redraw the crystal with the form deleted.

### Rotating the Crystal

Orientation of the drawing on the screen can be modified by using the 2, 4, 6, 8, and 5 keys on the numerical pad (right side of keyboard).

### Identifying a Face

Miller indices of any face on the crystal can be instantly identified by using the IDENTIFY FACE option under the EXPLORE menu.

### Locating a Form

All faces in a chosen form can be easily identified by using the LOCATE FORM option under the EXPLORE menu.

### Locating a Face

Any face can be located by using the LOCATE FACE option under the EXPLORE menu.

### 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 under the EXPLORE menu.

## EXERCISES WITH COMPUTER GENERATED CRYSTALS

### Cube - Octahedron crystals:

The cube {100} and octahedron {111} are common crystal forms on isometric crystals. In theory if {100} and {111} are present (one or both are absent on many crystals) they can occur in any combination of relative development. (Crystal structure and environmental conditions during crystallization determine which forms occurs and how extensively they develop.) We will examine the appearance of isometric crystals showing a range of relative developments of these two forms.

#### Draw a Cubo-octahedron

Under the heading ISOMETRIC select class  $m\bar{3}m$  (short for  $4/m\bar{3}2/m$ ) then click the "OK" button.

Enter the following Miller indices and central distances:

Cube	1	0	0	1.0
Octahedron	1	1	1	1.7

After entering the "1.7" hit return and click the DONE key to exit the data entry cycle.

The computer will draw your crystal. The octahedron faces appear as tiny triangles at each corner of the cube. Note that the 1.7 central distance for {111} was almost too great; if {111} had been spaced further away, say 1.8, the octahedron faces would not have been present at all.

#### Draw Cubo-Octahedron combinations

Use the "Adjust face size" routine (see Hand-out) to redraw the crystal with the following central distances.

Cube	Octahedron
1	1.4
1	0.6
1	1.0

#### Interfacial angles

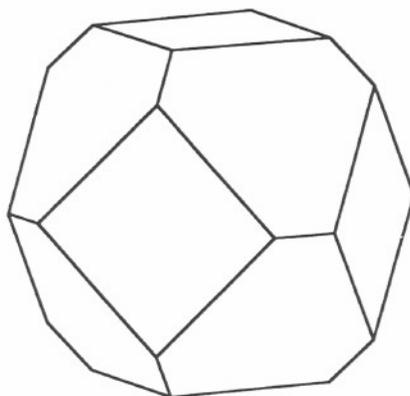
Use the "Interfacial angles" routine to find the following interfacial angles:

$$(001) \wedge (111) = \underline{\hspace{2cm}}$$

$$(111) \wedge (111) = \underline{\hspace{2cm}}$$

Identifying faces

Use the "Identify a Face" routine to assign Miller indices to every face on this crystal.



Find the symmetry axes

Use the numeric pad keys to rotate the crystal until you have a view directly down a 2-fold, 3-fold, and 4-fold axis. List Miller indices of the face perpendicular to each of the following axes:

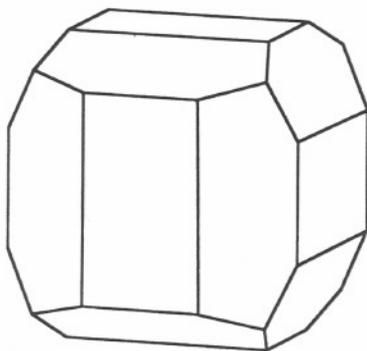
3-fold \_\_\_\_\_ 4-fold \_\_\_\_\_

**Pyritohedron**

Select BEGIN AGAIN from the EDIT menu; this will rerun SHAPE. From the ISOMETRIC column choose mb3 (for  $2/m\bar{3}$ ). Enter the form  $\{102\}$  with CD = 1.0; press return then select DONE to exit the entry loop. SHAPE will draw a pyritohedron.

The drawing below shows that the cube can occur with the pyritohedron. Use the "Add a New Form" routine to add the cube  $\{100\}$  to your crystal. Keeping the  $\{102\}$  CD=1.0 use SHAPE to find the CD for the cube that will duplicate the cube-pyritohedron drawing below.

$\{100\}$  Central Distance = \_\_\_\_\_



### Interfacial angles

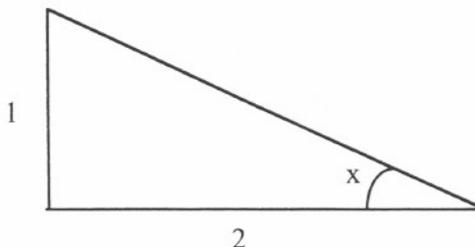
Use the "Interfacial angles" routine to find the interfacial angle  $(001) \wedge (102) = \underline{\hspace{2cm}}$   
Compare this value with the acute angle "x" shown in the right triangle with sides of one and two (i.e., a face formed by stacking identical cubes in a 2:1 ratio).

$$\tan x = 1/2 = 0.5$$

$$x = \text{atan}(0.5)$$

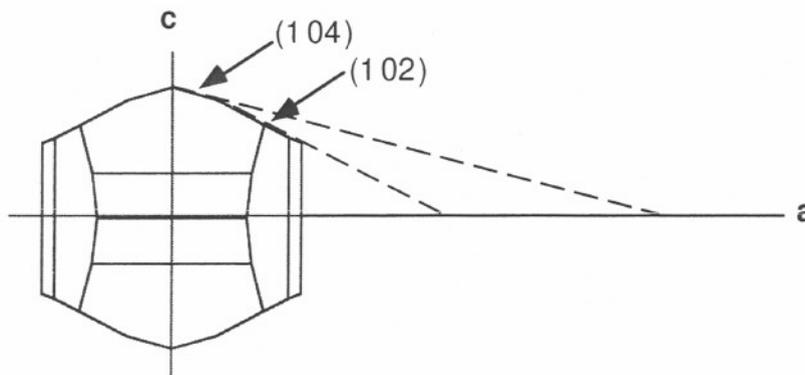
$$x = \underline{\hspace{2cm}}$$

use your calculator



### Multiple pyritohedra

Use the "remove a form" routine to delete the cube. Add a second pyritohedron with indices  $\{104\}$  and  $CD = 1$ , to your crystal. Is the orientation of  $(104)$ , relative to  $(102)$  consistent with a stacking of 4 units along **a** and 1 on **c**?        (the drawing below shows the crystal rotated to provide a side view and the faces extended to intercept the **a**-axis).



### Locate Forms & Faces

Use the "Locating Forms" routine to examine the faces in both  $\{102\}$  and  $\{104\}$ . Can you find face  $(201)$ ? If not delete  $\{104\}$  and add  $\{201\}$  to your form list. What does this result tell you about the forms  $\{102\}$  and  $\{201\}$  in class  $2/m\bar{3}$ ?

\_\_\_\_\_

### **Quartz**

The development of positive  $\{101\}^*$  and negative  $\{011\}$  rhombohedra often make alpha-quartz (class 32) appear to have 6-fold symmetry. In most cases, however, the two rhombohedra are not equally developed, thereby revealing the true 3-fold symmetry. We can examine this situation using SHAPE. [\*Note: for hexagonal and trigonal crystals, which normally have indices  $\{hkil\}$ , SHAPE ignores the "i" index as this value can be calculated from  $i = -(h + k)$ .]

Select "Begin again" from the EDIT menu; this will rerun SHAPE. Under the TRIGONAL column select 32 (the symmetry of quartz). At the bottom of the screen enter dimensions of the quartz unit cell:

$$a = 4.9 \quad \text{and} \quad b = 5.4$$

Enter the following forms and central distances:

1 0 0	1	(the hexagonal prism)
1 0 1	1	(the positive rhombohedron)
0 1 1	1	(the negative rhombohedron)

Select DONE to exit the form entry loop.

This calculation should produce a "Hexagonal-appearing" quartz crystal.

Locate Forms

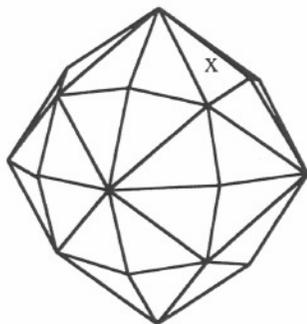
Use the "Locating a Form" routine to determine which faces are in {101} and which are in {011}. Adjust the faces (use Adjust Face procedure) using the following central distances.

(100)	1.0
(101)	1.5
(011)	1.7

Redraw the crystal. Note that the six terminating faces are not related by symmetry (i.e., they do not belong to a single form).

**The hexoctahedron**

Select "Begin again" from the EDIT menu; this will rerun SHAPE. Under ISOMETRIC select class m3m (short for  $4/m\bar{3}2/m$ ) then click the "OK" button. Enter the indices (321) and CD= 1, the press return and DONE. A 48-faced form, called the hexoctahedron will appear. Use the Identify Face option to identify the face marked with an "x" on the hexoctahedron.



The indices of the face "x" are \_\_\_\_\_

Add a new hexoctahedron with indices (642). Explain what happens and why.

For fun add at least two additional hexoctahedra, each with indices other than 1, 2 or 3, to your crystal.

## HOMEWORK PROBLEM

Solve the problems below using SHAPE

1) The study of a particular tetragonal crystal gave the following data:

- Form {001} has 2 faces
- Form {100} has 4 faces
- Form {111} has 4 faces
- Form {101} has 8 faces
- Form {121} has 8 faces

To which crystal class must this crystal belong? Explain your answer (i.e., how were the other possibilities eliminated?).

2) The study of a particular trigonal crystal revealed that the following forms were present:

- Pedion
- Hexagonal prism
- Ditrigonal prism
- Trigonal prism
- Trigonal pyramid

To which crystal class must this crystal belong? Explain your answer.

## TWINNING EXERCISES

In most cases the relationship between individual domains within a twinned crystal can be described by rotation about a twin axis or reflection across a twin plane. Both of these operations can be performed using SHAPE.

### I. Twinning by Reflection

#### A. The Gypsum Fish-tail Twin

The common "fish-tail" gypsum twin is described as "twinned on (100)." This means that the "fish-tail" contact twins can be generated by reflecting one half of a gypsum crystal across the (100) plane, to generate the twinned crystal. Using SHAPE, this operation is performed as follows:

1. Enter SHAPE: From the start-up screen:

- a. select **2/m** from the monoclinic section
- b. enter unit cell parameters  
**a** = 5.68      **b** = 15.5      **c** = 6.29      **B** = 113.8, then click OKAY
- c. enter the following forms and CD's

1 2 0	1.0	
0 1 0	0.5	
-1 1 1	1.0	then click ACCEPT and DONE

2. To twin the crystal: select the **Twins** option under the **TWINS/EPITAXY** menu.

3. From the dialog box headed **‡> TWIN MODE < ‡**

- a. choose "contact" and "hide interfacial edges"
- b. select the Okay button

4. From the dialog box headed **‡> TWIN OPERATOR 1 < ‡**

- a. choose "Reflection on" and enter 1 0 0 as indices of the twin operator
- b. click the ACCEPT button
- c. select the DONE button

5. From the dialog box headed **‡> COMPOSITION PLANE 1 < ‡**

- a. enter the indices 1 0 0 as the composition plane
- b. click the ACCEPT button
- c. select the DONE button

An inverted "fish-tail" gypsum twin will appear. The twin can be rotated into the standard orientation using buttons on the numeric pad (right end of the keyboard).

#### B. Staurolite Cruciform Twin

The distinctive staurolite cruciform twin can be formed by reflection across (031). This operation produces twin individuals that are almost, but not precisely, 90° apart. To simplify the drawing of this twin an untwinned staurolite crystal, showing the forms {110}, {010}, {201}, and {001} has been pre-drawn and stored under the file-name "Staurolite." The following steps will produce a staurolite twin.

1. Load the pre-drawn crystal by selecting the "Get data from a remake file..." option from the starting SHAPE screen and choosing "Staurolite" from the menu.
2. To twin the crystal: select the **Twins** option from the **TWINS/EPITAXY** menu.
3. From the dialog box headed †> **TWIN MODE** < †
  - a. select: **Interpenetration with intercrystalline edges**
  - b. for the query **Intra-facial edges** select:- hide
  - c. click the Okay button
4. From the dialog box headed †> **TWIN OPERATOR 1** < †
  - a. choose "Reflection" and enter 0 3 1 as indices of the twin plane
  - b. click the ACCEPT and DONE buttons

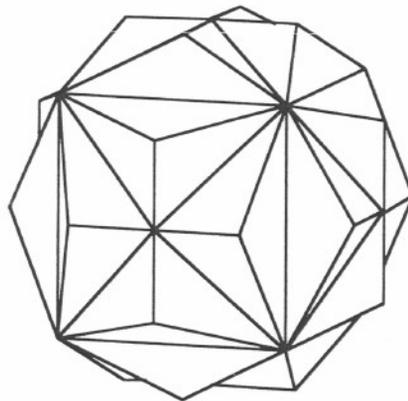
The staurolite twin will appear. The extraneous lines in the drawing can be removed by pressing "Command L" (i.e., the apple button & the "L" key on a Macintosh).

Measure the angle between twin individuals by using the "interfacial angles" routine to find the angle between (001) on crystal one, and (001) on crystal two. Angle = \_\_\_\_\_

## II. Twinning by Rotation

### A. The pyrite "iron cross" twin

The iron cross twin (shown below) is a penetration twin formed by a 90° rotation about the c-axis, the [001] direction.



Using SHAPE, this operation is performed as follows:

1. Enter SHAPE:- From the start-up screen:  
select **mb3** (short for  $2/m\bar{3}$ ) from the isometric section and click Okay
2. On the data entry screen enter the form {102} with CD = 1, select done
3. To twin the crystal: select the **Twins** option under the **TWINS/EPITAXY** menu.

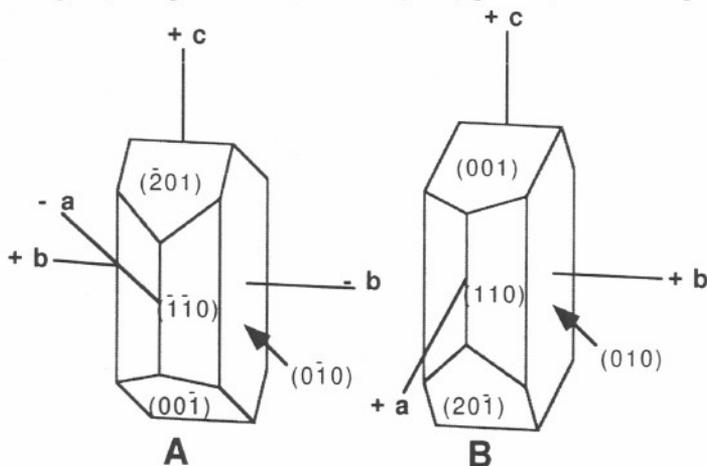
4. From the dialog box headed ‡> **TWIN MODE** < ‡
  - a. select: **Interpenetration with intercrystalline edges**
  - b. for the query **Intra-facial edges** select :- hide
  - c. click the Okay button
  
5. From the dialog box headed ‡> **TWIN OPERATOR 1** < ‡
  - a. choose "Rotation" and enter 0 0 1 as indices of the twin axis
  - b. enter a rotation angle of 90°
  - c. click the ACCEPT button
  - d. select the DONE button

SHAPE will then draw the twin. The final drawing can be cleaned up (extra lines removed) by pressing Command L (i.e., the apple button & the "L" key on a Macintosh).

**QUESTION:** Note that the **c**-axis in pyrite is a 2-fold symmetry axis. Predict what would happen if the angle in step 5. b. were 180°, rather than 90°. Try it to test the accuracy of your prediction.

#### Carlsbad Twining on the Computer

Carlsbad twins are penetration twins that commonly form in feldspars. The composition plane is {010} and the twin axis is the **c**-axis (i.e., the [001] direction). One twin individual is rotated 180° about the **c**-axis, relative to the other. In the illustrations below note that Fig. A shows how Fig. B would appear if rotated 180° about the **c**-axis. In the twin the two individuals are merged (interpenetrated) on the {010} planes, to form a penetration twin.



Drawing the Carlsbad twin is simplified by using a pre-drawn, untwinned monoclinic K-feldspar crystal. This drawing, which has been distorted somewhat to make the twin appear more realistic, is stored under the file-name "Carlsbad." The following steps will produce a Carlsbad twin.

1. Load this pre-drawn crystal by selecting the "Get data from a remake file..." option from the bottom of the starting SHAPE screen and choosing "Carlsbad" from the menu.
  
2. To twin the crystal: select the **Twins** option from the **TWINS/EPITAXY** menu.

3. From the dialog box headed †> **TWIN MODE** < †
  - a. select: **Interpenetration with intercrystalline edges**
  - b. for the for the query **Intra-facial edges** select:- hide
  - c. click the Okay button
  
4. From the dialog box headed †> **TWIN OPERATOR 1** < †
  - a. choose "Rotation" and enter 0 0 1 as indices of the twin operator
  - b. enter a rotation angle of 180°
  - c. click the ACCEPT button
  - d. select the DONE button

A Carlsbad twin will appear. The extraneous lines in the drawing can be removed by pressing "Command L".

**QUESTION:** Perform the Carlsbad procedure again, but this time substitute the b-axis [010] in place of [001]. Explain your result.

For fun generate the penetration twin formed when the form {211} in class 23, it twinned by a 90° rotation of the c-axis.

## NOTE TO INSTRUCTORS

This package contains two computer exercises that use SHAPE software to teach certain aspects of crystal morphology and twinning. Both exercises are designed to be self-contained; that is, once students become familiar with the computer and software, they can work through the material individually. It is intended that each student will have access to an individual computer.

SHAPE is a software package developed by Eric Dowty. It is commercially available from: Shape Software 521 Hidden Valley Road, Kingsport, TN 37663. Phone (615) 239-3258. Demo versions are available for both PC and Mac computers.

It is assumed that students performing these exercises have been introduced to the basic elements of symmetry, Miller indices, and crystal forms. "Exercises with Computer Generated Crystals" uses SHAPE to explore these concepts in an interactive computer format. The second package, "Twinning Exercises", allows students to draw reflection and rotation twins. Both exercises encourage experimentation and are aimed at students with modest mathematical backgrounds.

The twinning exercises call for previously saved crystal drawings in "Remake Files" named "Staurolite" and "Carlsbad." The staurolite file can be created with the following data:

Crystal Class: 2/m	{0 0 1}	1.7
a = 7.83	{1 1 0}	0.5
b = 16.62	{0 1 0}	0.7
c = 5.65	{2 0 1}	1.3
$\beta = 90^\circ$	{-2 0 1}	1.3

The carlsbad file can be created with the following data:

Crystal Class: 2	{0 0 1}	1.6
a = 8.5	{1 1 0}	1.0
b = 13.0	{1 -1 0}	1.0
c = 7.2	{-2 0 1}	1.3
$\beta = 116^\circ$	{0 1 0}	0.8
	{0 -1 0}	0.4

### Using *SHAPE*

The nuts & bolts of using SHAPE are summarized on the first two pages. The blocks entitled "Getting Started" and "Entering Crystallographic Data" outline the procedures for starting the software and providing the crystal symmetry, form indices, and central distances needed to draw a crystal. The block entitled "Modifying Crystals" describes the options available for "playing with a crystal." This information should be available for reference while in performing the exercises.

#### Major Disadvantage:

A computer laboratory with a bank relatively fast personal computers is recommended to fully implement the exercises.