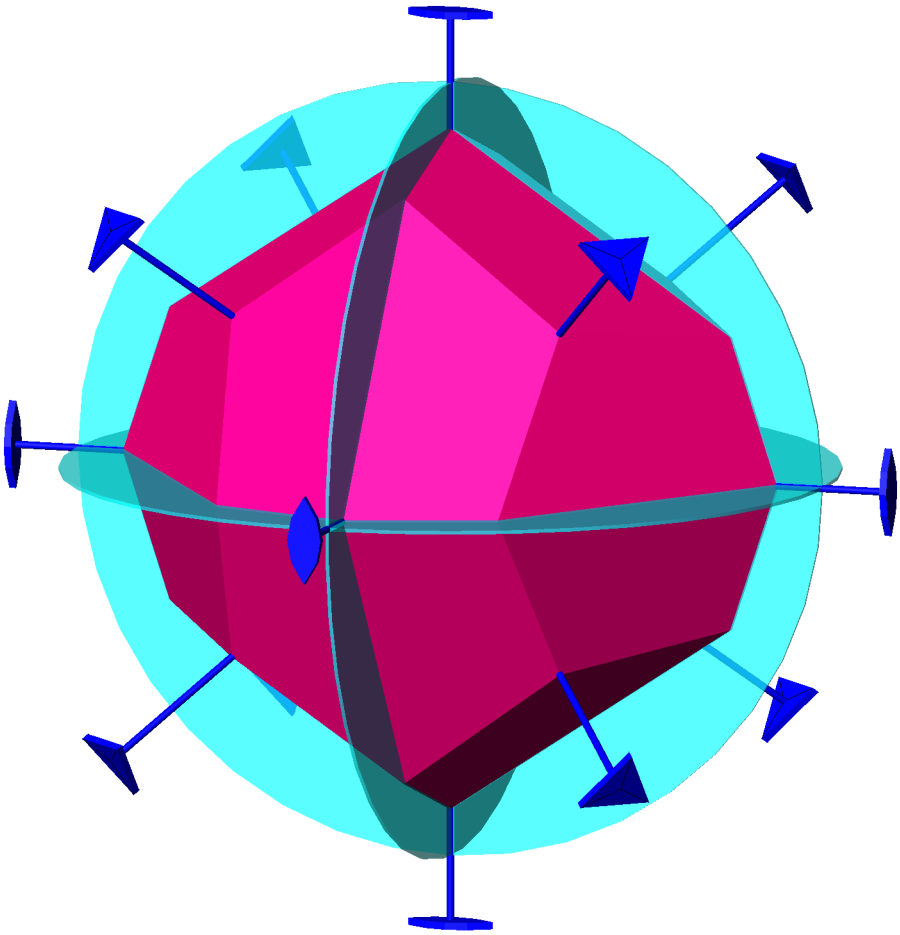

SHAPE

SHAPE
Version 7.4

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Table of Contents

1 Introduction

It may be helpful to read these topics before using SHAPE

1.1 Capabilities

SHAPE is a program to calculate and display the morphology and symmetry of single crystals, twins and epitaxial and other intergrowths. Some of the basic mathematical aspects of the program were described in a paper in The American Mineralogist (1980, V.65, p.465). However, many important improvements have been made since then in the capabilities and speed of the program.

To draw an individual crystal, it is necessary to enter only the crystal class, the unit cell parameters, and the indices and central distance for one face of each form. The crystal drawing can be rotated, translated and rescaled, and crystal axes can be added at will.

The central distances, which determine the prominence (area) of each form, may be derived from the unit cell and space group, using the Donnay-Harker morphological "law".

The crystal can be displayed in an orthographic projection rotated in a standard way (virtually identical to clinographic projection), or in a "straight-on" orthographic projection, and the view of the crystal can be combined with a stereonet showing the poles to the faces and the crystal axes. The mouse cursor can be used to index any of the visible faces. Any of the faces can be filled in with color (if a color display is used) or dot shading patterns. The entire crystal can be shaded, in color or black-and-white. Stereopairs of the image may be drawn, either as separate images or as superimposed anaglyphs (two-color).

The 3D Drawing Modes, which use OpenGL or Direct3D system software, allow a number of special effects, such as transparent faces. In these modes, the symmetry elements (rotation axes and mirror planes) may be shown.

Stereo output through quad-buffered OpenGL (or Direct3D on Windows) is available for appropriate hardware (suitable graphics cards, monitors, projectors and/or eyewear).

The central distance, and therefore the size, of each face may be adjusted on-screen by clicking with the mouse.

After having generated a single crystal, and even after having rotated it, the crystal may be twinned in any of several ways. Almost any kind of twin is possible, including many kinds of multi-crystal aggregates. Also, epitaxial intergrowths may be drawn, again including multi-crystal aggregates. All inter-crystal edges and corners may be drawn, and all unwanted lines may be removed from these plots, producing an absolutely perfect final

version.

Sections of crystals may be drawn for any orientation and at any level. Growth zoning may be modeled in section, using non-linear growth rates and/or different start and end times for multiple crystals. Also, non-crystallographic symmetry can be used to draw quasi-crystals.

Hard copies of the drawings can be made in several ways. The screen image can be reproduced with dot-matrix or laser printers - actually, with the high-resolution modes of these printers, the resolution of the image is much improved over the screen. Plots can also be made with most pen plotters. Finally, if neither a pen plotter nor a suitable dot-matrix printer is available, the coordinates of the corners and other information can be listed and the drawing can be made by hand.

Running the program is not difficult — the input is interactive and usually simple. However, a knowledge of elementary crystallography is assumed. Some examples, the first one in the form of a tutorial, are given after the instructions.

1.2 Starting Up

When you double-click on the SHAPE application icon, the Startup Window appears. Usually you will choose one of the buttons or select the **File** menu, both of which give the choice of starting a new file, opening an old file or importing data.

When you double-click on a SHAPE data file (.shp file) the file is read in and you see an message box giving you the choice of calculating the crystal or cancelling (see below).

The first time you run SHAPE you may want to check the dialogs in the **Settings** menu, especially the Preferences dialog. If you intend to use a pen plotter, you should select the Pen Plotter Settings command, and verify or change the settings as needed. Likewise, you many need to change or verify the PostScript Settings.

Opening an old crystal file. You can read in one of the sample files (in the \SAMPLES sub-directory), using the Open button or the command in the **File** menu. Alternatively, when SHAPE is not active, you can double click on one of the SHAPE data files (.shp files). Note that SHAPE for Windows cannot directly read files from SHAPE for DOS V4.1 or earlier - such files must be converted using the utility program FILEUP.

Entering a new crystal. You can enter a new crystal with the NEWFILE item in the **File** menu. This will step automatically through the Title/Axes, Symmetry, and Forms dialogs from the **Input1** menu.

After an old SHAPE data set has been read in or a new data set entered, you are asked if you want to "..calculate now". If you reply **Yes**, the crystal is calculated and should

appear in the Graphics Window after a short time. If you reply **No**, the Graphics window is blank when it opens; you can then modify the data for the crystal or the display parameters using the menus and dialogs, as described in Chapter III. When corrections or additions have been made, use the **Calculate** command in the **File** menu.

Importing data from a crystallographic file. The Import sub-menu in the File menu allows importation of unit cell, crystal class and space group from many types of crystallographic files.

The **Calculate** command in the **File** menu and the **Replot** command in the **Display** menu (both are also in the Dialog Bar - Left) are two of the most important and frequently-used in SHAPE. **Calculate** reproduces crystal faces by symmetry, locates corners and identifies edges, and then plots the crystal in the Graphics window. You must use this command if you change anything which affects the number and location of corners or edges. This includes many parameters in the dialogs of the **Input1** menu, although there are are also some parameters, mostly colors, whose changes do not require recalculation. **Replot** simply redraws the crystal without changing the configuration of faces, corners and edges. Changes in any of the parameters in the dialogs of the **Input2** menu can be put into effect with **Replot**.

1.3 Description of the Calculations

From the crystal class or point group, the program determines what symmetry operators to use in the calculations, and generates all the faces belonging to each form.

In order to find the crystal shape, the program solves for all intersections of three faces, which are the possible corners. However, if the crystal possesses mirror planes, it is only necessary to solve for a fraction of all the possible corners, and then reproduce the others by symmetry. For example, in class *m*3*m*, it is only necessary to find the corners in 1/48th of the crystal as a whole. This means that the calculations for crystals with mirror planes are faster than those for crystals without mirror planes; in class 432, it takes almost 8 times as long to calculate the general form (which contains 24 faces) as it does to calculate the general form in *m*3*m* (which contains 48 faces). After finding corners, each possible pair must be tested as defining an edge. For individual (non-twinned) crystals, this is the end of the calculation, although the crystal may be rotated to any orientation and rescaled as desired. Some simple tests distinguish between edges which are visible and those which are not, and no further processing of the image is required.

For contact twins, a composition plane (or planes) is added, and the superfluous portion of the crystal is removed. Then the crystal is reproduced according to the specified twin operation(s). For interpenetration twins, the individual is reproduced according to the twin operations, and then the intertwin corners and edges are located and drawn.

For epitaxial intergrowths, after generation of the two crystals they are rotated and

translated so that they are in contact on the specified face, with specified vectors in each crystal being parallel. The intergrowths can also be drawn in interpenetration geometry, like twins.

For most interpenetration and some contact twins and many epitaxial intergrowths there will be some edges of one individual which are partially or entirely behind and hidden by another individual (this problem does not arise in single crystals). Preliminary drawings of multi-crystal aggregates may thus have some extra or false lines. In order to produce an absolutely perfect final drawing, an additional procedure breaks each edge into segments defined by the intersections (in projection) with other edges, then determines whether each segment is hidden by any face. This can also eliminate edges lying within faces, which occur in penetration twins with parallel, overlapping faces.

For drawing sections of crystals, it is necessary to locate the intersection of crystal edges with the section plane, which is taken to be parallel to the screen or paper; these intersections are the corners of the section. For modeling linear growth zoning in single crystals or concentric twins, it is only necessary to rescale the crystal corners before solving for the section in each zone. For epitaxial crystals and non-linear zoning, it is necessary to repeat the entire calculation for each zone.

In 3D Drawing modes, the drawing procedure is somewhat different from the above. These modes use a depth buffer which contains the depth of the foremost object at each pixel, so that it is not necessary to solve explicitly for the intersections or front-back relationships of objects such as interpenetrating crystals. It also allows surfaces, such as crystal faces or mirror planes, to be translucent.

2 Types of Windows

SHAPE uses three types of windows besides dialogs and alerts: the Startup window; the main Graphics window; and . Each type of window has its own menu bar (in the window itself in Windows, and at the top of the screen in the Macintosh). The Help system also has its own windows and menus.

Note that under the Windows operating system the SHAPE windows are not confined to reside within a framework window, as in pre-V6.0 SHAPE.

All the current windows are listed in the Windows menu, and this menu can be used to switch between windows if some are not visible. When starting up SHAPE, the menus displayed in the Startup window include only a File menu, a Settings menu and a Help menu. Use the commands in the File menu to start a new SHAPE data set, read an old one from a file, or import data from a file with an external format.

After you have entered or read in the data for a SHAPE file, the main Graphics window

opens and the Startup window disappears; if you have elected not to Calculate, the Graphics window may be blank, otherwise it will show the current SHAPE drawing. Only one data set at a time is allowed in SHAPE, and there is only one main Graphics window. When this window is active, there is a File menu and various other specialized menus such as Input1for data input and modification and graphics output.

The List Results command in the **File** menu lists the relevant data to a Text window, as does the Section Data command (see the Sections or Growth Zones dialog (**Input1** menu). Each window actually displays the contents of a file, called respectively RESULTS.SHD, and SECTOUT.SHD. These files are written over again for each new SHAPE data set, so if they are to be preserved they should be saved with the Save As command in the **File** menu, using a different name.

Text windows are "children" of the main Graphics window, since their contents pertain only to the current structure, and they are destroyed if the Graphics window is closed.

2.1 Startup Window

See also Startup Window Menu Bar for all the menu commands available.

You should see this window only when there is no SHAPE data set in memory. To load a data set, use the New, Import or Open commands in the file menu, or the buttons with the same names.

2.2 Graphics Window

See also Graphics Window Menu Bar for all the menu commands available.

See the separate topics Dialog Bar - Left, Dialog Bar - Right and Dialog Bar - Epitaxial for help on the controls on the left and right-hand sides of the Graphics window. This window shows the structure drawing. The drawing may be rotated with the mouse or with controls in the Dialog Bar - Left and rescaled with those in the Dialog Bar - Right. Other types of rotation, rescaling, etc. are available with commands in the menus, especially Input2 and Display.

To switch to other windows (see Types of Windows), click on the other window if it is visible, or use the Window menu or an option in the Display menu.

2.3 Text Windows

This type of window has its own menu bar, with commands pertaining only to the modification, printing, saving etc. of the text file which is being edited. In Windows the menu bar is in the Window itself, and on the Macintosh it is in the standard position. On the Macintosh, to see the menu bar which allows modification of the SHAPE data set itself, return to the Graphics window by clicking on it if it is visible, or by using the

Windows menu.

The List Results command in the **File** menu lists the relevant data to a Text window, as does the Section Data command (see the Sections or Growth Zones dialog (**Input1** menu). Each window actually displays the contents of a file, called respectively RESULTS.SHD, and SECTOUT.SHD. These files are written over again for each new SHAPE data set, so if they are to be preserved they should be saved with the Save As command in the **File** menu, using a different name.

3 Menus and Dialogs

Startup Window - This window appears when starting SHAPE, or when the Graphics window has been closed.

Graphics Window - This is the main window for entry, alteration and display of crystal data sets.

Text Windows - These windows are used for the List Results and Section Data (see Sections and Growth Zones dialog in the **Input1** Menu) commands in the **File** menu of the Graphics window. It is a more-or-less standard text edit window.

3.1 Startup Window Menu Bar

File menu - Use the commands in this menu to start a new SHAPE data set or open a file for an old data set.

Settings menu - Use the commands in this menu to set operating parameters which are likely to remain constant for normal operation.

Help Menu - Onscreen help.

3.1.1 File Menu (Startup Window)

To start up SHAPE, you must select either **New** to enter an all-new data set, **Open** to open a previously-saved SHAPE data file or Import to read data from a crystallographic file.

New - Step-by-step input of a new SHAPE data set.

Open - Open an old SHAPE data file.

Import File - Import data from external crystallographic file types.

Print Setup - Select the printer and set its parameters.

Exit - Quit SHAPE.

3.1.1.1 New (Startup Window)

New Command [File menu**]**

If there is a data set in memory which has been modified, you are asked if you want to save the changes - see the Close command.

SHAPE steps through the three dialogs in the Input1 menu which provide the minimum data necessary for a problem; Title/Axes,Symmetry and Forms. You may need to select other commands in the **Input1, Input2** and **Display** menus to provide information for more complex problems or to set display parameters.

3.1.1.2 Open (Startup Window)

Open command [File menu **(Graphics Window) or** File menu **(Startup Window)]**

If there is a data set in memory which has been modified, you are asked if you want to save the changes - see the Close command.

Use this command to open an existing SHAPE data file. After the file has been read in, you are asked if you want to calculate immediately. If you click on OK, the crystal will be plotted in the Graphics window. If you decline to calculate immediately, you can modify the crystal or display parameters. When finished, use the Calculate command in the **File** menu.

You can create a new SHAPE data set with the New command, and import data from various crystallographic file formats with the Import File command.

Files written with SHAPE for DOS V4.1 and earlier cannot be read directly by SHAPE for Windows or Macintosh. You must use the DOS program FILEUP to convert these files to the newer "exchange" format.

3.1.1.3 Import File (Startup Window)

Dialog Box: Import File [File menu **(Graphics Window) or** File menu **(Startup Window)]**

If there is a data set in memory which has been modified, you are asked if you want to save the changes - see the Close command. Also, you have the option of importing the new data as an epitaxial crystal. If you select the epitaxial option, you will be routed to the Epitaxial Relations dialog after the file has been read.

SHAPE obtains only the title, the unit-cell parameters, the crystal class or point group and the space group from most import files - however the forms can also be obtained

from Free-Form (.inp) Files. The space group symmetry is only used in the Donnay-Harker Morphology option (Input1 menu).

If there is more than one data set or phase in the file, the **Data Sets...in Import File** dialog will present you with a list. The name of the SHAPE data file will be taken from the name of the file, and the title (Title/Axes dialog in the Input1 Menu) will be taken from the data set or phase. The extension .SHP will be appended to the structure file, replacing the original extension.

Read default display parameters . If this box is checked, the display parameters last saved (Settings menu) will be read for the new data set.

File Extension . The three-letter extension (.xxx) which identifies the file type may be specified here - only files of that type will be shown in the Open File dialog. To show all files, enter ".* ".

Source of symmetry (some formats lack this option). Space-group symmetry in the import files is given in one or both of two basic ways; as a space-group symbol or number, or in the form of matrices.

Symbol. If you select this option, the Hall symbol, the Hermann-Maughin symbol, and then the *International Tables* number will be used in that order if present (CIF files are the only type which is likely to contain the Hall symbol).

Use positions as xyz . If matrices are given, they are most often in the "xyz" form, in which symmetry operators are given as positions in the general equipoint as in the *International Tables for X-ray Crystallography*. This option also applies to cases in which the matrices are given in all-numerical format, such as ORTEP and RIETAN files - currently in all such cases there is no choice of symmetry format. SHAPE will try to identify the space-group from the matrices - for this to be successful, the space group must be in one of the standard settings used in SgInfo. The allowed settings are listed in the file HALL.DAT. SHAPE does not store the matrices, only the valid space-group symbols.

If the information for the symmetry option selected is not present, the other option will usually be tried. However, if identification of space-group symmetry fails, it may sometimes be necessary to re-import the file, with the other option selected. Whether the symbol or matrices are used to obtain the space group, it must be in one of the standard settings listed in the HALL.DAT file. If the setting in the file is not one of the standard ones, it may be necessary to select the space group manually in the Donnay-Harker Morphology dialog (Input1 dialog). The choice of origin in the space group is not used by SHAPE; however, the orientation may be important as SHAPE only uses certain orientations, in particular the unique axis must be b for monoclinic crystals and c in other cases (except for trigonal rhombohedral). Also, some trigonal, tetragonal and hexagonal

point groups may have alternate orientations of the symmetry elements with respect to the crystallographic *a* -axes - see Symmetry. It may be necessary to change the point group or crystal class to agree with the space-group setting.

Currently the following types of files are supported:

CCDC FDAT files from the Cambridge Crystallographic Data Centre.

SHELX .INS files from the program system of Prof. G. Sheldrick.

CIF - Crystallographic Information Files.

DBWS/LHPM Rietveld input files.

ICSD Inorganic Crystal Structure Database files. Three types of ICSD file are supported, classified according to source: 1) Files from the current CD-ROM database, accessed by the program RETRIEVE. The RETRIEVE files must be written from the DATA window using the PRINT option, not as export files (if there is sufficient demand, export files may be supported). That is, the file should be a copy of what is shown on the screen in the RETRIEVE program. 2) Files from the Canadian Scientific Numeric Database System (CAN/SND). This service may no longer be available. The files are referred to as CRYSTIN. 3) Files from the Netherlands CAOS information system. These files are also referred to as CRYSTIN.

ORTEP Original or ORTEP II atom information.

XTLVIEW Drawing program.

VIBRAT (.VBR) Graphic data files from VIBRAT or VIBRATZ (Shape Software).

ATOMS Structure drawing program (Shape Software).

RIETAN Rietveld program files.

GSAS Data files (.EXP) files from the Los Alamos Lab system.

AM MINERAL Data files from the American Mineralogist structure data base. This is currently available on the Internet at www.geo.arizona.edu/xtal-cgi.test.

FULLPROF . All-purpose refinement program.

RAVEL ATOMS This program is not the same as ATOMS by Shape Software, but is for EXAFS Analysis.

WIEN2K The program package WIEN2k performs electronic structure calculations of solids using density functional theory (DFT). CRYSCON will read the .struct input files, but will only recognize file extensions with three characters, so it may be necessary to rename the files, search manually in the File Open dialog (enter *.struct) or use the "all files" option.

IZA (zeolites). Files from the International Zeolite Association database.

FREE-FORM (.INP). Files of this type are read and written by ATOMS and CRYSCON (Shape Software). Atomic-coordinate information is ignored. All information needed for a SHAPE calculation can be entered with these files, and they should be easy to write with other software.

3.1.1.3.1 Import IZA file

Import IZA (International Zeolite Association) File [File menu]

See the Import File dialog for general aspects of importing atomic-structure data files.

The IZA has an extensive database of natural and synthetic zeolites available on the WWWeb, but does not seem to have an option for export of the data - it will be necessary to cut-and-paste the information into a text file.

Go to the Web page for the Database:

http://www.iza-structure.org/databases/

and select "**Collection of Simulated XRD Powder Patterns for Zeolites**". This should show a matrix of structure types by three-letter code - select one of these. You can also access structures in other ways, but you need to end up on a page showing options for X-ray powder diffraction together with the structure data. There should be lines for "Material name" ..."Composition:" ... "Crystal Data:" and others, with the fractional coordinates for the atoms in a table.

Mark the top right part of the page with your mouse, starting with the three-letter code centered at the top, and going below the atomic-coordinates table. Do not include the "Reset" and "Submit" buttons and material below this line. Do not include the column of options on the left of the page. Copy the marked information into the clipboard in the standard way.

Now, in a word processor, open a new text (ascii) file. Paste the clipboard contents into the file. Save the file, giving it a ".iza" extension if possible. Here is a sample (or look in the ZEOLITES subfolder for sample .iza files):

```
-------------
LAU
Material name:  Laumontite
Composition: |Ca4(H2O)18| [Si16Al8O48]
Refined composition: |Ca4(H2O)18| [Si16Al8O48]
Crystal data: Space group: C12/m1      (# 12)
 a =  14.8538 Å b =  13.1695 Å  c =  7.5421 Å
alpha =  90° beta =  110.323°  gamma =  90°

 X-ray Rietveld refinement, Rwp=0.115, Rp=0.090, RF2=0.046
  Comment: unique axis b, cell choice 1
Reference: Artioli, G. and Ståhl, K.
Zeolites, 17, 249-255, (1993)


Atomic coordinates Atom name Form factor x y z PP B(iso)
CA Ca 0.2601 0.5 0.737 1.0 3.4
SI1 Si 0.2368 0.3838 0.156 1.0 1.89
SI2 Si 0.0763 0.3834 0.325 1.0 2.13
AL1 Al 0.1315 0.3080 0.737 1.0 2.61
O1 O 0.260 0.5 0.219 1.0 0.79
O2 O 0.2084 0.3744 0.919 1.0 1.66
O3 O 0.1384 0.3838 0.552 1.0 0.55
O4 O 0.146 0.3454 0.203 1.0 2.92
O5 O 0.3205 0.3185 0.248 1.0 0.79
O6 O 0.043 0.5 0.267 1.0 0.71
O7 O 0.013 0.3083 0.743 1.0 2.53
H2O1 O2-(H2O) 0.029 0.171 0.0 0.5 2.45
H2O2 O2-(H2O) 0.401 0.5 0.026 1.0 5.92
H2O5 O2-(H2O) 0.5 0.467 0.5 0.5 3.16
H2O8 O2-(H2O) 0.1426 0.129 0.332 1.0 4.03
------------------------------
```

3.1.1.4 Page Setup

Page Setup command [File menu**]**

This allows setting of the paper type or size, the standard orientation (portrait or landscape) and the paper margins (except Macintosh). Margins will only be used in Text Windows.

---Macintosh only ------

Use the Page Margins dialog to set margins.

3.1.2 Settings Menu (Startup Window)

Preferences - Sets parameters for modes of operation.

PostScript Settings - Hardware settings for direct PostScript output.

Pen Plotter Settings - Hardware settings for the pen plotter or pen-plotter files.

Palette - Modify, save or read the RGB values for the 16-color palette.

Save Defaults - This saves default display parameters, mostly those in the **Input2** menu, for use when inputting a new crystal with the New command in the **File** menu.

3.1.2.1 Preferences

Dialog Box: Preferences [Settings Menu**]**

Scaling units. This sets either inches or centimeters as the units for overall use in SHAPE. This choice may be locally overridden for printing or other output (**File** menu) by the **Units** setting in some of the dialogs involved.

On-screen rotation increment (degrees) . This is the amount by which the image is rotated in the Dialog Bar - Left . This is the value which is in the dialog when it is first called; this value and not the latest value in the dialog itself is saved on quitting SHAPE.

On-screen rescaling factor (%) . This is the default amount by which the drawing is rescaled with the **Scale** button in the Dialog Bar - Right. This is the value which is in the dialog when it is first called; this value and not the latest value in the dialog itself is saved on quitting SHAPE.

Stereopair rotation angle . This is used in the Stereopair and Anaglyph modes set in the Drawing Modes sub-menu of the **Modes** menu or in the Dialog Bar - Left. Each view is rotated by this amount; about 3 degrees is normal. The value can also be set in the Dialog Bar - Right.

On-screen resizing factor. This is the factor by which the central distance of the selected form is increased by a click with the left button when in the **Resizing** Cursor Mode. Clicking on the right button decreases the central distance by the inverse of this factor.

Radius of stereonet symbols. This is the size, in inches or centimeters, of the symbols for crystal axes and face poles in the stereonet mode, selected in the **Modes** menu.

Sounds . This turns on or off the sounds emitted by SHAPE, for example at the beginning and end of calculation and/or plotting (some system sounds are unaffected).

Edges in faces. When different crystals in intergrowths have parallel and coincident faces, the edges lying in this common surface may or may not be realistic or meaningful, and you can elect to draw them or not. Usually the drawing is simpler and more satisfactory without them.

Always show composition-plane edges . Twins by reflection on the composition plane

should always match exactly at the junction, and a certain short-cut in the drawing of such twins is often useful. When this box is not checked, if the composition plane is forward-facing, edges with this composition plane are not drawn. This often allows simple twins to be drawn without using the **Remove Hidden Lines** option in the Display menu. However, if the twin is by reflection, the two individuals often do not match exactly on the composition plane, and visible edges may be omitted. Generally, for correct drawing of mismatching rotation twins this box should be checked, and also the **Edges in faces box** . If the **Always show composition-plane edges** box is checked, the **Remove Hidden Lines** option in the Display menu must be selected.

Screen start-up. This sets the color/black-and-white state of the screen at start of SHAPE. It can be changed with the Color command in the **Display** menu.

3.1.2.2 PostScript Settings

Dialog Box: PostScript Settings [Direct Postscript Output Dialog**] [** Settings Menu**]**

If you are using direct output to a printer you *must* select the **Port** ; this will be either "LPTn" or "COMn". Also, if you are using a serial port for the printer, you must set or verify the data transmission parameters, such as baud, parity, etc., even if the port currently shown is the correct one. This is done in the **Ports** item of the Windows **Control Panel** (not in SHAPE).

The page size, page margins and dots per inch/centimeter should be determined by the actual printer used for final output; if these are not correct, the drawing may not be scaled and/or placed on the page correctly.

The Transfer Function is analogous to the PostScript function of the same name. The linear option is standard; modify the function to get lighter or darker shading in PostScript print-out.

Preview Color . If you select a screen preview (TIFF bitmap sub-file) in the Direct PostScript Output dialog, and if color output is selected, you can specify the type of color or pixel depth used. The **Screen** option uses the color depth of the the current screen display. Black-and-white PostScript output always uses a 1-bit or black-and-white screen preview.

3.1.2.3 PostScript Transfer Function

Dialog Box: PostScript Transfer Function [Postscript Settings dialog**]**

The **Transfer Function** is analogous to the PostScript function of the same name. It changes the nominal gray values (0.0-1.0 for black-white) calculated by SHAPE as true illumination to values actually output. (Note that the PostScript gray scale, 0.0-1.0 for black to white, is in the opposite direction to the SHAPE gray scale, 0-15 for white-black;

the transfer function uses the Postscript gray scale.) If your printer gives gray shadings that are too dark (this is common, especially for lighter shades), you can increase the output values. Values in between the listed values are linearly interpolated. The actual gray values output to the printer or EPS file are changed; the transfer function itself is not part of the EPS file. Note that the gray-scale conversion also applies to lines of greater than single-dot width (single-dot lines are always black).

3.1.2.4 Pen Plotter Settings

Dialog Box: Pen Plotter Settings [Pen Plot dialog**] [** Settings Menu**]**

Current plotter radio buttons. There are several pre-programmed plotters; clicking on the Get Data button reads the pen-plotter data file (PPLOT) and obtains the commands and parameters. Even if your plotter is not listed here, you may be able to input the commands through the **Other** option. In this case, click on the Commands button to set or revise the commands and parameters.

Port . This should be either a serial or parallel port: "COMn" or "LPTn". Even if this box shows the correct port, if it is a serial port you should verify the baud, parity, stop bits and data bits in the **Ports** item in the Windows **Control Panel** . These parameters should be set to match the settings on your pen plotter (which are usually controlled by DIP switches).

Pen-change mode radio buttons. If you have a multiple-pen plotter, you can elect to run in the **Use single pen** mode with the pen number entered in the edit field, and conversely if you have a single-pen plotter you can draw with multiple colors, but you will have to change the pens manually. If you choose the **Change pens manually** mode, the plotter returns to the zero position after drawing all lines of each color, and a message box appears, prompting you to change pens.

Speed number . This is the parameter (see Commands) which controls velocity of the pen - for example for the Comrex, speed number 1 is slowest and 15 is fastest. Although some plotters, like the HP7475A, allow decimal speeds, you must use an integer here.

3.1.2.5 Pen-Plotter Commands and Parameters

Dialog Box: Pen-Plotter Commands and Parameters [Pen Plotter Settings dialog**]**

This allows you to enter or revise the pen-plotter commands and parameters, for non-standard pen-plotter types.

It is assumed that the plotter accepts ASCII commands that follow a simple syntax of "command, parameters, terminator". For example, the Hewlett-Packard command for moving the pen, raised, to the coordinates x,y is "PUx,y;". "PU" is the command, which should be entered (without parentheses) in the text box **Move - pen up** : x and y are the

parameters, which are always supplied internally by SHAPE; and the semicolon is the terminator required in the **Terminator** text box. Commas between parameters are also supplied by SHAPE. **Move - pen up** means move to the new coordinates with the pen up (not marking).

You must enter or edit the commands in the text boxes on the left of the dialog. If more than one command is required to perform the operation requested, give all the commands with any intermediate parameters and terminators required, but omit the last terminator. If your plotter does not use a command, just leave that field blank.

Following are comments on the plotter inputs. The type of variable required, and the maximum number of characters in case of a character variable, are given in parentheses. View samples by clicking on the selections in the Current Plotter group in the **[** Pen Plotter Settings dialog**]** dialog.

Commands

Move - pen up . (6 chrs) Move to the new coordinates with the pen up.

Move - pen down . (6 chrs) Move to the new coordinates with the pen down.

Raise pen . (6 chrs) Raise the pen without movement.

Pen speed . (6 chrs) This is the command which causes pen speed to be set or changed; the parameter is entered as a separate item in the Pen Plotter dialog.

Change pen . (6 chrs) This is required only for multi-pen plotters.

Start plot . (12 chrs) Initialize the plotter. May require no commands, or several.

End plot . (12 chrs) Terminate plotting. Like (12).

Terminator . (2 chrs) The character which signals the end of a command. In most cases the semicolon.

Parameters

Maximum x/y . (Decimal) Maximum x and y coordinates. These values establish the centering of the plot. Increments on the x and y axes are assumed to be equal.

x/y at finish . (Decimal) The "base" coordinates, in plotter units, to which the paper or pen will be returned at the end of the plot, or when pens are to be changed manually.

Units/inch(or centimeter) . (Decimal) This establishes the resolution of the plotter and is used in scaling. If your plotter instructions do not give this number, divide the maximum x or y coordinate (item 1 above) by its length in inches.

3.1.2.6 Palette

Dialog Box: Palette [Settings Menu**]**

The primary 16-color palette is used to set up a 256-color palette for 8-bit screen display or raster output, and also to set the primary choices for color in all cases (you can always select other colors using different RGB values). See Colors and Palettes for more detail. The default palette has the same RGB values as the "alternate" palette used in DOS versions of SHAPE, but rearranged to a more logical order.

You can read and write the RGB values to palette (.PAL) files. Two palettes are provided on file: STANDARD.PAL and ALTERNATE.PAL, which are respectively the standard IBM/DOS palette and the default alternate palette used in DOS versions of SHAPE. It is easy to write or modify the .PAL files directly; they simply contain the RGB values, from 0 to 255, separated by spaces (or commas).

3.1.2.7 Read/Save Defaults

Save Defaults Command [Settings Menu**]**

When inputting data for a drawing with the New command in the **File** menu, you can elect to use default values for display parameters, rather than set these in the dialogs of the Input2 menu. If no data set is in memory, the default display parameters are always read from disk; and if there is a data set in memory, you can use the current values or read the defaults from disk.

This option saves the current display parameters, i.e. values in the dialogs of the Input2 menu, to the file, so that they will be the default values for future input with the New command.

3.2 Graphics Window Menu Bar

File menu - In addition to the usual **New** , **Open** , **Print** etc., this menu has commands for listing input and generated data, and for for PostScript, pen plotter, raster or bit-map and Metafile output.

Modes menu - This sets the Display, Operating and Cursor modes.

Input1 menu - This contains dialogs involving mostly the basic data for the crystal, such as axes (unit cell), symmetry, forms, etc.

Input2 menu - This contains dialogs setting display parameters specific to each crystal.

Display menu - This contains commands and dialogs which set the overall display attributes of SHAPE, and modeless dialogs for rapid rotation and displacement of the crystal.

Rotation menu - This contains several options for rotating and aligning the crystal.

Settings menu - This contains settings for hardware, palette and preferences for modes of operation.

Window menu - This contains commands relating to the display or activation of the two kinds of windows - the Graphics window, and Text windows (see Types of Windows).

Help menu - Help system access.

3.2.1 File Menu (Graphics Window)

New - Step-by-step input of a new SHAPE data set.

Open - Open an old SHAPE data file.

Close - Close the current graphics window.

Save - Save a SHAPE data file.

Save as - Save a SHAPE data file with a new name.

Import File - Import data from external crystallographic file types.

Calculate - Reproduce faces by symmetry, locate corners and edges, and carry out twin operations.

Print - Print out the graphics image; see the List Results commands below for listing data and calculation results.

Print Setup - Select the printer and set its parameters.

List Results - List input data and calculation results to the file RESULTS.SHD and to a Text window.

Output group

PostScript - Direct output to a PostScript printer (bypassing the printer driver) or to an EPS file.

Pen Plot - Output to a pen plotter or HPGL file.

Raster Files - Writes raster or bit-map files in .PNG (plus .BMP, .PCX or .TIF in Windows) format.

Metafiles (Windows) or PICT (Macintosh) - Writes files to the clipboard or disk files.

Screen to Bitmap - Dumps the exact contents of the Graphics window to the clipboard or a raster file.

VRML Files - Writes files in the 3D Virtual Reality Modeling Language

POV-Ray Files - Writes files for the POV-Ray ray-tracing program.

3D-Printer Files - Writes files for 3D Printing programs.

Exit - Quit SHAPE.

3.2.1.1 New (Graphics Window)

[File menu (Graphics Window) or File menu (Startup Window)]

If there is a data set in memory which has been modified, you are asked if you want to save the changes - see the Close command.

SHAPE steps through the three dialogs in the Input1 menu which provide the minimum data necessary for a problem; Title/Axes, Symmetry and Forms. You may need to select other commands in the **Input1, Input2** and **Display** menus to provide information for more complex problems or to set display parameters.

3.2.1.2 Open (Graphics Window)

Open command [File menu (Graphics Window) or File menu (Startup Window)]

If there is a data set in memory which has been modified, you are asked if you want to save the changes - see the Close command.

Otherwise this command is the same as the Open command in the File menu of the Startup Window.

3.2.1.3 Import (Graphics Window)

The Import Submenu and Import dialog in the File menu of the Graphics Window are the same as the Import submenu and dialog box in the File menu of the Startup Window.

3.2.1.4 Close (Graphics Window)

Close Command [File menu - Graphics window]

When exiting SHAPE, closing the graphics window, reading another file or starting a new file, SHAPE tries to determine if you have made any changes in the problem currently in memory; if so, you are asked if you want to save the file.

First, it checks whether the orientation has changed from the Initial Orientation established during calculation. If so, you can save the current orientation as initial rotations. It also checks whether any dialog in the **Input1** and **Input2** menus have been opened.

You can also close a data set by using the Close icon on the Graphics window.

3.2.1.5 Save (Graphics Window)

Save command [File menu, Graphics window]

When called from the Graphics window, this saves the active data set to its current name and directory. If you have changed the orientation from that specified in the Initial Orientation dialog in the **File2** menu, you are asked if you want to save the current orientation. If you choose to do this, the current orientation will be converted to initial orientations on the observer x, y and z axes

When you save a data set for the first time, SHAPE displays the Save As dialog box so you can name your data set. If you want to change the name and directory of an existing data set before you save it, choose the Save As command.

3.2.1.6 Save As (Graphics Window)

Save As command [File menu, Graphics window]

If you have changed the orientation from that specified in the Initial Orientation dialog in the **File2** menu, you are asked if you want to save the current orientation. If you choose to do this, the current orientation will be converted to initial orientations on the observer x, y and z axes

To save a data set with its existing name and directory, use the Save command.

3.2.1.7 Calculate Command

Calculate Command [File menu]

This command must be used whenever an "intrinsic" or "input" parameter of the crystal, including most items in the **Input1** menu, is changed. For parameters which affect display only, such as line colors colors and other items in the **Input2** menu, use the

Replot command in the **Display** menu (shortcut Ctrl-R).

Generally, the time for recalculation is short on current computers, and it does no harm to use **Calculate** instead of **Replot.** One exception is when section edges have been added to the normal view of the crystal (see the Sections and Growth Zones dialog in the **Input1** menu). In this case, the **Calculate** command will cause disappearance of the section edges.

3.2.1.8 Print Graphics Image

Dialog Box: Print Graphics Image [File menu**]**

------ Linux only ---------

PostScript printing is standard in Linux, so for non-3D output printing is handled by the Direct PostScript option, not by the dialog below. However, for 3D output printing is controlled by this dialog.

------- Windows only----------

This command is for normal printer output through the printer driver (see below). If you have a PostScript printer, you should probably use the PostScript command in the **File** menu rather than this one for non-3D images; that command sends PostScript language commands directly to the printer, bypassing the printer driver. The PostScript language has a few capabilities which are missing from the system routines. Using Direct PostScript output may give somewhat different, and usually more correct colors, than using the Print option (although color inaccuracies may possibly be fixed by changing the settings of the printer driver in the Page Setup command).

In the case of 3D images (that is printing while in the 3D Display mode), SHAPE does not send drawing commands to the printer - rather the entire drawing (or sections thereof) must be imaged in memory, and this raster or bitmap image is sent to the printer.

------ Macintosh only ----------

Three different **Print Modes** may be used, depending on the settings in this dialog and the SHAPE Drawing mode - 1) Standard or QuickDraw, 2) Direct PostScript or 3) Bitmap.

Option 1) sends standard QuickDraw graphics commands (the same as those used for the screen) to a printer driver, which may be supplied by Apple or the printer manufacturer. The printer then makes the image in its own memory. You select the printer or printer driver in the **Chooser** option in the **Apple** menu (OS 8/9) or in the **Print Center** (OS X). This option sometimes results in poor quality output, with too-thick or irregular lines, patterns at a scale of 72 dpi instead of the true printer resolution, or incorrect colors. If this happens try one of the other options.

If you have a PostScript printer, for non-3D output you should probably select the **Direct PostScript** option - this causes SHAPE to send PostScript language commands to the printer instead of the QuickDraw drawing commands, although these commands are transmitted through the currently-selected printer driver. Some printer drivers, especially the standard LaserWriter drivers, may not print at the maximum resolution of the printer without this option. Note that direct PostScript printer output is only supported through this option, not through the PostScript item in the **File** menu. The **Pattern Series** selection is ignored - patterns are determined by the Printer.

Option 3) forms the image in memory, then sends it as a bitmap to the printer. This option is always used for 3D Display modes. This method may be very slow, but often gives higher quality than option 1).

------- End Linux/Macintosh/Windows only ----------

If the Standard printer dialog on OK box is checked, the Print dialog supplied by the operating system or the printer driver comes up after you click OK. Use that dialog to set the number of copies or in some cases the resolution. The orientation (portrait or landscape) can also be set in the Page Setup dialog in the File menu. If you have a color printer, you may need to
make a choice between color and black-and-white printing in one of the printer dialogs as well as with the Color printing checkbox in this dialog. This choice may be an option in the standard printer dialog above, or you may need to set it in the Page Setup option in the File menu. Background applies only to color printing; for black-and-white printing the background is always white (although you could print on black paper).

See Frames for details of the frame and frame units.

In this print option, for non-3D images, SHAPE sends standard graphics commands to the operating system, which passes them on to the printer driver, a piece of software which is normally written by the printer manufacturer (but sometimes by Microsoft in the case of Windows). For color printing, it is standard to send RGB values to specify colors for lines and files, and for black-and-white printing, it is standard to send gray-scale values (actually, RGB values with all three components equal). The printer driver interprets these values in terms solid areas and/or dot patterns of ink on the paper. No color printer can print all colors as solid areas; traditional printing uses as few as three or four colors, most commonly cyan, magenta, yellow and black, intermixed or dithered in dot-patterns to produce a full range of colors. Microcomputer printers may use more colors, but the principle is the same, and dot density is typically lower than in traditional printing, so it may be important to select colors which are as simple as possible in terms of red, green and blue or cyan, magenta and yellow (see Colors and Palettes)

Use SHAPE b/w patterns and Pattern series. Black-and-white printer drivers must interpret the gray values for fills as dot patterns of varying density. The patterns supplied

by the printer driver may or may not be satisfactory for the SHAPE user. Rather than send gray-scale values for fills, SHAPE can also send its own dot patterns, which have been carefully designed for its purposes. The Fine series is appropriate for small drawings which will not be reproduced photographically. The Coarse series simulates halftone screening and is appropriate for photographic reproduction. To be precise, at a printer resolution of 300 dots per inch, most of the patterns have a screen density of 53 lines per inch, at 45 degrees; this is about half the density of typical standard printing, so a reduction of about a factor of two is generallly satisfactory. Of course, different printer resolution would dictate different reduction factors. Note that this coarse/fine setting is the same as that in the Raster and Metafile or PICT files dialogs in the File menu.

------ Macintosh only ----------

SHAPE patterns are always used for b/w printing, but they may be rescaled or otherwise changed by the printer driver.

------- End Macintosh/Windows only ----------

Actually, different printer drivers may interpret the standard gray-scale commands in terms of patterns which are similar either to the fine or coarse series supplied by SHAPE. Some may convert the SHAPE patterns to their own patterns, and some may not accept the SHAPE patterns at all. Some may offer their own choice of pattern types or densities (typically in the printer dialog above or the Page Setup dialog in the File menu). Thus some experimentation may be necessary to find the best choice for patterns (i.e. printer-driver patterns, fine SHAPE patterns; or coarse SHAPE patterns). Gray lines of greater than one-dot width are always drawn by filling an outline with one of the SHAPE patterns - gray-scale values are not used because many printers will not print gray lines. Thus the coarse/fine setting is always used for wide b/w lines.

Maximum memory. This is used only when printing in 3D Drawing modes. Operating system support for printing in this mode is incomplete, and SHAPE itself must therefore draw raster or bitmap images and send these to the printer, rather than relying on the printer driver. Memory considerations similar to those involved in Raster Files therefore come into play.

Both Macintosh and Windows operating systems use virtual memory, which means that they pretend that a hard disk can be used in place of actual hardware memory chips. For some purposes this is useful, but when writing raster files it usually results in "disk thrashing", or constant reading and writing of data to the hard disk.

SHAPE is capable of imaging and writing raster files in segments or bands to avoid this problem. This requires repeating the entire drawing process for each band, but this usually is much faster than the reading/writing to disk involved in using virtual memory. To do this requires knowing how much actual chip memory is available. Unfortunately, at

present the operating systems do not provide this information in a usefule way. Thus the user may need to determine this by trial and error using the Maximum memory parameter. This is the same parameter which is set in the Raster Files dialog.

When the Maximum memory parameter is set to zero, SHAPE will simply ask the system for a block of memory large enough to image the entire drawing at once. If this amount of memory is greater than the amount of chip memory which is made available by the system (and this may be considerably less than the actual amount of chip memory in the computer), the operating system will use virtual memory, which is typically manifested by disk thrashing. If you change the Maximum memory to some amount than that require for the image (say half), SHAPE will only request this amount of memory from the system, and virtual memory may not come into play. A Maximum memory setting should be good for a given session, regardless of the size of the raster file; larger files will use more bands. However, the amount of memory available may depend on whether other applications are active.

The amount of virtual memory is determined by the available space on the hard disk. If this is insufficient, SHAPE will automatically use bands, but since virtual memory is being used, it may still be advantageous to use a Maximum memory value which will increase the number of bands.

3.2.1.9 Page Setup

Page Setup command [File menu**]**

This allows setting of the paper type or size, the standard orientation (portrait or landscape) and the paper margins (except Macintosh). Margins will only be used in Text Windows.

---Macintosh only ------

Use the Page Margins dialog to set margins.

3.2.1.10 List Results

Dialog Box: List Results [File Menu**]**

This will give a listing of input data as well as results for the current problem.

If the **List detailed information...** box is checked, all faces, corner and edges will be listed; otherwise only the number of faces and the orientation of the axes will be listed.

The **List angles between edges in faces** option gives angles within each face, not interfacial angles. For interfacial angles see Face at Cursor or Interfacial Angles.

Form Areas. This lists the area of each face and the total area for the form. This is in the arbitrary "central distance units". Note that it may not be possible to use any arbitrary magnitudes for central distances to match real units because of the finite tolerances used in several stages of the calculation - these tolerances assume central distances on the order of 1.0. Generally, problems with tolerances arise as the faces intersect at low angles and as the number of faces intersecting at a single corner increases.

3.2.1.11 List Section Data

This will list, in a Text Window, the results of the last Section/Zoning Mode calculation.

If there have been no section/zoning calculations, this item is not available.

3.2.1.12 Direct Postscript Output

Dialog Box: Direct Postscript Output [File menu**]**

--- Linux only ---------

PostScript printing is standard in Linux, so for non-3D output, including diffraction diagrams, printing is routed to this dialog, not the Print command in the File menu. Output can be directly to the printer or to an EPS file, as for Windows (below).

---- Windows only ----

This option can be used to write Encapsulated Postscript (EPS) files for transmission of graphics to other software, as well as for direct output to a Postscript printer. This direct output is generally superior to, as well as faster than, the output from the normal Print command in the File menu if your printer is PostScript. The Destination option sends output either directly to a printer or to a file in standard EPS (Encapsulated Postscript V3.0) format.

Screen Preview. Most word-processing and publishing software cannot display an EPS file on the screen unless the file has a special bitmap attached, called the screen preview. This is actually a sub-file in the TIFF format. The pixel depth of this file can be set in the PostScript Settings dialog (Settings button). The pixel depth of the preview is set to that of the screen, and the pattern series is set to fine (see Raster Files).

---- Macintosh only ----

This option can only be used to write Encapsulated Postscript (EPS) files for transmission of graphics to other software. For direct output to a Postscript printer, use the Print option.

Screen Preview. Most word-processing and publishing software cannot display an EPS file on the screen unless the file has a special attachment, called the screen preview. This

is actually a PICT in the resource fork of the file.

---- End Linux/Windows/Macintosh only ----

In 3D Display modes, SHAPE always writes data (or sends it to the printer) in the form of a bitmap (or "image" in PostScript terminology). Because of the facts that PostScript files must be ASCII (text), and that efficient data-compression schemes (other than the copyrighted LZW) are not supported in PostScript level 2, PostScript files for 3D drawings tend to be much larger than the best Raster formats, especially PNG. Thus the PNG Raster format is generally preferable for all 3D Display mode drawings.

The **Maximum memory** setting limits the amount of memory used for bitmap buffers when in the 3D Drawing Modes - see the Raster section for further details. The number of pixels on each raster line must be divisible by four - the image width will be increased if necessary to achieve this. Settings button (calls PostScript Settingsdialog). On or before first using the Direct PostScript Output command, you should set or verify the settings in this dialog, especially the port to which the printer is attached.

See Frames for details of the frame and frame units.

3.2.1.13 Pen Plot

Dialog Box: Pen Plot [File Menu]

On first using this command, be sure to click on the Settings button to set or verify the characteristics of the plotter, especially the plotter port.

This option can also be used to write HPGL vector files; set the **Destination** to **File** , and click on the Settings button and select **HPGL plotter** .

See Frames for details of the frame and frame units.

3.2.1.14 Raster (Bitmap) Files

Dialog Box: Raster (Bitmap) Files [File Menu]

--Windows/Linux Only ----------

This command can write files in four different formats (**File type**): Windows device-independent format (.BMP); PC-Paintbrush (.PCX); Tag-image-format (.TIF); and Portable Network Graphics (.PNG) files.

If the **Compress .BMP** box is checked, 4- and 8-bit .BMP files are compressed; 1- and 24- bit .BMP files are never compressed. Owing to a system bug, compression of 4-bit .BMP files may not work when banding is used (see below). TIF files are compressed with run-length encoding, which is one of the required formats under the TIFF 6.0

standard. However, some applications may not support this type of compression, or may reject .TIF files for other reasons.

--Macintosh only---------

This command can write files in the Portable Network Graphics (.PNG) format. The PICT Files option (File menu) can also write raster or bitmap files, in the PICT format.

--End Windows/Macintosh only----

See **Selection of File Format** below for information on choosing the format.

Each one of these may be either black and white or color. If black and white, the **pixel size** is 1-bit. For color files the pixel size is based on the current screen; 4-bit for standard VGA or other 4-bit display, 8-bit for 256-color display, and 24-bit for 16- or 24-bit display.

The images will look much the same as a screen image, except that for black-and-white files there is a choice of coarse or fine dot patterns to represent gray shades, as for printing and metafiles (see the Print dialog in the File menu). Fine patterns are appropriate for small images which will not be reproduced photographically, or for images which will be shown on the screen only; coarse patterns mimic halftone screens used in printing, and generally reproduce better photographically, especially when the image is reduced in size. Note that this coarse/fine setting is the same as that in the Print and Metafiles dialogs in the **File** menu.

See Frames for details of the frame and frame units.

Maximum memory . Windows and Macintosh use *virtual memory* , which means that it pretends that a hard disk can be used in place of actual hardware memory chips. For some applications this is useful, but when writing raster files it often results in "disk thrashing", or constant reading and writing of data to the hard disk.

SHAPE is capable of imaging and writing raster files in segments or bands to avoid this problem. This requires repeating the entire drawing process for each band, but this usually is much faster than the reading/writing to disk involved in using virtual memory. To do this requires knowing how much actual chip memory is available. Unfortunately, at present Windows does not provide this information in a way that can be used for both 16- (standard Windows 3.1) and 32-bit (Windows NT) systems. Thus the user may need to determine this by trial and error using the **Maximum memory** parameter.

When the **Maximum memory** parameter is set to zero, SHAPE will simply ask the system for a block of memory large enough to image the entire drawing at once. This amount of memory is printed out in the dialog which appears after starting the raster

imaging: "nnnn bytes required, mmmm bytes available - will require 1 bands". If this amount of memory is greater than the amount of chip memory available, Windows will use virtual memory, which is typically manifested by constant running of the hard disk for long periods. If you change the **Maximum memory** to some amount smaller than nnnn (say half), SHAPE will only request this amount of memory from the system, and virtual memory may not come into play. A **Maximum memory** setting should be good for a given session, regardless of the size of the raster file; larger files will use more bands. However, the amount of memory available may depend on whether other applications are active.

The amount of virtual memory is determined by the available space on the hard disk. If this is insufficient, SHAPE will automatically use bands, but since virtual memory is being used, it may still be advantageous to use a **Maximum memory** value which will increase the number of bands.

Testing has suggested that a Maximum memory setting of about 1 mb (1000 kb) may be the optimum, at least for simple drawings.

Note that from V5.0.1 SHAPE uses Windows system routines to draw bitmaps, rather than its own assembly-language routines, which were used in DOS versions and V5.0 for Windows. The only effect of this from the user's point of view is to remove complete freedom in determining the pixel size of color bitmaps.

Selection of File Format. The choice of format depends first of all on what formats are supported by the target software (paint program; publishing program; etc.). Beyond this the first choice should be PNG. For Windows the second choice should be PCX, and then TIF or BMP depending of what is supported and how much memory or disk space is available. For Macintosh, the only choice besides PNG is PICT , which is usually not as compact, but this may depend on the Macintosh operating system.

As of 1997, the preferred graphics file types for the internet were GIF and JPEG. However, GIF uses the LZW compression scheme copyrighted by Unisys Corp., which in principle charges a license fee for every application using it. JPEG files are compact but involve losses and degradation of the image and are thus not suitable for SHAPE files.

The PNG format is intended to be a replacement for GIF, and in fact is superior to most other formats, being lossless and giving very good compression for the type of images generated by SHAPE (although 3D images do not compress as well as standard-mode images). Essentially all major software vendors have subscribed to the PNG convention and releases from 1998 onward should support it.

Most TIF files also use LZW compression, but SHAPE does not use this type of compression because of the copyright problem. The run-length-encoding which SHAPE does use is supposed to be supported by all TIF readers, but in fact some do not support

it, and this algorithm does not work well for 24-bit (RGB) images.

There are dozens of raster graphics formats and it will never be possible for SHAPE to support all of them. SHAPE users who work with raster files should consider investing in a conversion program - there are many such programs which are not expensive. Hijaak, by Inset Systems, handles a great many raster, metafile and vector formats. The PNG home page (www.cdrom.com/pub/pnp) has links to many shareware and conventional commercial conversion packages.

3.2.1.15 Metafiles

Dialog Box: Metafiles [File Menu**]**

-----Entire topic Windows only ----------

Windows metafiles are basically vector images (but including fills) that can be rescaled without necessarily losing resolution. They record the drawing commands that are used for the screen or standard printer output, but the result may depend on the software or device for which they are intended. A metafile image may either be saved in the Clipboard, to be Pasted into another application, or written to a file.

SHAPE can write three types of metafiles. The original or standard metafile format has proven inadequate for transmitting scaling information, and many applications do not even accept Standard metafiles. Placeable metafiles, a format which was originated by Aldus Corporation, contain scaling information in an additional header. The standard and placeable metafiles have the .WMF extension. WMF or standard files are 16-bit format, i.e. use 2-byte integers. Enhanced metafiles are 32-bit format files which also contain scaling information. They are the preferred type of metafile for use in 32-bit Windows systems (Windows NT or Windows 95), but cannot be used in standard 16-bit Windows 3.1or Win32s.

Original (16-bit or .WMF) metafiles can be written with either of two Scaling Modes; Isotropic or Anisotropic. Isotropic supposedly keeps the same proportions. Generally, Isotropic is the best as it allows rescaling while preserving proportions. However, some applications only accept Anisotropic files, and some ignore the scaling mode completely. The type of image written by this option is strictly two-dimensional. It is also possible to write files containing three-dimensional images with the VRML Files and POV-Ray options.

When writing to a file, to prevent loss of resolution, SHAPE uses a standard scaling of 2540 dots or pixels per inch (1000/cm). However, some drawing applications may not read the scaling correctly (assuming 72 dpi) and it may be necessary to rescale the drawing after importation.

When writing to the clipboard, SHAPE uses the current screen resolution, which usually

is about 92 dpi. This is because most drawing applications assume screen resolution or 72 dpi. The clipboard image can be either 16-bit (.wmf) or 32-bit (.emf) according to the setting of the **Type** option.

See Frames for details of the frame and frame units.

Limitations of Metafiles. As designed and implemented by Microsoft, the metafile allows recording of all Windows drawing commands, so that a file image can be a copy of what is shown on the screen but rescalable. Unfortunately non-Microsoft drawing applications (e.g. Corel Draw, Adobe Illustrator) sometimes implement metafiles incompletely or incorrectly so that there are some limitations in metafiles written by this option, in order to allow them to work in as many applications as possible. It many be necessary to try many combinations of settings (Destination, Scaling mode, Type of file) to get satisfactory results in an importing program.

1) Resolution for the clipboard is now that of the screen, typically 72-96 dots-per-inch (dpi) - earlier versions of SHAPE used 2540 dpi. The lower resolution should not cause problems except for very complex drawings - if a drawing looks good on the screen, it should look good in a document. If the clipboard is unsatisfactory use a file.

2) Bitmap patterns for black-and-white images cannot be used. Fills are transmitted as gray shades which are interpreted by the importing application and/or printer.

3) A background is always present, to insure correct scaling. With some care, this drawing element may be removed in importing applications.

4) There is no clipping of the image, although some importing applications may use the drawing frame for clipping. For

5) Transmission of the image in Corel Draw with the Clipboard may require use of Edit/Paste Special rather than a simple Paste.

6) Adobe Illustrator generally does not do well with labels - is may be necessary to use an EPS file for Adobe Illustrator. Label backgrounds may not be transmitted in other applications.

If a metafile is not satisfactory, a raster file can be used. PNG raster files are often smaller than metafiles, especially for complex drawings. Also, many drawing programs now support import of EPS (Direct PostScript) files. EPS is usually the preferred type of file for Adobe Illustrator.

3.2.1.16 PICT Files

Dialog Box: PICT File (Clipboard) [File menu]

------ Entire Topic Macintosh Only -----------

Note that this type of output may be referred to elsewhere as Metafile output. This option can write images either to PICT files or the Clipboard, in either of two formats: (a) a rescalable 2-dimensional Picture or metafile, or (b) a raster image or bitmap.

For the 3D Drawing mode , this option writes a two-dimensional image and only bitmaps are available, but see the VRML Files option for files which actually contain three-dimensional data Macintosh **Pictures** , as used here, are images containing lines or vectors and fills of regions defined by lines, that can be rescaled without necessarily losing resolution. They record the drawing commands that are used for the screen or standard printer output, but the result may depend on the software or device in which they are used.

Bitmaps or raster images record every pixel, so they are not susceptible to undesirable modification by other software. Although most "painting" software can resize bitmaps, this usually causes a loss of quality, so it is best to save a bitmap in exactly the desired size. Note that you can also save bitmaps in the **PNG file** format (File menu), which is superior is some respects to PICT files.

If color output is selected, you can choose either 16- or 32-bit color depth - 8-bit (256-color) files cannot be written.

You can select the nominal dots per inch/centimeter, and this is written into the PICT file, but note that programs which read the file may ignore this and show the image at 72 dots per inch.

Background color. If this option, which applies only to Picture output, is on, the color selected in the Background Color dialog of the **Input2** menu will be applied in color output only. Background in b/w output is always white.

In the 3D drawing mode PICT (bitmap) output always has 32-bit pixel depth.

See Frames for details of the frame and frame units.

3.2.1.17 Screen to Bitmap

Dialog Box: Screen to Bitmap (.BMP) [File Menu]

This command writes a bitmap giving *exactly* what is shown inside the current graphics window, not including any overlapping windows. It will save a Device-Independent-

Bitmap (DIB) either to the clipboard or to a .BMP file.

This is appropriate for applications which will use the image on the screen. For applications which will use a printed image, either the Raster Files or Metafiles options will usually give better results.

You can also copy the current window to the clipboard with the **Print Screen** key (this is a standard Windows function). However, this includes the window title bar and border and parts of overlapping windows, whereas the **Screen to Bitmap** command only copies the graphics part or the client area.

3.2.1.18 VRML Files

VRML Files [File Menu**]**

Virtual Reality Modeling Language files were intended for exchange of virtual reality data on the Internet. However, they have become a de facto standard for interchange of 3D data of all types. SHAPE currently supports V1.0 ascii files.

VRML files can be viewed with the Netscape Navigator browser for Windows, using the Live3D plug-in or the SGI Cosmoplayer plug-in. The Microsoft Internet software for Windows 95 can also view VRML files. Since the files are text, they can also be viewed on any system. VRWeb for Windows 95/NT is a viewer which is independent of Internet browsers - it is smaller and faster than the browser plug-ins. Viewers may not support all features, such as transparency.

For the latest information on crystallographic applications of VRML see http://193.49.43/dif/3D_crystals.html or http://fluo.univ-lemans.fr:8001/vrml/intvrml.html.

The images will be very similar to those in the 3D Display mode on screen.

3.2.1.19 POV-Ray Files

POV-Ray File Output [File menu**]**

POV-Ray is a program which draws a 3D image pixel-by-pixel, calculating all possible light-ray paths. It allows for much more elaborate lighting effects than the OpenGL or Direct3D software used in the 3D Drawing Modes in SHAPE. Some obvious effects are refraction and internal reflection but there are many possibilities. Backgrounds and other objects may be added as well. The files are text (ASCII) and may be edited.

Since the calculation is much more elaborate than that done by OpenGL, this is not a method that can be used for real-time display on the screen - POV-Ray images may take many minutes to complete.

The POV-Ray package, with instructions, samples, etc., may be obtained from www.povray.org.

Since the primary purpose of the option is try to produce truly realistic drawings of crystals, symmetry elements are not presently included.

See Frames for details of the frame and frame units.

3.2.1.20 3D Printer Files

3D Printer File Output [File menu**]**

This is for the particular types of files which can be read by 3D printing software. StereoLithograpy (.stl) files should be universally read, but they are bulky and have no color information. Wavefront (.obj) files do allow color, although few low-cost printing programs accept color. Colors for different crystals in twins or epitaxial intergrowths are specified in the 3D Crystal color dialog in the Input2 menu.

Only the crystals themselves (their faces) will be put in the file - no edges, crystal axes, symmetry elements etc. and no face fill colors or striations.

Scale factor. The finite tolerances in SHAPE calculations are designed for central distances on the order of 1 A, so it may be convenient to use the scale factor in this dialog - usually a factor of 10 or more is required to convert to printer coordinates if the files are read in as millimeters.

Separate objects/colors. When multiple crystals are present, they may be designated as separate objects (with color and other 3D materials for .obj files). If not, all crystals are simply part of a single object. Some programs may ignore the separate objects, but some may allow movement or deletion of the separate objects. If this is selected for .obj files, a separate .mtl file is written to contain the color and material properties (specified in the 3D materials dialog).

The Windows program AccuTrans 3D will read VRML (.wrl) files written by SHAPE and convert them to .stl, .obj and many other formats.

3.2.1.21 Exit/Quit

Exit/Quit command [File **menu]**

Use this command to end your SHAPE session. SHAPE prompts you to save data sets with unsaved changes.

If you have changed the orientation from that specified in the Initial Orientation dialog in the **File2** menu, you are asked if you want to save the current orientation. If you choose to do this, the current orientation will be converted to initial orientations on the observer

x, y and z axes. If clinographic viewing is in effect at the time of saving, the initial clinographic viewing flag will be turned on. The initial rotations can be changed or deleted in the Initial Orientation dialog in the **File2** menu. See also Coordinate Systems.

3.2.2 Modes Menu

This has four submenus, for selecting the **Model, Drawing, Operating** and **Cursor** modes. The selections in the **Model, Drawing** and **Operating** mode submenus are also in the Dialog Bar - Left, turned on and off in the Display Menu. The **Cursor** modes are also in the Dialog Bar - Right.

The **Model** mode determines how the crystal(s) are displayed.

In **Standard** mode, there is an external view, and this view occupies the center of the viewing area unless it is deliberately displaced. In the original orientation, the view is down a*.

In **Stereonet** mode, the standard drawing of the crystal occupies the left half of the viewing area, and a standard Wulff Stereonet occupies the right half. The original viewing orientation of the crystal is different from that in the standard mode; it is viewed directly down the c crystallographic axis rather than the a* axis. If clinographic viewing is on for the standard view, it is ignored in the stereonet mode. Other rotations are transferred between the two modes.

In **Section/Zoning** mode, a section or successive sections of the crystal, parallel to the y-z plane, are drawn. The many parameters for this type of view are set in the Sections and Growth Zones dialog in the **Input1** menu and its subdialogs. This mode is not available in SHAPE Standard Edition.

The **Drawing mode** determines what method is used to draw the crystal(s). The drawing can be in 2D (two-dimensional) mode, for more schematic drawings; or in 3D (OpenGL) mode for more realistic representation as 3D objects. For actual stereoscopic viewing, either 2D or 3D can be shown as separated stereopairs, the Quad Stereo mode can take advantage of hardware which supports quad-buffered OpenGL or the Direct3D mode can show also stereo in Windows with appropriate hardware.

The **Operating mode** determines whether SHAPE uses procedures for normal crystals **(Crystal** or SHAPE mode) or for non-crystallographic symmetry **(Cartesian,** quasi-

crystal or QSHAPE mode).

Polyhedral solids with non-crystallographic symmetry such as icosahedral or pentagonal are often referred to as quasi-crystals (hence the name QSHAPE, formerly used for a separate version of SHAPE). The Cartesian mode is not available in SHAPE Standard Edition.

For normal crystallographic symmetry, SHAPE can simply permute and/or negate the indices of input forms to find all the symmetry equivalents. The form/face indices refer to intercepts on axes whose length and mutual inclination vary. It is only necessary to select one of the 32 crystallographic point groups or crystal classes.

For quasi-crystal symmetry, face/form indices always refer to Cartesian axes, and it is necessary to read a file containing the symmetry matrices. An auxiliary program, SYMGRP, can write these files, although the files containing matrices for the icosahedral and pentagonal groups are provided. Indices are integers for the Crystal mode, and decimal or floating-point numbers for the Cartesian mode. Cartesian-mode indices are always normalized automatically to a length of one.

Apart from the symmetry input and the integer/floating-point nature of indices, operation is almost identical in the two modes.

The **Cursor Mode** determines what happens when you click in the graphics window.

In the **Index** mode, when the left mouse button is clicked, the face is identified and certain other information is given (see Face at Cursor). If the right button is clicked on an edge or corner, you have the option of adding a face truncating that edge or corner - the indices of the new face will be the sum of the indices of the faces involved in the edge or corner.

The **Resizing** mode allows automatic adjustment of central distances and therefore face sizes. In this mode, clicking the left button on a face will increase the central distance of the *form* , and cause recalculation (the current orientation will be retained). Of course, increasing the central distance generally decreases the size of the faces in the form. Clicking the right button decreases the central distance. The amount of the increase or decrease is set in the Preferences dialog in the **Settings** menu. Clicking on a face of a twin will cause a change in all the twin individuals.

Note that the **Resizing** mode affects all faces of a form. If you want to change individual faces, distorting the crystal from ideal symmetry, select the **Remove Symmetry** button in the Dialog Bar - Right, or go the the Symmetry option in the Input1 menu and select the **Remove Symmetry** button.

When in the **Resizing** mode, there is a box in the upper left of the graphics window labelled "Resize mode off". Clicking in this box will revert to the **Index** mode.

In the **Rotate** mode, clicking and dragging in the major part of the graphics window causes rotation on either or both of the reference axes in the plane of the screen. Clicking and dragging near the left-hand or upper edges causes rotation on the axis perpendicular to the screen.

Summary of mouse cursor operations in graphics window. For Macintosh, "Right button" is obtained with the option key plus the mouse button.

Index (Identification) mode:

Left button - identifies face and form; successive clicks give interfacial angle.

Right button - identifies edges and corners; allow addition of new form truncating face or corner.

Resizing mode:

Left button - increases central distance of form selected - usually decreases area.

Right button - decreases central distance of form selected - usually increases area.

Rotate mode:

Left button - click and drag in main part of window rotates around axes in screen; click and drag near left or upper edge rotates around axis perpendicular to screen.

3.2.2.1 Model Mode Sub-Menu

Sub-Menu - Model Mode [Display menu]

The **Model** mode determines how the crystal(s) are represented.

The **Standard** mode is an external view, and this view occupies the center of the viewing area unless it is deliberately displaced. In the original orientation, the view is down a*. The crystal may be shown as a single crystal or as a stereopair; and it may be shown in 2D or 3D Drawing mode.

In **Stereonet** mode, the standard drawing of the crystal occupies the left half of the viewing area, and a standard Wulff Stereonet occupies the right half. The original viewing orientation of the crystal is different from that in the standard mode; it is viewed directly down the c crystallographic axis rather than the a* axis. If clinographic viewing

is on for the standard view, it is ignored in the stereonet mode. Other rotations are transferred between the two modes. This is shown in a 2D Drawing mode only.

In **Section/Zoning** mode, a section or successive sections of the crystal, parallel to the y-z plane, are drawn. The many parameters for this type of view are set in the Sections and Growth Zones dialog in the **Input1** menu and its subdialogs. This is shown in a 2D Drawing mode only.

3.2.2.2 Drawing Mode Sub-Menu

Sub-Menu - Drawing Mode [Display menu]

This sub-menu switches between 2D and 3D types of drawing, and also allows "true" stereoscopic drawing, that is drawing with quad-buffered OpenGL with appropriate hardware.

Graphics in the Standard Model mode can be either 2D, which uses the standard system software for drawing in two dimensions; or they can be 3D, which uses the system software (OpenGL) for drawing three-dimensional objects. The StereoNet and Sectors/Zoning Model modes are 2D only.

3D**.** Although a fully shaded drawing done in the **Standard** mode may have a highly 3-dimensional appearance, this option, which uses special system software not available on all machines, allows a number of extra options in terms of lighting and material properties and is the only Drawing mode in which symmetry can be shown. Switching into this mode requires loading the system software, which may take a few seconds.

The choices in this submenu are also in the Drawing Mode drop-down in the Dialog Bar - Left which is controlled from the **Display** menu.

The OpenGL system software (abbreviated OGL in some situations) is available on all platforms - Windows, Macintosh and Linux. It can always be used to get 3D images, but may require a special graphics card such as the nVidia Quadro series to show non-separated "true" stereo.

3D Quad Stereo. This is a special kind of OpenGL drawing mode, which uses quad-buffered display hardware to draw left- and right-eye images, which are alternated on screen or other viewing device at a high rate, or which may even be drawn on separate displays. Most systems require wearing special glasses, either shutter glasses or some type of polarizing glasses. Currently nVidia, in their Quadro line of display cards, provides the most widely available type of quad-buffered systems, which must be used with certain types of monitor. Quad-buffered OpenGL may also be supported by other hardware such as projectors and using software drivers other than nVidia, such as iZ3D and TriDef.

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Direct3D (Windows only). This is Microsoft's version of 3D software. The only reason for using this mode instead of the OpenGL modes is to support stereoscopic viewing with shutter glasses or polarizing monitors using those display cards which do not support quad-buffered OpenGL. This includes most of nVidia's display cards except Quadro cards.

Fullscreen Mode. Any of the display modes can be shown in fullscreen mode rather than in the graphics window. Change to fullscreen with the Fullscreen option in the Display menu or the Fullscreen button in the Dialog Bar-Left

3.2.2.2.1 2D Drawing Modes

These drawing modes can be selected in the Drawing Mode submenu in the **Display** menu, or in the Dialog Bar - Left**.**

This mode is actually very flexible, and supports representations ranging from very schematic line drawings to fully three-dimensional, but it will not show symmetry.

The alternatives to 2D modes are 3D Drawing modes, which give a more realistic appearance in full color, but are not generally suitable for schematic drawings. See Description of the Calculations for details on the difference between 2D and 3D Drawing modes.

Stereopairs. Selecting **2D Stereopair** causes two separate drawings to be made, which are identical except for the Stereopair Rotation Angle. Many people cannot view a stereopair directly because of the difficulty of getting the left and right eyes to focus on separate points at a short distance. However, various devices are available for such viewing, using lenses, mirrors or prisms.

Some people can view stereopairs by crossing their eyes, without artificial aids. For this, the Stereopair Rotation Angle should be negative.

Stereo viewing works best when Perspective is selected.

3.2.2.2.2 OpenGL Drawing Modes

These drawing modes can be selected in the **Drawing Mode** submenu of the Display menu, or the Dialog Bar - Left**.**

The **OpenGL** modes use the OpenGL system software for a more "realistic" appearance. Since this type of drawing automatically handles the interpenetration and intersection of solid objects (using a depth buffer), it allows the depiction of symmetry elements, that is rotation axes and mirror planes. See 3D Drawing modes for more details. Settings for

this mode are in the 3D Parameters dialog in the Input2 menu.

The **OpenGL Stereopair** mode shows two images, as in the 2D **Stereopair** mode, but they are drawn using the 3D method.

Although a fully-shaded SHAPE drawing in the 2D Drawing modes has an excellent 3-dimensional appearance, the term "3D drawing" is used to denote a method of drawing which is different in several respects. SHAPE uses the OpenGL software package for Windows, Linux and Macintosh. 3D Drawing modes give a more realistic appearance in full color, especially on screen, but are not generally suitable for schematic drawings, as there are no boundary lines. See below and in Description of the Calculations for details on the difference between 2D and 3D Drawing modes.

Stereopairs. Selecting **3D Stereopair** causes two separate drawings to be made, which are identical except for the Stereopair Rotation Angle. Many people cannot view a stereopair directly because of the difficulty of getting the left and right eyes to focus on separate points at a short distance. However, various devices are available for such viewing, using lenses, mirrors or prisms.

Stereo viewing works best when Perspective is selected.

In order to show non-separated stereo views with OpenGL, you must have an appropriate graphics card and viewing hardware, and you must select the
OpenGL Quad Stereo Drawing Mode

Some people can view stereopairs by crossing their eyes, without artificial aids. For this, the Stereopair Rotation Angle should be negative.

Older stereo drawing drivers from nVidia, which worked with shutter glasses but only on Cathode-Ray-Tube monitors, not flat-screen LCD monitors, supported OpenGL without quad-buffering. If you are using such a system, you do not need to select the SHAPE 3D Quad Stereo Mode; stereo images can be viewed in the **3D Single Drawing** mode. However, stereo will be shown only in Fullscreen display, not in a window. The stereo effect is turned on with a hot key or other switch for the hardware.

Difference Between 2D and 3D Drawing Modes.

In 3D drawing, the surfaces of three dimensional objects such as spheres and cylinders are converted to an assemblage of planar polygons. Then each polygon is drawn essentially independently. The critical difference from 2D Drawing modes is that a *depth buffer* is used in 3D imaging. This is an array of integers, one for each pixel in the display or output (or that portion which is currently being drawn). Each element, representing a pixel, holds the relative x coordinate (in the SHAPE observer coordinate system) of the foremost object or polygon. The color for this object is retained in the *color buffer*,

which is a similar array representing pixels; this array is actually the image itself. Whenever a polygon is drawn, each pixel which it contains is compared against the depth buffer; if the *x* coordinate of the pixel is greater, or closer to the observer than what is in that element of the depth buffer, the color for this pixel in the new polygon replaces the value in the color buffer. That is, the depth buffer keeps track of the front surface of the drawing, and ensures that only this front surface (not any hidden surfaces) are kept in the color buffer or image itself. It is also possible to have transparent or translucent objects, through which hidden surfaces may show partially, by mixing the color of the latest object with the color which is already in the buffer.

Actually, the "double buffer" method is normally used, the color buffer being kept in an area of memory and then copied to the screen memory when the drawing is completed. This is usually faster than drawing directly to the screen.

The 2D Drawing modes of SHAPE do not use a depth buffer. When necessary, the intersections of objects are solved analytically and only the required portions of each are drawn.

Using a depth buffer has the advantages that it is not necessary to solve analytically for intersections, nor to sort the objects with respect to depth (unless some objects are translucent). This may save considerable time, especially for complex drawings, since the time for sorting tends to increase exponentially with the number of objects. Since analytical solution of intersections is not necessary, it is possible to place essentially any objects into the drawing. in any location. This overcomes the problem in SHAPE 2D Drawing modes of sometimes-incorrect drawing of crystal edges. The 3D method allows more complex shading and lighting effects, such as specular highlights and multiple light sources. For a completely 3-dimensional image, on a computer which has sufficient memory, the 3D Drawing mode is superior to the SHAPE 2D Drawing mode.

However, there are disadvantages to the 3D method. The depth buffer may result in excessive memory requirements even for the screen (but some 3D accelerator cards may have special memory for the depth buffer). Because printers have much higher resolution than the screen, this causes even higher memory requirements, and for reasonable sized printed drawings it is usually necessary to do the printing in bands or segments.

3.2.2.2.3 OpenGL Quad Stereo Drawing Mode

This drawing mode can be selected in the **Drawing Mode** submenu of the Display menu, or the Dialog Bar - Left**.**

This is a special type of 3D Drawing mode which is available only for graphics hardware supporting OpenGL quad-buffered stereo. In this mode, left- and right-eye images are drawn and displayed by either of two methods:

1) Shutter glasses. The images are drawn independently and flashed alternately on the screen at a high rate - 120 times per second in the latest computer implementations, for example those supported by the nVidia Quadro series of display cards. A special monitor is required, and it must be viewed with special shutter glasses which blank out the left and right eyes alternately in synch with the images on the screen.

2) Polarized monitors or projections. The monitor or projector simultaneously or alternately (very rapidly) generates two images which are polarized at 90 degrees to each other, or with different circular polarizations. Some "3D" (stereoscopic) televisions have different polarizations (and different images) for alternate lines on the screen and some projectors and TV's use a checkerboard pattern. Theater 3D systems use this method. It does not require expensive shutter glasses, only relatively cheap polarizing glasses for each viewer.

See the Stereoscopic Display section in Reference for general requirements and procedures.

Two settings affect the perception of depth in stereo viewing:

1) The Stereopair Rotation Angle, set in a dialog in the Input2 Men, or in the DialogBar - Right. A value of about 1 to 3 degrees is usually appropriate (smaller when starting out in stereo viewing).

2) The Perspective distance which is set in a dialog in the Input2 Menu, or in the DialogBar - Right. A value of about 100 Angstroms is usually appropriate, but it may be smaller for small structures.

In viewing real life objects setting the perspective distance would fix the stereopair rotation angle because the human eyes are a fixed distance apart. However in viewing objects on an Angstrom scale the interocular distance is arbitrary, and thus it is possible to set both parameters - in effect the stereopair rotation angle fixes the interocular distance or the scale of the atomic structure relative to the viewer.

Not all stereo hardware supports OpenGL. The GeForce series of video cards from nVidia supports stereo viewing with shutter glasses, but only through the Windows 3D system software, Direct3D, for which a different drawing mode is available in SHAPE. Direct3D is only available on Windows systems, not Macintosh or Linux. Although hardware is indifferent to whether the program draws in 3D through OpenGL double-buffered, OpenGL quad-buffered or Direct3D, the proper driver software must be present. Polarizing monitors may or may not have drivers supporting OpenGL.

Older stereo drawing drivers from nVidia, which worked only on Cathode-Ray-Tube monitors, not flat-screen LCD monitors, supported OpenGL without quad-buffering, as well as Direct3D. This system worked with inexpensive shutter glasses, but if the refresh

rate of the monitor is less than 100 hz or so the flicker tends to be excessive. If you are using such a system, you do not need to select the SHAPE **3D Quad Stereo** Mode; stereo images can be viewed in the **OpenGL Single Drawing** mode. However, stereo will be shown only in Fullscreen display. The stereo effect is turned on with a hot key or other switch for the hardware.

Stereo viewing works best when Perspective is selected.

Certain high-end nVidia Quadro cards support quad stereo on Linux, using special "Professional" emitters and glasses. This mode is thus available in Linux, although it will not produce stereo images without this special hardware. This mode has not been tested on Linux.

Setting up nVidia 3D Vision for quad-buffered OpenGL. In the nVidia control panel, select Manage 3D Settings in 3D Settings. In the Global Settings tabe, the Global presets option can be set to "3D OpenGL Stereo". It may then be necessary to select the particular setting Stereo - Display Mode and set it to "Generic active stereo (with NVIDIA 3D Vision)".

If you have a recent Vidia Quadro card it may support 3D Vision stereo through Direct3D as well as OpenGL. There seems to be no advantage to using Direct3D if quad-buffered OpenGL is available, but if Direct3D is used, different settings may need to be selected in the nVidia Control Panel. The Global preset option should probably be "3D App - Default Global Settings". All the nVidia settings may change and it may be necessary to experiment to find the best combination.

In this mode, the "separation" of the images is controlled with the Stereopair Rotation Angle dialog in the Input2 Menu, or with the DialogBar - Right.

Not all stereo hardware supports OpenGL. The GeForce series of video cards from nVidia supports stereo viewing with shutter glasses, but only through the Windows 3D system software, Direct3D, for which a different drawing mode is available in SHAPE. Direct3D is only available on Windows systems, not Macintosh or Linux. Although hardware is indifferent to whether the program draws in 3D through OpenGL double-buffered, OpenGL quad-buffered or Direct3D, the proper driver software must be present. Polarized monitors may or may not have drivers supporting OpenGL.

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3.2.2.2.4 Anaglyph

In **Anaglyph** mode there are two views of the crystal, but instead of occupying separate halves of the screen or paper they are drawn in two different colors such as red and blue and superimposed in the center of the screen or paper. This type of drawing must be viewed with standard colored 3-D glasses, which have a red lens for the left eye and a green or blue lens for the right eye.

There are several settings for this mode, such as the background and line colors; see the Anaglyph Settings dialog in the Display Menu

3.2.2.2.5 Direct3D Drawing Mode

This is a 3D mode using the Microsoft Direct3D (DirectX) software, which is essentially equivalent to OpenGL. The main reason for selecting this mode is to display

stereoscopically using shutter glasses or a polarizing monitor, if you have a display card which supports stereo only using Direct3D, not OpenGL quad-buffering. See the Stereoscopic Display section in Reference for the requirements and procedures.

This mode also allows anaglyph (Red/Green or Red/Blue) stereoscopic viewing with appropriate software drivers. This requires only cheap plastic colored glasses. The nVidia GeForce graphics cards which support stereo viewing with shutter glasses also support anaglyph viewing - in the nVidia Control Panel, enable Stereoscopic 3D and select "3D Vision Discover" in the Stereoscopic 3D display type option. Since SHAPE has its own Anaglyph mode there is usually no reason to use the 3D Vision Discover mode.

Other software vendors such as iZ3D and TriDef supply drivers which may support anaglyph or various other kinds of stereoscopic viewing on your system.

In this mode, there is no face identification with the mouse; clicking and dragging with either the left or right button rotates the structure. The shortcut keys control rotation, scaling, etc.

Stereo Viewing with nVidia shutter glasses. The nVidia GeForce display drivers prior to V266 supported stereo viewing only in fullscreen mode, not in a window. If you have an old driver you will have to go into fullscreen mode (Fullscreen button in the Dialog Bar - Left) to see stereo, but you should download the updated driver from nVidia if possible. For smoothest operation of windowed stereo, in the nVidia Control Panel, under Stereoscopic 3D/Set up stereoscopic 3D, in the category "Select when the display is in 3D mode:" choose "Always". If this is set to "Only while 3D programs run", the entire screen may blank out while entering and exiting Direct3D mode and entering and exiting from fullscreen mode. If it is set to "Only while full-screen 3D programs run", there will only be stereo in fullscreen mode, not in the SHAPE graphics window.

In the Direct3D mode, fullscreen, there is no atom identification - the only action of the mouse is to rotate the structure. The shortcut keys have their full effect.

The nVidia settings *depth* and *convergence* are not available to the user in SHAPE, because they are controlled by the two SHAPE settings Stereopair Rotation Angle and Perspective Distance. Convergence affects the apparent overall distance of the object - whether it appears to be in front of or behind the screen. However, excessive displacement in either direction can cause difficult in the ability of the eyes to merge the two images (they may become excessively separated on the screen), and also increased prominence of "ghosts" or residual weak images in the wrong eye. Therefore SHAPE always sets the convergence distance equal to the perspective distance so that the center of the structure is essentially in the screen, not in front of or behind it. The stereopair rotation angle then sets the nVidia depth (the term "depth" does not refer to the position

of the object front-back, but to the apparent distance between the nearest and the furthest parts of the object).

The nVidia Keyboard Shortcuts or hot keys for changing depth and convergence have no effect in SHAPE, although using the depth keys will bring up a scale showing the relative degree of stereo effect.

3.2.2.3 FullScreen Display

Fullscreen command [Modes menu]; Fullscreen button [Dialog Bar - Left]

The **Fullscreen** option in the the Display menu or the **Fullscreen button** in the Dialog Bar - Left switches to full-screen display. One reason to do this is to take advantage of full-screen, full-color stereoscopic viewing using shutter glasses - the software and hardware for some of these systems will only work in full-screen mode. See below and the Stereoscopic Display section in Reference for the requirements and procedures.

Mouse buttons have the same effect as when in the **Identify Faces** Cursor mode in a window.

Left button down is for identifying faces, as in the normal windowed mode. If the left mouse button is clicked when not on a crystal, a dialog offering Quit or escape from the Fullscreen mode, plus the control options as in the shortcut keys, will appear.

Right button down and moving the mouse down causes rotation exactly as in the normal windowed mode.

To exit from Fullscreen display, press the **Escape key**; or **click with the mouse where there is no crystal**.

-- KEYBOARD CONTROLS FOR FULLSCREEN MODE

With V7.3, the SHAPE shortcut keys have been revised and greatly expanded.

-- IF THE KEYBOARD IS NOT FULLY ACTIVE IN FULLSCREEN MODE

On different platforms (Windows, Macintosh, Linux) or different releases or versions of the same platform, some or all of the keys may be inactive in Fullscreen mode. Thus if some or all of the above keyboard controls do not work, click with the mouse where there is no crystal, and you will be presented with a dialog giving the options explicitly, as well as the option to Quit or exit fullscreen mode.

--Windows Only

Full-screen, full-color stereoscopic viewing with shutter glasses and CRT Monitors. The following describes older technology for CRT monitors, not newer technology such as nVidia 3D Vision, which requires special shutter glasses and certain 120 Hz monitors. That technology is supported with the 3D Quad Stereo Drawing mode (and can work in a window, not only in Fullscreen mode) or with the Direct3D mode.

Stereo viewing works best when Perspective is selected.

Shutter glasses, with driver software for Windows operating systems, were available from some vendors. The most complete support is for nVidia cards, the stereo drivers for which are available for free online (www.nvidia.com). The requirements and general procedure for shutter-glasses viewing are as follows.

1) You must have a cathode-ray-tube (CRT) monitor. Flat-screen monitors will not work because the refreshing mechanism is different. Stereo only works in 3D Single Drawing mode, not 2D modes.

2) You must install the stereo software driver for your particular graphics card onto the computer. You may also need an up-to-date driver for the card itself. For nVidia cards, install the latest standard (non-stereo) driver for your card, and then the (separate) stereo driver, according to the instructions at www.nvidia.com. For other cards you will need a third-party stereo driver, which may be provided with the glasses. The driver must support OpenGL.

3) Install the glasses (or the wireless station), typically by inserting a "dongle" where the monitor cable plugs into the computer (graphics card).

4) Turn on the Full-Screen mode in SHAPE, then turn on the stereo mode, usually by using a "hot key". It may be best to turn stereo on after entering full-screen mode in SHAPE, and turn it off before exiting.

Flickering in stereo mode is caused by a monitor refresh rate that is too slow. This usually may be reset in the Windows Display control panel and/or in the stereo driver software. On switching into full-screen mode, SHAPE first tries the current screen size, bit-depth and refresh rate. If this fails, then it tries successively smaller screen sizes. If you get a message saying that the switch into full-screen mode has failed, you can try changing the bit-depth (for example from 32- or 24-bit to 16-bit) or the refresh rate in the Windows Display control panel or in the stereo driver software.

The Website www.stereo3d.com has some basic technical information about shutter-glasses stereo, but the information on specific hardware and vendors may be out of date because the technology and marketing are currently moving very rapidly.

Caution: use shutter glasses or other hardware and driver software at your own risk - stereo drivers may have a tendency to crash your system. SHAPE software is not responsible for any damage to your hardware or software through use of these devices.

3.2.3 Input1 Menu

Title/Axes - Title and crystal axes or unit cell for the main crystal.

Symmetry - Symmetry of the main crystal.

Forms - Crystal forms (symmetry-equivalent faces) present on the main crystal.

Twins - This reproduces the main crystal according to specified twin operations.

Epitaxy - This adds additional crystals in defined orientation.

Sections/Growth Zones - This provides settings and parameters for the **Section/Zoning** Display mode selected in the **Modes** menu.

Face/Form Fills - This allows filling of specified faces and/or forms with colors or black-and-white patterns.

Shading - This turns on shading in color or black-and-white according to the angle of the faces from the specified illumination vector.

Striations - This adds striations to specified forms.

Interfacial Angle - This computes the angle between the normals between any two specified faces, even if they are not actually present.

Donnay-Harker Morphology - This derives a list of forms sorted according to X-ray d-spacing, or reticular area - such lists often correlate well with the forms observed.

3.2.3.1 Title/Axes

Dialog Box: Title/Axes [Input1 Menu] [Epitaxial Relations dialog]

The title may contain up to 63 characters.

In Crystal operating mode, select the crystal system, and axis-length and angle boxes appropriate for this system will appear. In Cartesian or QSHAPE mode, the axes must be Cartesian.

See also Coordinate Systems.

When called from the **Input1** menu, this dialog can only modify the main or host crystal of an epitaxial intergrowth. Epitaxial guest crystals are modified from the Epitaxial Relations dialog.

3.2.3.2 Symmetry - Point Group or Crystal Class

Dialog Box: Symmetry - Point Group or Crystal Class [Input1 Menu] [Epitaxial Relations dialog]

This dialog lists all the 32 crystallographic point groups, or crystal classes. The orientation is as indicated by the Herman-Maughin or International symbol. Note that a capital "B" preceeding an axis denotes an inversion axis, such as "bar-3". The orientation is as given by the H-M symbol, and in some cases two orientations are possible - see below.

The **Remove Symmetry** button offers the option of converting all faces which have been generated by symmetry to forms, and reducing the symmetry to group 1. The crystal can then be distorted from the ideal habit by changing the central distances of individual faces (through the Forms List dialog). This option is not available unless the crystal has been calculated.

When called from the **Input1** menu, this dialog can only modify the main or host crystal of an epitaxial intergrowth. Epitaxial guest crystals are modified from the Epitaxial Relations dialog.

Note that space-group symmetry is needed for the Donnay-Harker Morphology option - the point group is normally derived from the space group, and this may cause replacement of the point group specified in this dialog, if the two are not the same.
Alternate Orientations . There are two listings for each of five crystal classes, for which alternate orientations are possible. The pairs are 321 - 312, 3m1 - 31m, B3m1 - B31m, B42m - B4m2 and B6m2 - B62m. In these symbols, the first number or letter after the high-order axis (3, 4 or 6) indicates either a set of two-fold symmetry axes parallel to the *a* crystallographic axes, or a set of mirror planes perpendicular to the *a* crystallographic axes. The next letter or number indicates symmetry elements aligned on the directions bisecting the *a* crystallographic axes. If there is no symmetry in the *a* -axis directions, there is a number 1 as a placeholder. A final 1 is usually dropped, as in 321 = 32.

Versions of SHAPE prior to V6.0 allowed only the first orientation of each of these pairs. In V6.0, it is possible to import crystallographic data including the space group, and it is necessary to specify the space group for the Donnay-Harker Morphology option. Since the standard settings of space groups may have either of the orientations of each pair (for example P321 and P312 are different space groups), it is necessary to include both to correlate the morphology with the structure axes. It is possible to describe the morphology in terms of the orientation which does not correspond to that of the space group in the *International Tables* , but the unit cell in this orientation is non-primitive, the *a* axes are longer in relation to the *c* axis, and the indices of actual faces are different.

Since pre-V6.0 SHAPE only allowed one orientation, it is possible that forms entered may be incorrect. Most errors of this sort may be corrected simply by changing the symbol in this dialog, for example from P321 to P312. It is also possible that older morphological data may not correspond with the X-ray axes, which use the orientation as given in the *International Tables* . In this case, if the old morpological data are to be used with the X-ray axes, it is necessary to transform the indices.

3.2.3.3 Cartesian Symmetry

Dialog Box: Symmetry - Cartesian Matrices [Input1 Menu **] [** Epitaxial Relations dialog**]**

<Cartesian Mode>

SHAPE in the Cartesian mode (selected with the **Operate** command in the Modes menu, or by reading in a Cartesian file) requires a file containing the Cartesian symmetry matrices. The auxiliary program SYMGRP writes files which are normally given the suffix .SYM. If you type the name into the edit box, give the full name of the symmetry file, including the .SYM suffix. Some such files, namely those for pentagonal (C5, S10, D5, C5v, C5h, D5h and D5d) and icosahedral (I and Ih) point groups, have already been provided. For other point groups, it will be necessary to run the auxilliary program SYMGRP to generate the file before running SHAPE; see section IV-7 of the Instructions.

The **Get Symmetry** button reads the file and fills out the symbol, number of matrices and centric/non-centric state, which are printed out below the file name. If this button is not clicked, the file will be read when exiting the dialog.

The file name as entered in the edit box is saved in the data file for the crystal. If the complete path is not given, the Cartesian symmetry file should be in the same directory as the data file. If the file cannot be found when the **Get Symmetry** button is clicked or when exiting the dialog, you will get an error message and a chance to locate the file with a standard file dialog. The complete path name, as determined in this way or with the **Browse** button, will then be saved in the data file.

The Cartesian matrices themselves are saved in the SHAPE data file, and the Cartesian symmetry file is read only in this dialog.

The **Remove Symmetry** button offers the option of converting all faces which have been generated by symmetry to forms, and reducing the symmetry to group 1. The crystal can then be distorted from the ideal habit by changing the central distances of individual faces (through the Forms List dialog). This option is not available unless the crystal has been calculated.

When called from the **Input1** menu, this dialog can only modify the main or host crystal of an epitaxial intergrowth. Epitaxial guest crystals are modified from the Epitaxial Relations dialog.

In order to display the symmetry elements themselves in the 3D display mode, the .SYM file must give the orientation of these elements. Old files do not have this information: the new version of SYMGRP supplied the orientation information, but in some cases it may be necessary to modify the files manually - see Symmetry Element Display.

3.2.3.4 Forms List

Dialog Box: Forms List [Input1 Menu**] [** Epitaxial Crystals Dialog**]**

This lists the forms for the current crystal - this is the main crystal if this dialog is called from the Input1 menu, or an epitaxial crystal if called from the Epitaxial Crystals Dialog.

Multiply central distances by factor. Most calculations in SHAPE depend on finite tolerances to decide whether corners are not outside of any face, whether a corner derived from one triplet of faces is coincident with another, etc. Sometimes there are errors, for example extra corners, missing edges, or missing faces (in the Shading or Face Fill options, or in 3D mode). See Precision, Tolerances.. for more details. In many cases such errors can be eliminated by changing all central distances by the same factor, which effectively changes the relative tolerances. An increase in central distance is most likely to help, although a decrease may be required in some cases. If the **Multiply all parameters by factor** box is checked, parameters which involve absolute central distance units will be multiplied by the factor. Such parameters include fixed scale factors (Scaling); Perspective distance; Striation spacing; fixed Displacements of the crystal; Crystal Axes and Labels; Growth Rate and time parameters; and sizes of cylindrical edges and symmetry elements in the 3D modes (3D Parameters)

Clicking on the **Add** or **Revise** buttons calls up the **Add/Revise Form** dialog (Standard or Cartesian).

When called from the **Input1** menu, this dialog can only modify the main or host crystal of an epitaxial intergrowth. Epitaxial guest crystals are modified from the Epitaxial Relations dialog.

Imaginary faces, edges and corners . The user is responsible for specifying enough forms to make a complete crystal. After having generated all symmetry-equivalent faces and computing corners and edges, SHAPE applies some simple tests to see if a closed shape has been defined. If a closed shape does not seem to have been defined, you have the option of computing again to define imaginary edges and corners. This is done by adding "imaginary" faces at a central distance just greater than the most distant real corner, or about 1.5 times the largest central distance if no corners have been found. These faces are those of the unit cell, except for trigonal and hexagonal crystals, which use a trigonal or hexagonal prism. The edges which terminate the real faces against these imaginary faces are drawn with a different color (see Line Colors) and in the printed output (List Results dialog, File menu) these edges and associated corners are marked as Imaginary. These imaginary edges are not visible from the back side of the real faces unless **Back edges** are selected in the Line Attributes dialog (Input2 menu).

For the Cartesian or QSHAPE mode of operation, the imaginary faces are (100), (-100), (010), (0-10), (001), (00-1) and all their symmetry equivalents. This may lead to a very large number of faces and correspondingly long calculation times.

3.2.3.4.1 Add/Revise Form

Dialog Box: Add/Revise Form [Forms List Dialog **]**

<Standard Mode - see also Add/Revise Form (Cartesian)>

The central distance is the perpendicular distance from the center of the crystal to the faces of the form in question: the greater the distance, the smaller the area of the face (calculated areas are printed in the List Results option in the File menu). Also, if there are many forms, the greater the distance the less prominent the form (the smaller the area of the faces). Decimal values may be used for the central distance, but not for the indices. Use the **Next Form** button to add a form.

You can use negative central distances to define a crystal which does not lie on the origin; see the rutile twin example in Chapter 5 of the Instructions.

For hexagonal and trigonal crystals with hexagonal axes, four indices, (hkil), are commmonly used, but one of the first three is redundant. In SHAPE, you must omit the third, or i index.

The **Form letter** may be used to label each face in the conventional way. Whether numerical indices, form letters or no labels at all are shown is set in the Labels dialog in the Display menu.

The color, b/w pattern and pen number are used primarily for sections and growth zones and may be used for form fills.

The **Rate Constants** button pertains to growth zones. It brings up either the Exponential Growth-Rate Constants dialog or the Growth Intervals dialog, depending on the **Exponential/Discontinuous** setting in the Growth Zone Settings dialog. The rate parameters can also be set from the latter dialog.

See the Forms List dialog for the addition of imaginary faces, edges and corners if the real faces do not define a closed shape.

3.2.3.4.2 Add/Revise Form (Cartesian)

Dialog Box: Add/Revise Form (Cartesian) [Forms List Dialog**]**

<Cartesian Mode - see also Add/Revise Form (standard).>

The central distance is the perpendicular distance, from the center of the crystal to the faces of the form in question: the greater the distance, the smaller the area of the face. Also, if there are many forms, the greater the distance the less prominent the form (the smaller the area of the faces). Use the **Next Form** button to add a form.

The form indices and central distance are all decimal numbers. The indices will be normalized to length one after entry. Five or six significant figures are sufficient.

You can use negative central distances to define a crystal which does not lie on the origin; see the rutile twin example in Chapter 5.

The color, b/w pattern and pen number are used primarily for sections and growth zones.

The **Rate Constants** button pertains to growth zones. It brings up either the Exponential Growth-Rate Constants dialog or the Growth Intervals dialog, depending on the **Exponential/Discontinuous** setting in the Growth Zone Settings dialog. The rate parameters can also be set from the latter dialog.

See the Forms List Dialog for the addition of imaginary faces, edges and corners if the real faces do not define a closed shape.

3.2.3.5 Twins

Dialog Box: Twins [Input1 Menu**]**

There are basically two types of twins: contact and interpenetration. Interpenetration twins simply reproduce the main crystal according to the twin operator supplied. Normally, interpenetration twins should be drawn with intercrystal edges; these edges are located after the individuals are reproduced.

Clicking on the **Add** or **Revise** button calls up the **Twin Operator** dialog (Standard or Cartesian).

If you select the **contact** option, and supply one or more composition planes with the Composition Planes button, the composition planes are added to the crystal, truncating it as necessary, then the crystal is reproduced according to the twin operations supplied. No intercrystal edges are found for contact twins.

Note that all twin individuals are identical, and that composition planes always pass through the center of the crystal (central distance zero). Of course interpenetration twins may look different after the intercrystal edges are located. To draw twins in which the individuals are not identical, use Epitaxial Crystals.

Edges in faces. When different crystals in intergrowths have parallel and coincident faces, the edges lying in this common surface may or may not be realistic or meaningful, and you can elect to draw them or not. Usually the drawing is simpler and more satisfactory without them.

Always show composition-plane edges . Twins by reflection on the composition plane should always match exactly at the junction, and a certain short-cut in the drawing of such twins is often useful. When this box is not checked, if the composition plane is forward-facing, edges with this composition plane are not drawn. This often allows simple twins to be drawn without using the **Remove Hidden Lines** option in the Display menu. However, if the twin is by reflection, the two individuals often do not match exactly on the composition plane, and visible edges may be omitted. Generally, for correct drawing of mismatching rotation twins this box should be checked, and also the **Edges in faces**

box . If the **Always show composition-plane edges** box is checked, the **Remove Hidden Lines** option in the Display menu must be selected.

Scale successive interpenetration twins, by factor (1-x), x = . Interpenetration twins often have coincident faces. In 3D Drawing Modes, if the two individuals are assigned different colors, this usually causes the coincident areas to have a mottled appearance, which may shift in pattern as the crystal is rotated. This option rescales each twin individual by a small amount, (1 - x) where x is the value entered, so that the faces of the second individual just underlie those of the first, and so on. Appropriate values are approximately 0.00001 (10^-5), so that the second crystal is 0.99999 times as large as the first and so on.

This option should be used only for 3D modes - in Standard or 2D mode it will usually disrupt the drawing of edges when the **Remove Hidden Lines** option in the Display menu is chosen. After changing values, you must click **Calculate** as the corner locations of twins are changed permanently.

3.2.3.5.1 Twin Operator

Dialog Box: Twin Operator [Twins Dialog**]**

<Standard Mode - see also Twin Operator (Cartesian)>.

A twin operator may be either reflection on a rational plane or rotation on a rational vector. Normal twins according to the system commonly used for feldspars should be entered as reflection twins, giving the indices of the composition or twin plane. For parallel twins enter the indices of the twin axis is the twin operator.

For rotation twins, the rotation angle is normally an integral fraction of 360 degrees. A rotation angle is not needed for reflections twins - the angle will be set automatically to 180.

Note that composition planes must always be entered separately, even if the twin is by reflection.

Parent twin. With SHAPE V6.1.2, twins may be derived from other twins, not just the main crystal. This should simplify entry of many multiple twins. All twins must still be identical, and have a common center point at the origin (see the Lamellar Albite Twins example for methods of doing lamellar twins which do not have a common center).

Note that the number required here is the twin operator number, which is 0 for the main crystal, 1 for the first twin, and so on. After calculation, the crystals are numbered 1 for the main crystal, 2 for the first twin, and so on - if you click with the mouse on a crystal, you will get the crystal number, not the twin operator number.

3.2.3.5.2 Twin Operator (Cartesian)

Dialog Box: Twin Operator (Cartesian) [Twins Dialog**]**

<Cartesian Mode - see also Twin Operator (standard)>

A twin operator may be either reflection on a rational plane or rotation on a rational vector. Normal twins according to the system commonly used for feldspars should be entered as reflection twins, giving the indices of the composition or twin plane. For parallel twins enter the indices of the twin axis as the twin operator.

Indices will be normalized to length one.

For rotation twins, the rotation angle is normally an integral fraction of 360 degrees. A rotation angle is not needed for reflections twins - the angle will be set automatically to 180.

Note that composition planes must always be entered separately, even if the twin is by reflection.

3.2.3.5.3 Composition Planes

Dialog Box: Composition Planes [Twins Dialog**]**

This lists all the composition planes. Note that each composition plane is added to every twin individual - i.e. the composition planes are added before the main crystal is reproduced.

Compositions planes always pass through the center of the crystal - the central distance is zero.

Clicking on **Add** or **Revise** , or double-clicking on an individual entry takes you to the **Composition Plane** dialog (Standard or Cartesian) for entry or revision of data for individual composition planes

3.2.3.5.4 Composition Plane

Dialog Box: Composition Plane [Composition Planes **dialog]**

<Standard Mode - see also Composition Plane (Cartesian)>

The composition plane may be an indexed rational plane, or it may be the rhombic section. Rhombic sections must correspond in sequence number to a twin rotation axis entered in the Twin Operator dialog. That is, if a rhombic section is the second composition plane, the second twin operator must be a twin axis to which this rhombic section is to be parallel. If the composition plane is not a rhombic section, it need not be

parallel to any twin axis.

You should be aware that in rotation twins the two individuals may not match across the composition plane, even if the composition plane is parallel to the twin axis. If the composition plane is a rhombic section, it will pass through identical sections of the two crystals in terms of unit-cell geometry, but the faces may not match if they are not those of the unit cell.

3.2.3.5.5 Composition Plane (Cartesian)

Dialog Box: Composition Plane (Cartesian) [Twins Dialog**]**

<Cartesian Mode - see also Composition Plane (standard).>

The composition plane may be an indexed rational plane, or it may be the rhombic section. Rhombic sections must correspond in sequence number to a twin rotation axis entered in the Twin Operator dialog. That is, if a rhombic section is the second composition plane, the second twin operator must be a twin axis to which this rhombic section is to be parallel. If the composition plane is not a rhombic section, it need not be parallel to any twin axis.

You should be aware that in rotation twins the two individuals may not match across the composition plane, even if the composition plane is parallel to the twin axis. If the composition plane is a rhombic section, it will pass through identical sections of the two crystals in terms of unit-cell geometry, but the faces may not match if they are not those of the unit cell.

3.2.3.6 Epitaxial Crystals

Dialog Box: Epitaxial Crystals [Input1 Menu**]**

This option allows many complicated intergrowths of different crystals, as well as off-center twins, to be drawn. In epitaxial intergrowths, in principle a face of one crystal lies on a face of another crystal, either of the same or a different species. The mutual orientation must be further specified by the vectors within the faces which are parallel. Although the mutual orientation is described in terms of the faces, the crystals may after a period of growth be interpenetrating, or one may partially or completely enclose the other. In practice the "face-on-face" relation may only specify the mutual orientation, not position, and this option can be used to draw crystals with almost any kind of relation.

There are four ways to generate an epitaxial guest crystal: you can **Duplicate** the selected crystal; you can **Add** a new crystal with manual entry of the symmetry and forms; you can **Read from File** (that is from a .SHP data file); or you can Import an external file.

If you choose the **Read from File** option, the file in question must have been saved by SHAPE for Windows or in the ASCII "exchange" format with SHAPE for DOS V4.2. If you duplicate or read from a file, you will be transferred immediately to the Epitaxial Relations dialog.

To Import an epitaxial crystal, go directly to the Import option in the File menu (instead of this dialog). When the file has been read, you will be transferred immediately to the Epitaxial Relations dialog.

The host crystal is always crystal number 1; thus epitaxial guest crystals are always numbered from 2 upwards.

Orientation of crystals through epitaxial relationships involves a series of complex operations and is inherently less precise than orientation with twin operations. Occasionally, errors in drawing may result from this lack of precision. Twin operations should be used instead of epitaxy whenever possible to generate intergrowths.

Intercrystal edges are located only once during the calculation, after all crystals have been oriented and translated. If there are any crystal which actually do interpenetrate with one another, this box should be checked. If all epitaxial crystals are of the contact variety, it may be unchecked.

3.2.3.6.1 Epitaxial Relations

Dialog Box: Epitaxial Relations [Epitaxial Crystals Dialog**]**

<Standard Mode - see also Epitaxial Relations (Cartesian)>

The are basically three groups of information that must be supplied for each epitaxial crystals. At the top of the dialog is the type of contact geometry.
Contact adds a contact plane, with the same indices as the guest alignment face (see below), similar to the composition plane of a twin, to the guest crystal at a specified central distance; if you select this option the distance should be entered in the box below the host and guest indices. When the guest crystal is first generated, there may or may not be a crystal face with these indices; if there is, the central distance for the epitaxial plane should be less than that of the normal crystal face. That is, the epitaxial contact plane should truncate the guest crystal, not sit off in space. After the guest crystal is generated, it is rotated and translated so as to contact the host crystal on the specified faces. The specified alignment face of the host crystal should be one which is actually present; otherwise you will get an error message.

Interpenetration does not add a contact plane or try to match faces by translation. It simply establishes the mutual orientation and sets the crystals at a specified center-to-center distance. This distance is in central distance units and should be entered in the box below the host and guest indices. The host crystal remains at the center and the center of

the guest is displaced to the specified distance along the perpendicular to the epitaxial face.

In the middle of the dialog, you must specify the orientations of the host and guest crystals, by giving the indices of a face (khl) and a vector [uvw] parallel to this face for the host and for the guest. The face and the vector of the guest will be brought parallel to the corresponding elements of the host. If the vector is not parallel to the face, you will get an error message, and be asked to try again. A vector parallel to a face satisfies the relation uh + vk + wl = 0 .

Note that if the host and guest crystals are the same, and you enter the same face and vector for each, the two crystals are not in parallel orientation. Rather they are in twin orientation, related by rotation of 180 degrees around the alignment vector. Parallel orientation is attained by giving for the face on the guest crystal, the negatives of the indices for the face on the host crystal.

You have the option of specifying translations in addition to that parallel to the intercrystal vector. Movement can be made in either of two mutually perpendicular directions, specified with respect to the epitaxial plane on the host crystal: 1) parallel to the vector in this face which was used to orient the crystal; and 2) perpendicular to this vector, still in the plane of the face. Displacements are specified in central distance units. A right-handed system is formed by 1) the host-crystal vector; 2) the alignment vector in the host crystal face; and 3) the vector perpendicular to the alignment vector in the crystal face.

In the lower part of the dialog, enclosed in two boxes, are the data for the guest crystal. If the current epitaxial crystal is a duplicate of another crystal or has been read in from a file, these data may already be present; if not, you will have to click on the **Revise Title/Axes, Revise Symmetry** and **Revise Forms** buttons to enter these data. The dialogs called up are the same as those for entry of the main crystal, i.e. Title/Axes,Symmetry and Forms List. You must always use these buttons to modify epitaxial crystals - when called from the **Input1** menu, the Title/Axes,Symmetry and Forms List only modify the main or host crystal.

Clicking on the **Rescale** button will change all the central distances of the guest crystal by the factor entered in the **Rescale factor** box. This does not affect the distance entered for a contact plane.

3.2.3.6.2 Epitaxial Relations (Cartesian)

Dialog Box: Epitaxial Relations (Cartesian) [Epitaxial Crystals Dialog**]**

<Cartesian Mode - see also Epitaxial Relations (standard)>

The are basically three groups of information that must be supplied for each epitaxial

crystals. At the top of the dialog is the type of contact geometry.
Contact adds a contact plane, with the same indices as the guest alignment face (see below), similar to the composition plane of a twin, to the guest crystal at a specified central distance; if you select this option the distance should be entered in the box below the host and guest indices. When the guest crystal is first generated, there may or may not be a crystal face with these indices; if there is, the central distance for the epitaxial plane should be less than that of the normal crystal face. That is, the epitaxial contact plane should truncate the guest crystal, not sit off in space. After the guest crystal is generated, it is rotated and translated so as to contact the host crystal on the specified faces. The specified alignment face of the host crystal should be one which is actually present; otherwise you will get an error message.

Interpenetration does not add a contact plane or try to match faces by translation. It simply establishes the mutual orientation and sets the crystals at a specified center-to-center distance. This distance is in central distance units and should be entered in the box below the host and guest indices. The host crystal remains at the center and the center of the guest is displaced to the specified distance along the perpendicular to the epitaxial face.

In the middle of the dialog, you must specify the orientations of the host and guest crystals, by giving the indices of a face (khl) and a vector [uvw] parallel to this face for the host and for the guest. The face and the vector of the guest will be brought parallel to the corresponding elements of the host. If the vector is not parallel to the face, you will get an error message, and be asked to try again. A vector parallel to a face satisfies the relation $uh + vk + wl = 0$.

Note that if the host and guest crystals are the same, and you enter the same face and vector for each, the two crystals are not in parallel orientation. Rather they are in twin orientation, related by rotation of 180 degrees around the alignment vector. Parallel orientation is attained by giving for the face on the guest crystal, the negatives of the indices for the face on the host crystal.

You have the option of specifying translations in addition to that parallel to the intercrystal vector. Movement can be made in either of two mutually perpendicular directions, specified with respect to the epitaxial plane on the host crystal: 1) parallel to the vector in this face which was used to orient the crystal; and 2) perpendicular to this vector, still in the plane of the face. Displacements are specified in central distance units. A right-handed system is formed by 1) the host-crystal vector; 2) the alignment vector in the host crystal face; and 3) the vector perpendicular to the alignment vector in the crystal face.

In the lower part of the dialog, enclosed in two boxes, are the data for the guest crystal. If the current epitaxial crystal is a duplicate of another crystal or has been read in from a file, these data may already be present; if not, you will have to click on the **Revise**

Title/Axes, Revise Symmetry and **Revise Forms** buttons to enter these data. The dialogs called up are the same as those for entry of the main crystal, i.e. Title/Axes,Symmetry and Forms List. You must always use these buttons to modify epitaxial crystals - when called from the **Input1** menu, the Title/Axes,Symmetry and Forms List only modify the main or host crystal.

Clicking on the **Rescale** button will change all the central distances of the guest crystal by the factor entered in the **Rescale factor** box. This does not affect the distance entered for a contact plane.

3.2.3.7 Sections and Growth Zones

Dialog Box: Sections and Growth Zones [Input1 Menu**]**

In the Section/Zoning mode, a section is drawn through the current crystal or crystals, parallel to the screen or paper (observer x = constant). Sections and growth zones are shown only when the **Display** mode, in the **Modes** menu, is set to **Section/Zoning.** This dialog and the sub-dialogs it controls set the parameters for sections and growth zones.

The radio buttons at the top give the choice between the two main modes: **Single section outline,** which is useful for identifying the orientation of a crystal in a section of rock or other material; and **Growth zones,** which plots repeated sections at intervals according to various growth models. The **Growth Zone Settings** button brings up another dialog for additional growth zone settings.

A section, whether single or repeated as growth zones, is taken parallel to the y and z observer axes (see Coordinate Systems), at the x coordinate specified in the **Section height** box. This coordinate should not be larger than the dimension of the crystal in the x direction, or nothing will be shown.

In the non-fixed scaling modes (see Scaling), you can scale the **Section only** to occupy the viewing area, or you can include the entire crystal (**All corners**). Typically the latter mode is used if you are displaying a drawing of the crystal along with the section.

The coordinates of section corners can be listed to a file and/or to a Text window.

The colors, b/w patterns and pens can be specified for the different types of edges shown in a section; these colors are different from the the standard colors for edges in the Line Colors and Line Patterns and Pens dialogs in the **Input2** menu.

With the **Add** button you can add edges representing the current section to the drawing of the crystal as a whole. The crystal can then be rotated to better show the orientation of the section. These edges disappear the next time the crystal is recalculated. You must

replot after exercising this option.

Some basic facts and terminology must be understood in order to be able to use the suboptions for growth zoning.

The lines which appear in a section plot, or section edges, are the intersections of crystal faces with the section plane. If such a line of intersection is not also an exterior crystal edge, the resulting line will be called a *one-face edge.* If it is a crystal edge, then the result is a *two-face edge,* since the two faces intersect the section plane along this line.

A *sector* is ideally a pyramidal polyhedron which has one external face at its base, and the center of the crystal at its apex. If growth rates are not constant with time, faces and therefore sectors may be created or annihilated, and the geometry may be more complex, but a sector is always defined by a single crystal face. If the growth is linear, a section through the crystal center will show a sector as a triangular area, and if growth zones are drawn, there will be lines parallel to the crystal face. However, if a triangular area passing through the center is bounded on the outside of the crystal by a two-face edge, the area observed is not a sector, but the boundary between two sectors - those defined by the two faces which intersect at the edge.

In idealized drawings such as those made by SHAPE, special relations are very common because of symmetry and default setting geometry. In particular, the section often passes through the exact center, and two-face edges may often be seen. In real sections of crystals in rocks or synthetic materials, which are usually random with respect to height of the section and orientation of the crystal, relationships are in general less special and more complex; two-face edges are less common, and sectors and sector boundaries are very seldom seen in their entirety.

3.2.3.7.1 Growth Zone Settings

Dialog Box: Growth Zone Settings [Sections and Growth Zones Dialog**]**

Growth model radio buttons. There are three basic growth models; linear, exponential and discontinuous. The last two are considered to be non-linear. For linear growth, the rates are derived from the central distances, and the values in the **Total time** and **Time interval** boxes (below) are not used.

Linear growth. If the growth is linear (rates constant with time), and a single crystal or simple twins are being drawn, the calculation of zones is simple. The final shape of the crystal is taken to be specified by the central distances entered in the Forms List dialog (**Input1** menu), and it does not have to be recalculated; it is simply rescaled for each successive zone, the scale factors being determined from the **Number of zones.**

If multiple epitaxial crystals are being drawn, the entire calculation must be repeated for

each zone, as for non-linear growth below. Each crystal attains the size determined by the central distance of its forms. The main crystal does this in total time 1.0 - it always has start time 0.0 and end time 1.0. The start and end times of the epitaxial crystals (see **Start** button below) are given relative to the main crystal. If an epitaxial crystal is given a negative start time, or an end time greater than one, the total growth interval will be extended appropriately.

Non-linear growth. If the growth is by either the exponential or discontinuous models, the increment to the central distance for each form is calculated from the **Time interval** , using either the Rate Constants in the exponential model or the rates entered for each interval using the Intervals button. The growth of the main crystal starts at time zero, and ends at the **Total time** specified in the edit box. For epitaxial crystals, each epitaxial crystal starts and ends at the time specified using the Times button at the bottom of the dialog. As in the case of linear growth, the start and end of the growth process will be extended if epitaxial crystals start before or end after the main crystal. However, the start and end times for non-linear growth are absolute (in whatever units you may be using).

The non-linear method, i.e. repetition of the entire calculation for each zone, is always used for epitaxial intergrowth, even if the **Linear** growth model is selected.

When you click on either the **Rate Constants** or the **Intervals** button, you are first presented with the Forms List for Growth-Rate Constants dialog. This simply gives a list of the current forms, for each of which you must specify or confirm the rate constants. Selecting a form from that dialog then presents you with the Exponential Growth-Rate Constants dialog for exponential growth, or the Growth Intervals dialog for discontinuous growth. See help for these dialogs for further information on growth-rate parameters

For proper drawing of epitaxial crystals, the box for **Intercrystal edges** in the **Epitaxial Crystals** dialog should usually be checked. Similarly, for interpenetration twins specify the option with intercrystal edges.

When using scaling options (1) or (2) in the Scaling dialog (**Input2** menu), it is impossible to scale a non-linear growth-zone drawing before it is completed. However, the overall scale factor for the next calculation is obtained from the last zone. Thus it may be necessary to repeat the calculation with the **Calculate** command in the **File** menu, or the **Calculate** button in the Dialog Bar - Left to get proper scaling. If you are using scaling option (3)- Fixed in./cm. per central distance unit, it is up to you to insure that the drawing does not go off scale.

Linear: number of zones. In linear growth, the crystal will be divided into zones representing equal increments of growth time. Strictly speaking, this number of zones applies only to the host in epitaxial intergrowths; see **Times** below for the number of zones for guest crystals.

Non-linear: Total time. This is the end time for the main or host crystal if epitaxial crystals are present. Epitaxial guest crystals may actually start before the zero time or after the end or total time for the host crystal - see **Times** below. The time unit is arbitrary and may be considered to be seconds, hours or any other appropriate unit.

Non-linear: Time interval. An entire calculation will be carried out, and a zone drawn, for each interval.

Marker zones. If you are using wide lines to fill in the growth sectors (see Filling Sectors below), you can insert marker zones of a contrasting color at specified intervals, to show the orientation of growth and the relative rates.

Sector boundaries. If this box is checked, lines are drawn connecting corners in the section which are defined by the same combinations of faces. If a face appears or disappears on a corner between zones, no line is drawn, since this changes the identity of the sector boundary. If you find that too many sectors are thus undefined, the solution is to increase the **Number of zones** for linear growth, or decrease the **Time interval** for non-linear growth (see Filling Sectors below).

Pause after each zone. If this box is checked, the calculation will pause after the appearance of each zone outline. Pressing any key will cause the next zone to plot.

Colors for one-face edges. In section, growth sectors are defined by one-face edges (see Sections and Growth Zones). All these edges may be given a single or default color, or you may specify a color for each form, so that sectors may be more easily correlated with external forms. Two-face edges always have the colors specified in the sub-dialogs called with the **Line Colors** and **Patterns/Pens** buttons in the Sections and Growth Zones dialog.

Epitaxial crystals - start and end times (Start Button). This allows epitaxial guest crystals to start or end growth at different times relative to the host crystal. For linear growth, the times specified are relative to the main crystal; that is values of 0.0 and 1.0 mean that the epitaxial crystal in question (numbered starting with two for the first guest crystal) starts and ends at the same time as the host. Values of 0.5 and 1.5 mean that the guest crystal starts at half the **Total time** and ends at half again the **Total time** after the host crystal has ended.

For linear growth, epitaxial guest crystals reach the full size specified by the central distances of their forms in the time allotted (end minus start), and thus the number of zones will be less than that specified in the **Number of zones** box if the total time (end minus start) for this crystal is less than one.

For non-linear growth the times are absolute, in whatever time units are currently being used. The ultimate size of each crystal and number of zones is determined by the growth-

rate equations.

Filling Sectors. To minimize the problem of undefined sector boundaries, and to make it easier to identify sectors, it may be desirable to make the section lines so close together as to touch or almost touch. This can be done by increasing the **Number of zones** for linear growth or decreasing the **Time interval** for non-linear growth; it is made easier by increasing the width of the lines (Line Attributes dialog in the Input2 menu). If the sectors are completely filled in, **Marker zones** may be used to show the orientation of the growth.

3.2.3.7.2 Colors for Sections and Growth Zones

Dialog Box: Colors for Sections and Growth Zones [
Sections and Growth Zones Dialog **]**

These are colors which only appear when the **Display** mode (**Modes** menu) is set to **Section/Zoning.** See the Sections and Growth Zones dialog for further definitions of terms.

One-face edges are the intersections of single crystal faces with the section plane. The same color is used for front section edges (visible edges) when the section edges are added to a normal view of the crystal with the **Add** button in the Sections and Growth Zones dialog.

Two-face edges are the intersections of crystal edges with the section plane. That is, the crystal edge lies in and is parallel to the section plane.

Sector boundaries. These lines are drawn between section corners involving the same faces. They may be undefined when the morphology of a section changes.

Back edges are the back section edges (invisible edges) when the section edges are added to a normal view of the crystal with the **Add** button in the Sections and Growth Zones dialog.

Marker zones are lines which may be added (actually, substituted for the section edges) at specified intervals to growth zoning, especially when wide lines are being used to fill in sectors.

3.2.3.7.3 Line Patterns and Pens for Sections

Dialog Box: Line Patterns and Pens for Sections and Growth Zones [
Sections and Growth Zones Dialog **]**

These are colors which only appear when the **Display** mode (**Modes** menu) is set to **Section/Zoning.** See the Sections and Growth Zones dialog for further definitions of

terms.

One-face edges are the intersections of single crystal faces with the section plane. The same color is used for front section edges (visible edges) when the section edges are added to a normal view of the crystal with the **Add** button in the Sections and Growth Zones dialog.

Two-face edges are the intersections of crystal edges with the section plane. That is, the crystal edge lies in and is parallel to the section plane.

Sector boundaries. These lines are draw between section corners involving the same faces. They may be undefined when the morphology of a section changes.

Back edges are the back section edges (invisible edges) when the section edges are added to a normal view of the crystal with the **Add** button in the Sections and Growth Zones dialog.

Marker zones are lines which may be added (or actually substituted for the section edges) at specified intervals to growth zoning, especially when wide lines are being used to fill in sectors.

3.2.3.7.4 Exponential Growth-Rate Constants

Dialog Box: Exponential Growth-Rate Constants [Forms List Dialog**] [** Forms List for Growth-Rate Constants Dialog**]**

If the exponential growth model is specified in the Growth Zone Settings dialog, a rate equation, in terms of central distance units and any time units desired, must be specified for each form. The equation is exponential in form:

rate = a1 + a2 t^b2 + a3 t^b3 + a4 t^b4

where t is time. Most continuous functions can be approximated by an equation of this form with a MacLaurin expansion. The coefficients of the equation must be specified for each form; the forms are listed in sequential order, ignoring the crystal to which they belong in the case of epitaxial intergrowths. As a default, the a1 coefficient is simply taken to be the central distance; that is, the default is a linear rate which gives the same crystal shape as that specified by the original central distances, when total time is 1.0. Other a coefficients are set to zero. The default values for b2 through b4 are one, two and three respectively (b1 is not used).

Appearance and disappearance of forms in non-linear growth. In either the exponential or discontinuous models, forms may appear and disappear during growth. If the growth rate of a form is so large that it does not appear on a crystal after a given interval, its

central distance is adjusted so that it lies just outside the current corners and edges. When the current growth rate for a form is sufficiently small relative to the other forms over a given growth interval, that form will appear, regardless of how large its rate may have been in previous growth intervals. Thus the central distance of a form is not the integral of the rate equation, if the form does not appear for any time.

3.2.3.7.5 Growth Intervals

Dialog Box: Growth Intervals [Forms List Dialog**] [** Forms List for Growth-Rate Constants Dialog**]**

In the discontinuous growth model, the total growth time is divided into intervals for each form, with a different constant growth rate for each interval. Zero is a possible growth rate. Two constants must be given for each interval, for each form; the **Growth rate** and the **End time.** The first interval starts at the start time for the crystal (which is zero for the main crystal, but may be less than zero for epitaxial crystals), and succeeding intervals start at the end of the previous interval. These times are absolute, although the main crystal always starts at time zero. Sixteen intervals are allowed for each form (but see the README file for the latest number).

Appearance and disappearance of forms in non-linear growth. In either the exponential or discontinuous models, forms may appear and disappear during growth. If the growth rate of a form is so large that it does not appear on a crystal after a given interval, its central distance is adjusted so that it lies just outside the current corners and edges. When the current growth rate for a form is sufficiently small relative to the other forms over a given growth interval, that form will appear, regardless of how large its rate may have been in previous growth intervals. Thus the central distance of a form is not the integral of the rate equation, if the form does not appear for any time.

3.2.3.7.6 Forms List for Growth-Rate Constants

Dialog Box: Forms List for Growth-Rate Constants [Growth Zone Settings Dialog**]**

This dialog gives a list of the current forms, for each of which you must specify or confirm the rate constants. Selecting a form and clicking on the **Revise** button then presents you with the Exponential Growth-Rate Constants dialog for exponential growth, or the Growth Intervals dialog for discontinuous growth, depending on the exponential/discontinuous setting in the Growth Zone Settings dialog. See help for these dialogs for further information on growth-rate parameters.

3.2.3.7.7 Start and End Times for Epitaxial Crystals

Dialog Box: Start and End Times for Epitaxial Crystals [Growth Zone Settings Dialog**]**

This allows epitaxial guest crystals to start or end growth at different times relative to the host crystal. For linear growth, the times specified are relative to the main crystal; that is values of 0.0 and 1.0 mean that the epitaxial crystal in question (numbered starting with two for the first guest crystal) starts and ends at the same time as the host. Values of 0.5 and 1.5 mean that the guest crystal starts at half the **Total time** and ends at half again the **Total time** after the host crystal has ended.

For linear growth, epitaxial guest crystals reach the full size specified by the central distances of their forms in the time allotted (end minus start), and thus the number of zones will be less than that specified in the **Number of zones** box if the total time (end minus start) for this crystal is less than one.

For non-linear growth the times are absolute, in whatever time units are currently being used. However, the host crystal of epitaxial intergrowths always starts at time zero, so times for guest crystals may be negative. The ultimate size of each crystal and number of zones is determined by the growth-rate equations, constants for which are specified in the Exponential Growth-Rate Constants dialog for exponential growth, or the Growth Intervals dialog for discontinuous growth.

3.2.3.8 Face or Form Fills

Dialog Box: Face or Form Fills [Input1 Menu**]**

This dialog lists the current face and/or form fills.

Clicking on the **Add** or **Revise** buttons calls up the **Face or Form Fill Data** dialog (Standard or Cartesian).

Show crystal edges . If this box is checked (the default), crystal edges are shown with the normal colors (Line Colors and Line Patterns and Pens dialogs in the **Input2** menu); if not, edges are not drawn. This checkbox has no effect if there are no fills or shading. Back edges should be set to **None** in the Line Attributes dialog (**Input2** menu).

The **Fill all Forms** button will use the current form colors, set in the **Face or Form Fill Data** dialog (Standard or Cartesian).

Note that Shading (**Input1** menu) takes precedence over fills. You can turn shading on or off without affecting fills.

3.2.3.8.1 Face or Form Fill Data

Dialog Box: Face or Form Fill Data [Face or Form Fills Dialog**]**

<Standard Mode - see also Face or Form Fill Data (Cartesian)>.

Specify the indices, face/form, color and b/w pattern number for each fill in this dialog.

You can specify the crystal number for intergrowths; if this number is zero, all faces or forms with the given indices will be filled. SHAPE currently has hidden line removal algorithms (for multiple crystals), but these do not apply to faces, so it is not able to sort out the overlapping relations among faces of interpenetrating crystals, so fills are not generally satisfactory in interpenetration intergrowths. They may be successful in contact intergrowths, but only if part of one crystal is not hidden by another.

3.2.3.8.2 Face or Form Fill Data (Cartesian)

Dialog Box: Face or Form Fill Data (Cartesian) [Face or Form Fills Dialog**]**

<Cartesian Mode - see also Face or Form Fill Data (Standard) >

Specify the indices, face/form, color and b/w pattern number for each fill in this dialog.

You can specify the crystal number for intergrowths; if this number is zero, all faces or forms with the given indices will be filled. SHAPE currently has hidden line removal algorithms (for multiple crystals), but these do not apply to faces, so it is not able to sort out the overlapping relations among faces of interpenetrating crystals, so fills are not generally satisfactory in interpenetration intergrowths. They may be successful in contact intergrowths, but only if part of one crystal is not hidden by another.

3.2.3.9 Shading

Dialog Box: Shading [Input1 Menu**]**

Single crystals can be shaded in color or black and white. Shading is not likely to be successful in intergrowths if one crystal hides the faces of another. Except for the illumination vector, this dialog does not apply to the 3D mode - the separate settings for that mode are in the 3D Parameters dialog in the Input2 menu.

Illumination vector . Shading is based on the cosine of the angle between the normal to the face in question and the illumination vector. This vector points toward the light source. Any units can be used when entering the vector, but it will always be normalized to length one.

Darkest shade (fraction). This option "softens" the shading by allowing the presumed illumination of the darkest zone to be other than zero. Small values of this fraction, such as 0.1 or 0.2, are usually appropriate. It is 0.0 by default.

Darkness angle (degrees). For an isolated object in a vacuum, the intensity of illumination should vary from maximum to minimum as the angle varies from 0 to 90 degrees. However, this would be a very "hard" illumination, and SHAPE allows for a

"softening" or diffusing of the illumination in two alternative ways, by darkness angle or by darkest shade. The darkness angle, or the angle at which the illumination becomes zero or minimal, can vary from 90 to 180 degrees.

Color. If shading is to be shown on a 24-bit or other unrestricted device, you can select any RGB color. However, for compatibility with a range of devices it is best to use simple colors, starting with the first 8 colors (excepting black) in the standard Palette. If the face color is the same as the back edge color (Line Colors), and if back edges are enabled (Line Attributes), there may be an illusion of transparency.

Palette settings for 256-color display. SHAPE can set up the palette for 8-bit or 256-color displays in either of two ways. The primary palette (see the Palette dialog in the Settings menu) has 16 colors, which are always available for lines. Each of these, except black, can be used as the basis for 16 color zones, shading towards black; or colors 1-7 can each be used as the basis of 32 zones. If you select 16 zones, you can select any of the 15-non-black colors in the Palette with the **Select Color** button. If you select 32 zones, which generally gives better results for crystals with many faces, the only colors which can be shown are 0-7. If you select any of colors 8-15, they will be forced to one of the colors 0-7. Black, number 0, will not be shaded.

Multiple crystals . In many cases shading is incorrect for multiple crystals, especially for interpenetration intergrowths - the standard method of drawing is designed mainly to draw edges, not surfaces. There are liable to be problems with shading whenever the Remove Hidden Lines option (Display menu) is used. The 3D display mode avoids all problem of this sort.

3.2.3.10 Striations

Dialog Box: Striations [Input1 Menu]

Striations are evenly spaced lines on the faces of the given form. These lines are drawn parallel to an actual edge.

Striations are often useful in showing crystal symmetry which is lower than that of the form exhibited. For example, pyrite, group mB3, often grows in cubes, which have the full symmetry of group m3m. However, striations on the cube faces are often present, which bring out the fact that 4-fold axes are not present.

A maximum of 20 forms (not faces) may be striated.

The specifications for striations on individual forms are in the Striation Data dialog, which is accessed with the **Revise** or **Add Striation** buttons.

Randomize . This causes the striations to be randomly dashed lines - it does not randomize the spacing of the striations. The **Max. line** parameter is the maximum length

of the solid segments, while **Max. interval** is the maximum length of the blank interval between solid segments. Both solid and blank segments are randomized in length within these intervals. Lengths are in central distance units (c.d.u.), i.e. the same arbitrary units as the central distance for the forms.

Striations in 3D mode are always lines, not cylinders.

3.2.3.10.1 Striation Data

Dialog Box: Striation Data [Striations dialog]

Striations are defined by giving the indices of a face belonging to the form which is to be striated, and the indices of a face which makes an actual edge with the first face. This edge is the striation direction.

The spacing of the lines is in central distance units (c.d.u.), i.e. the same arbitrary units as the central distance for the forms.

Striations will be applied to all faces of the form. For twins or epitaxial intergrowths, the number of the individual may be specified, or a value of zero in the **Crystal No.** (number) box will apply the striations to all individuals. Of course in epitaxial intergrowths the two specified faces may not exist on all crystals, which will result in an error message.

3.2.3.11 Interfacial Angle

Dialog Box: Interfacial Angle [Input1 Menu]

This will calculate the angle between the normals to any two faces. After entering the indices for face 1 and face 2, the **Get Angle** button will cause the angle to appear at the botton of the dialog.

Note that the angle between the last two faces clicked is automatically given when in the Indexing or Face Identification cursor mode.

3.2.3.12 Donnay-Harker Morphology

Dialog Box: Donnay-Harker Morphology [Input1 Menu]

This option will give a list of forms with central distances as a function of X-ray d-spacing or relative reticular area.

According to the Law of Bravais, later extended by Donnay and Harker, the morphological importance of a form is inversely related to the interplanar spacing, or X-ray d-spacing. Since the d-spacings depend on the presence of non-primitive Bravais lattices, screw axes and glide planes, it is necessary to know the space group as well as

the unit-cell parameters.

This relationship is essentially empirical, and the quantitative relationship between d-spacing and growth rate is difficult to establish. Analysis of the equation for growth rate by the surface-nucleation mechanism (E. Dowty, "Crystal Growth and Nucleation Theory", in R.B. Hargraves, Ed. , Physics of Magmatic Processes), suggests a relationship of the form

$$R = k1\ d \exp(- k2\ d)$$

where k2 is inversely proportional to the supersaturation (or supercooling in the case of growth from the melt). Of course this is a great simplification, and ignores the influence of different surface energy on different faces.

For small values of k2, corresponding to large supersaturation or rapid growth, the rate of growth may show a maximum as a function of d-spacing. For the mechanism of growth by the spiral dislocation mechanism, there is apparently no inverse dependence of growth rate on d-spacing, rather the principal influence seems to be surface energy (included in k2 in the above equation). Thus the Bravais/Donnay-Harker law seems to apply to slow growth by the surface-nucleation mechanism, and adherence to this law is not expected in all cases, particularly rapid growth in the laboratory.

SHAPE offers the choice of three functions for the dependence of growth rate or central distance on d-spacing; a simple inverse dependence (R = 1 / d), the above exponential relation, and the above relation without the d in the pre-exponent.

The function (R = 1/d) has special consequences, in that it necessarily causes some faces to lie *exactly* on corners or edges. For example, in the orthorhombic group *mmm* , the first-ranked forms are {100}, {010}, and {001} - these are the only forms which appear as actual faces. However, the faces of forms {110}, {101} and {011} lie exactly on the edges and those of form {111} lie exactly on the corners. The faces of these forms appear in the listings for each corner, which may cause confusion. Because of the finite precision of the calculation, there may sometimes be extra corners or other anomalies (see Precision, Tolerances, etc.)

Whichever relation is chosen, SHAPE generates a set of hkl form indices consistent with the symmetry. The forms are sorted according to the growth rate or central distance, and normalized to the smallest growth rate. This list of forms will replace any forms currently present.

The space group may be specified by typing in either the H-M (Herman-Maughin or International) symbol, the Hall symbol, or the number of the space group in the *International Tables for X-ray Crystallography* . However, because of different possibilities for origin and orientation, the best way to specify the space group is by

selection in the list box. This selection is not entered until the selection is double-clicked or the **Select** button is clicked.

SHAPE requires monoclinic crystals to be in the second setting, i.e. unique or symmetry axis b, rather than c. If you enter a symbol which does not explicitly give the orientation, such as C2/c, the second setting will be assumed. Do *not* enter a symbol which does not conform to this standard (such as P112/m)

It is important to realize that an empirical list of forms in order of morphological importance for a given crystal usually represents a statistical compilation, not a typical or ideal morphology. To put it in another way, such compilations or observations are usually based on frequency of occurrence of forms, rather than measurements of central distance for any particular case, or averages of such measurements. While such a list may have dozens of entries, actual crystals typically show a small number, perhaps only 1 or 2 for a cubic crystal. Presumably the ideal relative growth rates as predicted theoretically on the basis of crystal structure and geometry alone are modified in each case by environmental factors, such as composition of the growth fluid and overall growth rate. The Bravais-Donnay-Harker list as derived by SHAPE should thus be considered as a ranking of forms in order of probability of occurrence.

Note that space groups in some trigonal, tetragonal and hexagonal point groups may have alternate orientations of the symmetry elements with respect to the crystallographic axes - for example P321 and P312 are different space groups. These differences in orientation are now included in the choices of point group in the Symmetry dialog, and it may be necessary to change the point group or crystal class to agree with the space group.

You may only make a D-H list of forms for a single crystal - if you use this option for an epitaxial intergrowth, all crystals except the main one will be deleted. In order to apply D-H morphology to an epitaxial crystal, you must do that crystal separately and save the results in a file (**Save** or **Saveas** in the File menu). Then that file may be read as a second or subsequent crystal in the Epitaxy option (Input1 menu). Of course it is advisable to remove any forms which do not appear in the actual calculated crystal - forms are marked as PRESENT or ABSENT in the Listing of calculation results (File menu).

3.2.4 Input2 Menu

Line Colors - Controls colors of front and back edges, etc. in color display or output.

Line Patterns and Pens - Controls gray shades or patterns of front and back edges, etc. in black-and-white display or output.

Line Attributes - Controls appearance of back edges, dashing and widths of lines.

Perspective - Controls drawing in perspective versus straight projection.

Background Color - Controls background color (ignored for b/w display or output).

Crystal Axes - Controls display of crystal axes.

Initial Orientation - Controls the orientation which is imposed after calculation and before first viewing.

Scaling - Controls scaling modes and factors.

Centering and Displacements - Controls displacements and automatic centering of the image.

3D Parameters - Controls the 3D display mode, including display of symmetry operators.

3.2.4.1 Line Colors

Dialog Box: Line Colors [Input2 Menu]

Back edges are those which are not visible if the crystal is opaque.

Display of **Crystal Axes** is controlled by the Crystal Axes dialog in the **Input2** menu.

Stereonet display is controlled by the **Display** command in the **Modes** menu.

See the Forms List dialog for the automatic addition of **Imaginary** faces, edges and corners if the real faces do not define a closed shape.

3.2.4.2 Line Patterns and Pen Numbers

Dialog Box: Line Patterns and Pen Numbers [Input2 Menu]

Back edges are those which are not visible if the crystal is opaque.

Display of **Crystal Axes** is controlled by the Crystal Axes dialog in the **Input2** menu.

Stereonet display is controlled by the **Display** command in the **Modes** menu.

3.2.4.3 Line Attributes

Dialog Box: Line Attributes [Input2 Menu]

Back edges - those not visible if the crystal is opaque - may be specified as none (not shown at all), dashed or solid.

Dash length and dash ratio . The dashes are used for back edges of crystals and display of Crystal Axes. Length or repeat distance is in inches/centimeters, and the length factor is the actual length of the solid part divided by the repeat distance. Note that when using Frames in output the dash length remains the same - it may be desirable to decrease the length for very small plots.

Widths are specified in inches or centimeters (choice of units is in the Preferences dialog in the Settings menu). Values of 0.0 will give one-dot width. **Output** pertains to all types of non-screen output except pen plot. Widths of pen plots can only be changed by using different pens.

See also the Line Colors and Line Patterns and Pen Numbers dialogs.

3.2.4.4 Background Color

Dialog Box: Background Color [Input2 Menu**]**

The best color for background may be neither white nor black - sometimes gray brings out shading better. The background for black-and-white display and output is always white.

3.2.4.5 Perspective

Dialog Box: Perspective [Input2 Menu**]**

If perspective is not in effect, or turned off, the drawing is simply a perpendicular projection down the observer x axis. If perspective is on, the drawing is projected from a point (x,0,0), where x is the perspective distance, onto the plane (0,y,z), that is a horizontal plane passing through the crystal center. Scaling applies to this plane, but obviously fixed scaling has limited intrinsic meaning in perspective drawing; generally the scaling mode **Each View Maximum** (set in the Scaling dialog in the Input2 menu) should be used when perspective is in effect.

The perspective distance is the distance *x* of the projection point from the projection plane, or in other words the distance from which the crystal is viewed (distance from the center of the crystal to the eye). Smaller distances will accentuate the "perspective"; larger distances will cause the plot to appear more like a straight-on projection. The perspective distance should be considerably larger than the distance of the furthest corner from the center (or the plane x=0) in the positive x direction.

3.2.4.6 Stereopair Angle

Dialog Box - called from: Input2 Menu

When either 2D Stereopair, OpenGL Stereopair, OpenGL Quad Stereo or Direct3D Stereo Drawing mode is selected, two images of the structure will be drawn.

The left or left-eye image will be rotated by the stereopair **Rotation angle** clockwise from the normal orientation, and the right-eye image will be rotated the same amount counter-clockwise. If shading is active the illumination vector will be rotated along with the structure. The stereopair rotation angle is typically about 3 degrees, although the proper angle may vary depending on the perspective distance, the actual viewing method, etc.

If the hard copy of stereopairs is to be viewed directly or with a small viewer, a frame size in the dot-matrix or pen plot of 4 to 5 inches across will give a distance between the two images about equal to the normal interocular distance.

Few people can directly view a stereo pair as shown on the full screen because the images are considerably further apart than the eyes. However, if a negative rotation angle is used, some people can view the image by crossing their eyes.

The two images are separated in the 2D Stereopair and OpenGL Stereopair but superimposed by viewing hardware in OpenGL Quad Stereo or Direct3D Stereo modes.

The rotation angle can also be set in the DialogBar - Right

3.2.4.7 Crystal Axes

Dialog Box: Crystal Axes [Input2 Menu**]**

You can superimpose crystal axes onto the drawing. Crystal axes cannot be drawn on stereopairs.

The crystal axes are scaled initially to be about the same size as the crystal. Thus the **Scale factor** is initially 1.0. The axes are always shown in front of the crystal(s), except in 3D mode. For hexagonal and trigonal (non-rhombohedral) crystals, the a3 axis is plotted, although it is not listed in print-outs.

If the **Include in scaling** box is checked the displaced axes will be included in any automatic Scaling or Centering operations (as selected in the Input1 menu).

The **Displacements** can be used to separate the crystal and axes, for example to put a small axial cross in a corner of the drawing. Note that you can also move the crystal with the Centering and Displacements command in the **Input2** menu or the Center button in the Dialog Bar - Right . The Scale Grid can assist in these displacements.

If you click on the **Locate with Mouse** button, the next click in the graphics window will relocate the axes to that point.

Front-back displacement is used only in the 3D mode.

If perspective viewing is on, the axes are projected as if they intersected at the origin,

although they are drawn as if they were in front of the crystal.

If the **Dashed** box is checked, the c axis is shown solid, the b axis is dashed with the dash intervals set in Crystal Edges dialog in the **Input2** menu, and the a axis is dashed with half these intervals. The crystal and the axes are projected independently, even if they are separated by displacements - that is, if you are looking directly down the a-axis direction in the crystal, you will also be looking directly down the a-axis in the axial cross.

Labels can be added to the positive end of each axis. The **Font** for axis labels is the same as that set in the face Labels dialog (Display menu). However, the size of the letters may be different from that in face labels - this is controlled by the **Scale factor for labels** .

In the 3D display mode in Perspective, there may be slight errors in the intersection of the axes at very short perspective distances (less than 20).

3.2.4.8 Initial Orientation

Dialog Box: Initial Orientation [Input2 Menu**]**

Any initial **Cartesian rotations** specified here will be be applied to the x, y and z crystal Cartesian axes (see section IV-4) in that order after the faces, corners, etc. are located and before the crystal is first displayed.

If the **Clinographic viewing** box is checked, the clinographic rotation (see Coordinate Systems) will be applied at the end of the calculation, after any initial Cartesian rotations. It may be turned off with the Clinographic Viewing command in the **Rotation** menu (or the ClinographicViewing command in the **Display** menu).

When exiting, SHAPE checks to see if the orientation has changed from the initial orientation defined in this dialog. If so, you have the option of saving the current orientation. This orientation will be converted into initial rotations on x, y and z, plus initial clinographic viewing if that is in effect. You can also save the current orientation with the Save/Recover Orientation dialog in the Rotation menu.

Summary of orientation operations . SHAPE first sets the *c* crystal axis parallel to the *z* viewer axis, and the *a* * crystal axis (perpendicular to *b* and *c*) parallel to *x* . This is the *original* orientation. Next, the initial Cartesian rotations, if any, are applied. Finally, the clinographic rotations, if selected, are applied. This is the *initial* orientation.

The initial orientation might also be termed the "preferred" orientation, since this is the one orientation which can be saved, and returned to with the Save/Recover Orientation command in the **Rotate** menu.

3.2.4.9 Scaling

Dialog Box: Scaling [Input2 Menu**]**

Scaling and displacement operations do not apply to the actual values of corner coordinates and face coefficients, which are permanently set by axis lengths and the central distances of the faces. Rescaling and displacement apply only to the plotting coordinates in screen, dot-matrix or pen-plotter displays.

Scale mode . There are three mode of scaling:

Maximize size for each view . In this mode, the crystal is scaled in each orientation so that it is just smaller than the viewing area. The actual scale will therefore change whenever the crystal is rotated. Hard copy is scaled the same way and what you see is essentially what you get.

Universal maximum. In this mode, the crystal is scaled so that its maximum dimension is just smaller than the minimum dimension of the plotting areas; thus, rotations can be made without changing the scale and without going out of bounds. Again, hard copy is scaled the same way and what you see is essentially what you get.

Fixed scale factors. This suboption allows you to set the scale to a fixed number of inches or centimeters per central distance unit for the dot-matrix and/or pen plot, or simply to reduce or enlarge the image from the automatic scaling modes.

The **Rescale factor** applies only to the **Maximize...** and **Universal...** modes. Both these modes scale the drawing to the dimensions of the screen (window) or the frame, and then apply this rescale factor. When you click the up- or down-size (or "zoom") button in the Dialog Bar - Right), this changes the rescale factor unless you are in the **Fixed...** scaling mode. (This is a change from pre-V6.0 SHAPE - formerly clicking one of these buttons when in the **Maximize...** or **Universal...** modes would switch to the **Fixed...** mode.

Scaling for the screen and normal printer output (Print command in the **File** menu) depends on the resolutions (dots per inch or centimeter), which are obtained from the software drivers for these devices. The correct scaling for a particular printer may not be attained until you have used that printer for the first time. Resolution for the printer may often be reset in the Print Setup dialog in the **File** menu. The resolution for the Pen Plotter is set in the Pen Plotter Settings dialog, and that for a direct PostScript printer is set in the Postscript Settings in the **Settings** menu.

The Dialog Bar - Right allows "zooming" or incremental adjustment of the scale factors.

When displaying symmetry operators in the 3D mode, scaling in the **Maximize size** or **Universal maximum** modes is based on the presumed maximum extent of symmetry elements, which in turn are based on the maximum distance for corners - the ratios governing the relative sizes of crystal and symmetry elements are set in the 3D Parameters dialog (Input2 menu). Thus the scaling for in the **Maximize size** mode is practically identical to that in the **Universal maximum** mode.

3.2.4.10 Centering/Displacement

Dialog Box: Centering/Displacement [Input2 Menu]

Automatic centering will center the crystal in the current viewing area. This is done for each view, and any displacements entered under **Constant Displacements** are ignored.

In most cases, the easiest way to scale and position a drawing onto a printed or typed page is to use the frame options in the Print command or other options in the **File** . However, the displacements in this section can be used to position the drawing within the frame defined in those suboptions.

The displacements are used only in plotting and are not actually part of the corner coordinates. Note that the center of rotation is not changed by these displacements - that is, the crystal is always rotated about its own zero of coordinates. Thus any desired rotations should always be made before using displacements.

The Dialog Bar - Right (**Display** menu) allows incremental displacements, and centering of the viewing area on a particular projection point in the crystal. Displacements made there will affect the displacements in this dialog (**Centering/Displacement**), and may be removed here.

The Scale Grid command in the **Display** menu is useful for showing the actual scaled location of the crystal and in estimating displacements.

3.2.4.11 Reset Scaling/Centering

Dialog Box: Reset Scaling and Centering [Input2 Menu]

This dialog allows reversion to the Scaling and Centering/Displacement modes and settings in effect before various interactive changes, or selection of the default settings (Universal Maximum scaling and Automatic centering).

Current makes the current settings permanent - after this these settings will be the "Last" settings.

Last returns to the values set in the last calculation, or the last reset with this dialog. Current settings are erased.

Default selects Universal Maximum scaling and Automatic centering, so the structure should

remain the same size and completely in view at all times.

Cancel will exit the dialog without any change - the current and last settings will be preserved.

You can always adjust the settings in the Scaling and Centering/Displacement dialogs in the Input2 menu.

This dialog can be called from the DialogBar-Leftwith the Reset Scaling button.

3.2.4.12 3D Parameters

These parameters apply to VRML and POV-Ray files as well as 3D Drawing Modes mode.

3.2.4.12.1 3D Display Modes

These drawing modes can be selected in the **Display Mode** submenu of the **Display menu** , or the Dialog Bar - Left .
Although a shaded SHAPE drawing in the **Standard display mode** using Shading (Input1 Menu) has a good 3-dimensional appearance, the term "3D drawing" is used to denote a method of drawing which is different in several respects. SHAPE uses the OpenGL system software package for Windows, Macintosh and Linux and the Direct3D package for Windows (only).

In this type of drawing, the surfaces of three dimensional objects such as spheres and cylinders are converted to an assemblage of planar polygons. Then each polygon is drawn essentially independently. The critical difference from non-3D modes is that a *depth buffer* is used in 3D imaging. This is an array of integers, one for each pixel in the display or output (or that portion which is currently being drawn). Each element, representing a pixel, holds the relative *x* coordinate (in the SHAPE observer coordinate system) of the foremost object or polygon. The color for this object is retained in the *color buffer* , which is a similar array representing pixels; this array is actually the image itself. Whenever a polygon is drawn, each pixel which it contains is compared against the depth buffer; if the *x* coordinate of the pixel is greater, or closer to the observer than what is in that element of the depth buffer, the color for this pixel in the new polygon replaces the value in the color buffer. That is, the depth buffer keeps track of the front surface of the drawing, and ensures that only this front surface (not any hidden surfaces) are kept in the color buffer or image itself. It is also possible to have transparent or translucent objects, through which hidden surfaces may show partially.

Actually, the "double buffer" method is normally used, the color buffer being kept in an area of memory and then copied to the screen memory when the drawing is completed. This is usually faster than drawing directly to the screen.

The non-3D display modes of SHAPE do not use a depth buffer: the back edges are drawn and then the front edges and faces (except for the **Anaglyph** mode). When necessary, the intersections of objects are solved analytically and only the required

portions of each are drawn.

There are two main advantages to using the 3D display mode in SHAPE. First, display of symmetry elements (rotation axes and mirror planes) is supported only in the 3D modes, because the intersections of these objects with each other and with crystal faces and edges is too complex for the methods used in standard modes. Second, correct shading of multiple crystals (twins and epitaxial intergrowths) can only be guaranteed in 3D modes, for similar reasons.

The 3D modes also allows for more elaborate lighting effects (see Lighting Equation and Material Parameters), although these are not of as much use for simple polyhedra as for other objects. The shading of curved surfaces (which in SHAPE means only cylindrical edges and crystal or symmetry axes, and some symmetry symbols) is more satisfactory in that the color (shading) at each point in a polygon is linear interpolated from the values calculated from "normals" supplied for each corner. Since this may call for very fine gradations in color, the greater the color resolution of the device (the more color bits per pixel) the better the result will be. 3D drawing will work with an 8-bit (256-color) display driver, but is usually much better with 16-, 24- or 32-bit display. The color resolution may be set in the Display control panel of Windows 95/98/NT.

The 3D modes usually draw only *surfaces* , not edges or intersections of surfaces. To show edges it is necessary to specify them independently and draw them as cylinders or lines.

Note that OpenGL does not support shadows, refraction and many other effects which make for a truly realistic drawing of a transparent object like a crystal. The freeware ray-tracing program POV-Ray can do much of this, and SHAPE can optionally write data files readable by POV-Ray (see List Results).

3D drawing is a raster method, and therefore is not supported in pen plots or metafiles - it is supported for the screen, dot-matrix, laser or ink-jet printing, and Raster Files.

3.2.4.12.2 Crystal Colors

Dialog Box: Crystal Colors [3D Display Parameters **dialog]**

This allows specification of separate colors for each individual in twins and epitaxial intergrowths.

The list box gives the RGB components for each crystal. Crystal number 1 is the main crystal. The R, G and B components for the selected crystal may be modified in the edit boxes at the bottom of the dialog, or you can modify the color graphically by clicking on the **Select Color** button.

In some twin and epitaxial intergrowths, the faces of two or more individual crystals may

be coincident, i.e. may overlap in places. If the crystals are given different colors, the color of the overlap areas is not predictable; parts of this area may be one color and parts another.

3.2.4.12.3 3D Display Parameters

Dialog Box: 3D Display Parameters [Input2 Menu]

This dialog controls parameters for the 3D Display mode, which is selected with the combo box in the Dialog Bar - Left, or with the Modes/Display Menu.

You can **Show Edges** and/or **Show Faces** , but of course you must check one or the other of these boxes unless you want to show symmetry elements only.

Edges may be simple **Lines** or **Cylinders** of the specified **Radius** . Lines have the thickness (in inches or centimeters) currently set in the Line Attributes dialog (Input2 menu). Keep in mind that lines are three-dimensional objects (with a ribbon shape), and they may interpenetrate with and be partially obscured by other objects such as crystal faces. If edges are to be wider than a few pixels it is usually better to use cylinders (note that cylinder radius is in central distance units, not cm/in). If lines are used it may be best to use a similar color for edges and faces. The edge colors are set in the Line Colors dialog in the Input2 menu. Striations in 3D mode are always lines, not cylinders.

Faces may be completely opaque (**opacity** = 1.0), or translucent/transparent. If the **opacity** value is greater than 0.98, faces will be assumed to be completely opaque - drawing opaque surfaces is faster.

If the **Show Symmetry** box is checked, all rotation axes and mirror planes will be shown. Attributes of this display may be changed with the **Symmetry** button (Symmetry Element Display dialog)

The **Materials** button (3D Materials dialog) allows changing the reflective/emissive properties of the objects.

If the **Use Face/Form Fills** radio button is checked, the selected faces or forms (Face or Form Fills dialog, Input1 menu) will have the particular color specified. Any faces or forms not specified will have the overall crystal color. If the **Use Crystal Color** radio button is checked, the given color will be applied to all faces. All faces, whether using fills or not, will be shaded according to the current illumination direction and materials parameters.

If there is more than one crystal (twin individuals or epitaxial crystals), and the **Use color for each crystal** box is checked, a separate color for each one will be used. The colors for the second and subsequent crystals must be set with the **More Colors** button (Crystal Colors dialog).

The **Illumination direction** is the direction in observer Cartesian coordinates (see Coordinate Systems) from which the light is coming. This is the same vector as in the Shading dialog (Input1 menu).

There is only one light, of the Directional type (not Positional) - that is, all rays are parallel.

3.2.4.12.4 3D Material Parameters

Dialog Box: 3D Material Properties [3D Display Parameters dialog]

In the 3D Display mode the material properties of objects determine the way the objects interact with the light sources.

The color observed at a given point is a resultant of the light source and the material properties; that is, the RGB coefficients of the **Ambient** , **Diffuse** and **Specular** components of the light source(s) are multiplied by the specified colors of the objects, and by the material coefficients in this dialog, then the results are limited to the range 0.0-1.0. See Lighting Equation for details. In SHAPE, there is only one light source, color white, which has rays coming from a constant direction (parallel rays), rather than from a single point.

Ambient light has no direction or origin and is considered to bathe all objects uniformly. Having a significant ambient component causes non-illuminated parts of objects to be other than black. It thus "softens" the illumination in a somewhat similar way to the **Darkest Shade** and **Darkness Angle** parameters (Shading dialog) in the **Standard** display mode.

Diffuse color is usually the main component of the appearance of objects. The intensity of the color is dependent on the angle between the light ray and the normal to the surface in question.

Specular reflection only occurs when the normal to the surface in question is close to bisecting the angle between the incident light and the vector from the point on the surface to the eye. It produces bright highlights on a curved surface. The larger the **Shininess** coefficient, the smaller will be the bright specular highlight on a curved surface. The shininess coefficient has a maximum of 128 because of computational restrictions, but values on the order of 5-30 are usually realistic.

In SHAPE, specular reflection is always white, that is it does not depend on the color of the object, only the color of the light source (which is white). Specular reflection does not currently work well for crystal faces and mirror planes because faces at the reflection angle will give an essentially solid white appearance, rather than a bright spot. This is because the angle is calculated for the corners of the face, and interpolated for each point

in the interior of the face. In order to produce bright-spot highlights on flat surfaces, it would be necessary to subdivide the surface on a fine grid, and use point light sources rather than parallel illumination.

Emission is similar to ambient, except that there is no dependence on the color of any light source. A high value of emission can make an object look like is is glowing.

These material properties are specified separately for cylindrical edges and symmetry axes, and for crystal faces and mirror planes.

3.2.4.12.5 Symmetry Element Display

Dialog Box: Symmetry Element Display [3D Display Parameters **dialog]**

In the 3D Display Mode, rotation axes and mirror planes may optionally be shown.

Rotation axes can be shown as simple lines, or cylinders of the specified **radius** . The standard symbol for each axis, in a 3-dimensional, "extruded" form, will be shown on each end of the axis.

All rotation axes will be the same **Color**.

Mirror planes are actually shown as plates of the specified **Thickness** .

If the **Opacity** is greater than 0.99, they are drawn as totally opaque, which is faster. The planes may be circular or disk shape, or square. Note that the circular outline of disks always consists of line segments, and the number of such segments in VRML files is determined by the viewer, not SHAPE. Thus disks may have an unacceptably polygonal appearance in some VRML file viewers.

Transparency of mirror planes is something of an approximation. Some color combinations for background, crystal edges, faces and mirror planes may work better than others.

Scale factors. These factors determine the relative sizes of the symmetry elements and the crystal. In the **Maximize size for each view** and **Universal maximum** scaling modes (Scaling dialog, Input2 menu), the drawing is scaled to the minimum dimension of the screen or the frame for printed or file output. When symmetry elements are shown, it is generally best to reduce the scale of the crystal relative to them. The rotation axes should usually be largest, so that the symbols at the ends are not obscured. If they are given scale factor 1.0, they will be scaled so that they occupy the space which would be occupied by the crystal in the absence of symmetry elements. Similarly, the scaling for the mirror planes and crystal should be reduced with respect to this original scaling - factors of about 0.7 and 0.6 respectively are reasonable. In the **Fixed** scaling mode the scale

factors specified in the Scaling dialog apply to the crystal, and the factors for symmetry axes and planes are scaled relative to the crystal.

The **Symbol size** determines the maximum dimension of the symbols drawn on both ends of each symmetry axis. The thickness is twice the cylinder radius for the axes (above).

There is a sample of each crystallographic symmetry group or crystal class in the \GROUPS subfolder or directory.

When in the Cartesian or QSHAPE mode (not supported in the Standard Edition), information on the symmetry operators must be present in the .SYM file (Cartesian Symmetry). This information follows the actual symmetry matrices in the form of lines beginning with the keyword SYMOP. This is followed by three floating-point values giving the orientation of the symmety element in Cartesian coordinates, and an integer giving the order of the symmetry element. An inversion axis is denoted by a negative sign. A mirror plane is denoted by order -2, and the coordinates are for the perpendicular to the plane.

Only one symmetry operator of each independent set should be given - the rest are generated by the symmetry matrices. In many cases these operators are just those which are required to generate the symmetry group in the program SYMGRP, and SYMGRP will now write out the generating operators as SYMOP lines. However, in some cases additional sets of operators are generated. SYMGRP will add a mirror plane perpendicular to any rotation axis of even order if a center of inversion is present, but there are still some cases in which operators may have to be added manually. For example, the non-centric icosahedral group *I* can be generated with only one three-fold axis and one five-fold axis (actually, only one operation of each), but a set of 2-fold axes is implicit in the group and must be added.

See the .SYM files in the \SYM subfolder for examples, which include the icosahedral and pentagonal groups.

Note that some trigonal, tetragonal and hexagonal point groups may have alternate orientations of the symmetry elements with respect to the crystallographic axes - see Symmetry.

3.2.5 Display Menu

Replot - Replots the image (does not recalculate).

Color - Switches the screen between black-and-white and color.

Remove Hidden Lines - For intergrowths, removes segments of lines of one crystal that are hidden by another.

Scale Grid - Superimposes a scale grid for location of the crystal or parts thereof.

Clinographic Viewing - Switches clinographic viewing on and off.

Anaglyph - Settings for the two-color Anaglyph Drawing mode.

Labels - Settings for face indices labeling.

Dialog Bar - Left - This is a vertical toolbar which resides along the left edge of the Main window. It combines the functions of the former Rotate and Quick Commands dialog
Dialog Bar - Right - This is a vertical toolbar which resides along the right edge of the Main window. It contains a list of form and some common commands.

Dialog Bar - Epitaxial - This allows movement of epitaxial crystals.

3.2.5.1 Replot Command

Replot Command [Display menu**]**

This command redraws the image without recalculation. Changes in most items in the Input2 menu can be put into effect with this command (although these dialogs all have an automatic replot check box). It can also be used after some changes in the items in the Input1 menu, such as colors. For changes which affect the number of faces, corners and edges and their relative locations, use the Calculate command in the **File** menu or the Calculate button in Dialog Bar - Left.

3.2.5.2 Color Command

Color Command [Display menu**]**

This switches between full-color and black-and-white screen display (all types of output have independent color switches). Displays with more than 16 colors may show true gray-scale rather than the dithering which is used in actual black-and-white output. You can set the default or start-up status of this switch in the Preferences dialog in the **Settings** menu.

Even if your display is color it may be useful to view the image in black-and-white to see what it will look like in black-and-white files or printing.

3.2.5.3 Scale Grid

Dialog Box: Scale Grid [Display Menu**]**

This option allows you to locate and size the crystal, so that it can be rescaled or displaced. It will draw a square grid at the given absolute intervals. The center of coordinates is shown by a star at the center of the screen, and the current location of the

center of the crystal by another star. These two center points differ only if you have entered displacements or turned on automatic centering with the Centering/Displacements dialog in the **Input2** menu or with the Dialog Bar - Right . The grid is removed only by replotting with the **Grid plotting on** box unchecked.

See Input Colors/Patterns/Pens for general aspects of input

3.2.5.4 Clinographic Viewing Command

Clinographic Viewing Command [Display menu**]**

This turns clinographic viewing on and off, with automatic replot. See also Clinographic Viewing in the **Rotation** menu, which does the same thing without automatic replot. Set the inital state of clinographic viewing in the Initial Orientation dialog in the **Input2** menu.

See also Coordinate Systems.

3.2.5.5 Anaglyph Settings

Dialog Box: Anaglyph Settings [Display **Menu]**

Rotation angle. This is the angle by which each of the views is rotated away from the non-stereo position. This angle is the same as the angle for separate stereopair views, which is also set in the Preferences dialog (**Settings** menu).

View colors and Background . The colors of the two images are completely different depending on the background. For screen viewing, the background is normally black, and the left-eye image is red, while the right-eye image is blue, green or cyan. Which of the latter three colors works best depends on the particular glasses you are using. The color of the combined, 3-D image is white, violet, or yellow. In most cases, images on the screen work best with red-cyan rather than red-blue.

For printed images, the background is normally white, and the right-eye image is red, while the left-eye image is green, cyan or blue, again depending on the glasses. The color of the combined, 3-D image is normally black.

Anaglyph drawings can be shaded, but the color will be ignored and the crystal will be shown as white. On the screen, if the color where the two images overlap is not white, try changing from red/blue to red/cyan or vice versa.

It is certainly possible to use a white background on the screen, but a black background for printing is not usually very satisfactory, because of bleed (widening) of the black background pixels onto the colored lines. Lines must be many pixels wide to avoid this problem.

The success of the 3-D image relies on proper combination of colors during drawing. When part of the right-eye image is superimposed on part of the left-eye image, the colors must be added, instead of the right-eye image just replacing the left-eye image. That is, where a red image and a blue or cyan image coincide on a black background the color should be white (or violet), instead of blue (or red). For Windows, this appears to be done incorrectly for 8-bit (256-color) screen modes and correctly for 16- and 24-bit screen modes. Color combination for index Labels does not seem to be done correctly even in the 16- and 24-bit screen modes. However, these aspects may also depend on the particular graphics card installed in your machine. For printing, the rules for combining colors are completely different, and the results you get may depend on the printer driver and printing mechanism.

In summary, you may need to experiment with the **View colors** and **Background** settings to get the best results.

3.2.5.6 Labels

Dialog Box: Labels [Display Menu]

This option can cause either form letters or the numeric indices of each face to be written. The label is written at the center of the face, which is located by averaging the corners. Labels are not written in the Cartesian mode. Face indices may be shown with or without the standard parentheses or brackets. The form letters are entered for each form in the Add/Revise Form dialog in the Input1 menu.

You can **Label back faces** , but only if back edges are shown (Line Attributes dialog, Input2 menu). You can select the Colors for the labels for front and back faces: usually these should be the same as the colors for the front and back edges set in the Line Colors dialog, Input2 menu.

The negative **Signs for indices** may be above each number, in conventional crystallographic style, or before the number, in normal mathematical style (positive signs are never shown). If the chosen font is not fixed-width (see below), signs above may not work correctly. In D3D (Windows) drawing mode signs are always before the numbers.

The labels can be offset by uniform amounts across and up, or the observer y and z directions.

If you select **Opaque** , rather than **Transparent** , there will be a white block behind each label. However, this is not recommended for indices because the small bars over the numbers, denoting negative signs for the index, are actually formed by writing underscores on another line above the numbers.

It is best to select a fixed-width **Font** such as Courier, because the correct location of the negative sign bars above the numbers depends on letters having a constant width. Fixed-

width fonts typically have "fixed" or "mono" in the name. The font in PostScript output will always be Courier.

In the 3D display mode, the position in space of the labels depends on whether actual planar faces are shown (3D Parameters dialog, Input2 menu). If faces are not shown, the labels are written at the center of each face. If faces are shown, the labels are all in a plane which is in front of the entire crystal.

3.2.5.7 Dialog Bar - Left

Dialog Bar - Left

This is actually a special type of Control Bar, residing on the left or right side of the Main window. It can be turned on or off with the **Dialog Bar - Left** command in the **Display** menu. The Left-hand dialog bar combines the functions of the former Rotation and Quick Commands modeless dialogs. The Dialog Bar - Right contains the list of forms, and another set of common controls.

Only those controls are visible which can have an effect on the current state of the problem. For example, when SHAPE is first started up, only the Open button is shown.

The upper part controls rotation of the structure in simple ways (for more ways to rotate or align the structure, see the commands in the Rotation menu). The current orientation is shown at the top. The a, b and c axis labels are attached to the positive ends of the axes, and the part of the axes extending forward (positive x) are drawn with heavier lines. In normal or standard view, the rotation buttons below this are for rotation on x, y and z, respectively; positive angle (clockwise looking outward on the axis) is on the left, and negative rotation on the right. In stereonet view you are looking down on the c-axis, so the pairs of buttons are for z, y and x going downward. The angle of rotation is in the box below the buttons. The initial value of this angle is set in the Preferences dialog in the Settings menu.

If the **Auto** box is checked, the rotation occurs as soon as each rotation button is clicked. If this box is not checked, the rotations are accumulated into a matrix, and the drawing is not replotted until you click on the **Replot** button lower in the dialog (or select **Replot** from the Display menu).

The buttons beneath **Auto** duplicate some common commands, all from the File menu except **Replot** , which is also found in the Display menu. You can use Open to start up SHAPE by reading in a file.

Replot - Replots the image (does not recalculate).
Calculate - Reproduce faces and locate corners and edges, etc..
Open - Open an old SHAPE data file.
Save - Save a SHAPE data file.

Save as - Save a SHAPE data file with a new name
Print - Prints using the standard printer.

The Model Mode drop-down or box controls the Model Mode - this duplicates a submenu in the **Modes** menu.

The Drawing Mode drop-down or box controls the Drawing Mode - this also duplicates a submenu in the **Modes** menu.

The Fullscreen button switches from normal windows to display using the entire screen. From SHAPE V7.3 this can be done with any combination of Model and Drawing Modes and on Macintosh, Windows or Linux.

3.2.5.8 Dialog Bar - Right

Dialog Bar - Right

This is actually a special type of Control Bar which resides on the right side of the Main window. It can be turned on or off with the **Dialog Bar- Right** command in the **Display** menu. The Right-hand bar contains a list of forms, and some common commands. The Dialog Bar - Left contains another set of common controls.

The current forms are given in the list box at the top of the dialog bar. To modify a current form, double-click on an entry in the list. This brings up the Add/Revise Form dialog. To **Add** or **Delete** forms, use the buttons below the list box. If epitaxial crystals are present, the **Add** button will add a form to the crystal whose form is currently selected in the list box.

The **Cursor Mode** radio buttons control the operation of the mouse cursor.

In the **Identify Faces** cursor mode, clicking the left mouse button on a face brings up the Face at Cursor dialog, which provides information about the face and form. Clicking the right mouse button on an edge or corner allows insertion of a new form truncating this edge or corner and its symmetry equivalents. Only visible or front edges may be selected. The indices of the new form will be the sum of all the faces involved in the edge/corner. The alert box which asks your permission to add this form gives the indices as a raw sum (e.g. 202), but before the form is actually added the indices will be reduced by any common factor (e.g. to 101). In the case of twins, the new form will be added to all twin individuals, but in the case of epitaxial intergrowths, only the crystal which is selected will be affected. The cursor shape for this mode is a simple cross.

The **Resize** cursor mode allows automatic adjustment of central distances and therefore face sizes. In this mode, clicking the left button on a face will increase the central distance of the *form* , and cause recalculation (the current orientation will be retained).

Of course, increasing the central distance generally decreases the size of the faces in the form. Clicking the right button decreases the central distance. The amount of the increase or decrease is set in the Preferences dialog in the **Settings** menu. Clicking on a face of a twin will cause a change in all the twin individuals. The cursor shape for this mode is a cross with arrowheads on all arms. When this mode is in effect there is a white block in the upper left corner of the graphics window saying "Resize mode off". This block is a reminder that clicking on any face will actually change the shape of the crystal, and clicking in the block will cause reversion to the **Identify Faces** cursor mode.

The **Rotate** cursor mode allows rotation of the drawing, by clicking and dragging. Clicking and dragging near the center of the plotting area causes rotation on the y and z Cartesian reference axes (see Coordinate Systems) - the effect is as if the cursor "grabs" a point on the front of the crystal. Clicking and dragging near the left or upper edges of the plotting area causes rotation on the z Cartesian reference axis, which is perpendicular to the screen. The cursor shape for this mode is a quasi-circular rotation arrow.

The **Remove Symmetry** button allows for distortion from ideal symmetry, by complete removal of all symmetry. Each current generated face is converted to a form, whose central distance may then be adjusted (e.g. with the **Resize** cursor) independently of the other faces related to this one by the original symmetry.

The **Show Symmetry** check box controls the display of symmetry elements (rotation axes and mirror planes), which is possible only in the 3D display mode. See 3D Parameters.

Clinographic Viewing . This turns on and off the rotations which give the standard

The **Set Center** button defines a new center point - use this to "focus" or "zero in" on a specific area or point in the plot. After clicking on this button, an alert box informs you that the next mouse click in the graphics window will define a new center point. After clicking on a point, the drawing will then be displaced so that that point will be at the center of the viewing area. It may be more useful to think of the result as the viewing area being centered on the point selected.

With the **Rescale** buttons, you can "zoom" in or out. When in the **Maximize...** or **Universal...** scaling modes, this changes the rescale factor (see Scaling). In the **Fixed...** mode, clicking on these buttons simply changes the fixed scale factors. The actual rescale factor applied is 1/(1+x) for down scaling, and (1+x) for up scaling, where x is the amount in the edit box converted from percent to a fraction.

The **Reset Scale** button calls the Reset Scaling and Centering dialog. This allows reversion to the last setttings, before interactive changes with the **Set Center** or **Rescale** buttons (above), or in the **Fullscreen 3D** mode.

Summary of mouse cursor operations in graphics window. For Macintosh, "Right

button" is obtained with the option key plus the mouse button.

Index (Identification) mode:

Left button - identifies face and form; successive clicks give interfacial angle.

Right button - identifies edges and corners; allow addition of new form truncating face or corner.

Resizing mode:

Left button - increases central distance of form selected - usually decreases area.

Right button - decreases central distance of form selected - usually increases area.

Rotate mode:

Left button - click and drag in main part of window rotates around axes in screen; click and drag near left or upper edge rotates around axis perpendicular to screen.

3.2.5.9 Dialog Bar - Epitaxial

Dialog Bar - Epitaxial

This is actually a special type of Control Bar, residing on the right side of the Graphics window, but just to the left of the Dialog Bar - Right. It can be turned on or off with the **Dialog Bar - Epitaxial** command in the Display menu.

This dialog bar is only for positioning the epitaxial crystal(s) with respect to the main crystal. To change the orientation (i.e. host plane and vector and guest plane and vector) go to the Epitaxy dialog in the Input1 menu. The Crystal which is being positioned is set with the choice box at the top. The main crystal is number 1, so the first epitaxial crystal is number 2.

The **Distance** is measured between the center of the epitaxial crystal and the the center of the main crystal, perpendicular to the Host Plane.

The **Displacement Parallel to vector** is in the direction of the Host vector listed above in the dialog bar. The displacement Perpendicular to this vector is in the epitaxial plane. To show the new position, click the Calculate button.

3.2.6 Rotation Menu

Cartesian Axes - Rotate on the viewer or reference axes.

Crystal Vector - Rotate on a rational crystal vector [uvw].

Clinographic Viewing - This turns clinographic viewing on and off, with optional replot.

Align Face or Vector - Align the crystal with a face in the screen or a vector perpendicular to it.

Save/Recover Orientation - Remove all rotations made since the calculation or the Initial Orientation, or save the current orientation as the Initial Orientation.

Current Orientation - Gives the exact current orientation of the crystal(s).

Continuous Rotation - Initiates continuous rotation of the crystals(s) about a specified axis.

Rotation Movie - Writes a video file in .SWF - Flash platform-independent format or Windows- or Macintosh-specific format.

3.2.6.1 Rotate on Cartesian Axes

Dialog Box: Rotate on Cartesian Axes [Rotation menu**]**

This rotates the crystal on one of two sets of Cartesian axes. If clinographic viewing is off, the crystal is always rotated about one of the axes belonging to the observer system: x coming straight out towards the observer, y in the plane of the screen or paper pointing to the right and z upwards. If clinographic viewing is on, you can choose to rotate about the clinographic axes, which have been rotated in a certain way from the observer axes (see Coordinate Systems).

Each time you click the **Rotate** button, a rotation is added to a master rotation matrix; the number of such rotations is listed at the bottom of the dialog box. When you have finished rotating, click the **Done** button and the master rotation matrix is applied to the crystal. If you click **Cancel** , no rotations are applied.

In Standard mode, the clinographic and observer axes are roughly similar. However, in Stereonet mode (selected in the Modes menu), they are distinctly different. In this mode, you are considered to be viewing the crystal down the c axis, instead of down the a* axis (or approximately so, if clinographic viewing is on). Thus the clinographic z axis comes directly out of the screen or paper, the x axis is downward and the y axis is to the right - in other words the clinographic axes are rotated by 90 degrees with respect to the observer axes. As noted in Coordinate Systems, when rotating about the clinographic axes, the crystal can be considered to be rotating in its own coordinate system, while the user may have different points of view: in Standard mode with clinographic viewing off, looking directly down the x axis; in Standard mode with clinographic viewing on, looking down a direction which is up and to the right from the x axis; and in Stereonet mode,

looking directly down the z axis.

3.2.6.2 Rotate on Structure Vector

Dialog Box: Rotate on Crystal Vector [Rotation Menu**]**

This will rotate about a rational crystal direction [uvw], regardless of the current display mode or orientation of the crystal. If you are drawing a molecule and have used Cartesian reference axes, the rotation direction is simply a vector with the coefficients u, v and w in the original molecule axis directions a, b and c. The indices or coefficients refer to a coordinate system fixed with respect to the crystal (always rotating with it). In Crystal (not Cartesian) SHAPE the indices must be integers, but this is not a bar in practice to rotation about irrational vectors, since the indices may take very large values.

Each time you click the **Rotate** button, a rotation is added to a master rotation matrix; the number of such rotations is listed at the bottom of the dialog box. When you have finished rotating, click the **Done** button and the master rotation matrix is applied to the crystal. If you click **Cancel** , no rotations are applied.

3.2.6.3 Clinographic Viewing

Dialog Box: Clinographic Viewing [Rotation Menu**]**

This will switch on and off the rotations of -18.4 degrees on z and 9.5 degrees on y, applied in clinographic display mode. This in effect changes the viewpoint of the observer between the clinographic position, down the vector [621] referred to the observer Cartesian axial system, and a straight-on position, down the x axis. This command is included in the menu for convenience; the same operation is performed by the Clinographic Viewing command in the **Display** menu, although choosing that command always causes a replot.

See also Coordinate Systems.

3.2.6.4 Align Face or Vector

Dialog Box: Align Face or Vector [Rotation Menu**]**

<Standard Mode - see also Align Face or Vector (Cartesian)>

This will rotate a specified face (hkl) to lie flat in the screen or paper (face-normal parallel to x observer), or a vector (uvw) to be perpendicular to the screen or paper. To align a face, it is also necessary to specify a vector lying in the face which will be vertical in the screen or paper (z direction). Conversely, to align a vector, it is necessary to specify a face, containing the vector, whose normal will be vertical. If a vector [uvw] lies in a face (hkl), the indices satisfy the condition hu + kv + lw = 0. If clinographic viewing is in effect, it is turned off when the face is aligned, to simplify any subsequent rotations.

You can elect to use a default alignment vector or face. The default vector will be the intersection of the face (hkl) with the face (100), whose indices are given by the cross product (hkl)x(100). If the face (hkl) is (100), the default alignment vector will be the vector [001]. For aligning a vector the algebra is just the same, with interchange of face and vector.

3.2.6.5 Align Face or Vector (Cartesian)

Dialog Box: Align Face or Vector (Cartesian) [Rotation Menu**]**

<Cartesian mode - see also Align Face or Vector (standard)>

This will rotate a specified face (hkl) to lie flat in the screen or paper (face-normal parallel to x observer), or a vector (uvw) to be perpendicular to the screen or paper. To align a face, it is also necessary to specify a vector lying in the face which will be vertical in the screen or paper (z direction). Conversely, to align a vector, it is necessary to specify a face, containing the vector, whose normal will be vertical. If a vector [uvw] lies in a face (hkl), the indices satisfy the condition hu + kv + lw = 0. If clinographic viewing is in effect, it is turned off when the face is aligned, to simplify any subsequent rotations.

In the Cartesian mode, faces and vectors are equivalent - that is, to align a face is also to align a vector with the same indices.

You can elect to use the default alignment vector or face, instead of specifying it. The default vector will be the intersection of the face (hkl) with the face (100), whose indices are given by the cross product (hkl)x(100). If the face (hkl) is (100), the default alignment vector will be the vector [001].

3.2.6.6 Save/Recover Orientation

Dialog Box: Save/Recover Orientation [Rotation Menu**]**

The first two options will counteract all rotations made by the dialogs in the **Rotation** menu as well as any made on-screen with dialogs in the **Display** menu, and take you back to one of two settings. The *original* orientation means the orientation before any rotations, including the rotations of the Initial Orientation dialog in the **Input2** menu, have been made. The *initial* orientation is that attained after the rotations of the Initial Orientation dialog - that is initital Cartesian rotations and initial clinographic rotations - have been made, if any of them were actually used. See also Coordinate Systems.

The third option will save the current orientation as initial Cartesian rotations, plus initial clinographic rotation if clinographic viewing is currently in effect. These settings can be viewed and changed in the Initial Orientation dialog in the **Input2** menu.

Summary of orientation operations . After calculation, SHAPE first sets the *c* crystal axis parallel to the *z* viewer axis, and the *a* * crystal axis (perpendicular to *b* and *c*) parallel to *x* . This is the *original* orientation. Next, the initial Cartesian rotations, if any, are applied. Finally, the clinographic rotations, if selected, are applied. This is the *initial* orientation.

3.2.6.7 Current Orientation

Dialog Box: Current Orientation [Rotate **Menu]**

This gives the current orientation in terms of the face normals and crystal vectors which are a) in x observer direction (see Coordinate Systems), perpendicular to the screen or paper; and b) in the z observer direction, vertical in the screen.

Note that the List Results command in the **File** menu gives the directions of the crystal axes in the observer Cartesian system.

3.2.6.8 Continuous Rotation

Dialog Box: Continuous Rotation [Rotate **Menu]**

This dialog initiates a continuous rotation about any of the three Cartesian observer axes (x out of the screen or paper, y to the right and z vertical).

The **Delay** (in integral seconds) is the time after finishing one view and beginning the next; it does not include the time required to draw the view.

To stop the rotation, press any key. You will then see a dialog allowing you to abort the rotation or to continue it.

Sounds are turned off during this rotation, the cursor is invisible, and the double-buffer drawing method is used (Preferences dialog, **Settings** menu). When you finish continuous rotation, the previous settings are restored.

3.2.6.9 Rotation Movie

Dialog Box - Rotation Movie [Rotation Menu**]**

This will write a movie or video file in .AVI (Windows), .MOV (Macintosh) or .SWF - Flash (all platforms) format. These files consist of a series of bitmap (raster) images. The structure will be rotated from its current attitude about the selected **Axis** , with the selected **Rotation increment**, until the sum of rotations exceeds the **Maximum rotation**.

A normal motion picture uses 30 **Frames per second** , but typical computer videos use less than this. In fact, some computers may not be able to handle 30 frames/sec for large images.

For .SWF - Flash files (only) you can add a sound track from a .mp3 file.

Note that movie files may be very large (many megabytes) even if compressed. For Macintosh, the compression mode is automatically selected by the System software, and is supposedly optimal for the resolution (**Pixel size**) selected. In Windows, you are presented with a dialog showing the available codecs (COmpression-DECompression algorithms), and you must select one. Finding the optimal codec may be a matter of trial and error - performance usually varies with the **Pixel size** and the actual number of colors used. Some codecs compress very effectively, but cause degradation of the image - SHAPE images should usually be compressed with a lossless compression method. Some codecs which have been found to be good for typical SHAPE images are the CorePNG and Lagarath codecs.

See Frames for details of the frame and frame units.

3.2.7 Settings Menu (Graphics Window)

The Settings Menu in the Graphics Window is identical to the Settings Menu in the Startup Window.

3.2.8 Windows Menu

The Windows menu lists all the possible windows in SHAPE - those which do not actually exist are greyed out.

Select a window to make it active, or bring it to front.

When a Text window is active, the first item in the menu is a **Font** selector, which acts on the entire text in the window.

3.2.9 Help Menu

This gives access to the online Help system, and to the About dialog with copyright and other information.

On the Macintosh, the About dialog will appear in the Apple menu (OS 8/9) or in the Application menu.

3.2.9.1 About

About command [Help menu]

Use this command to display the copyright notice and version number of your copy of SHAPE.

3.3 Text Window Menu Bar

These windows are used for the List Results command in the **File** menu of the Graphics window and for listing of corner information in Sections and Growth Zones - see Types of Windows. They are standard Windows text or edit windows. To switch to the SHAPE graphics window, which has the menus and commands for altering and displaying crystal data, use the **Window** menu, or click on the Graphics window if it is visible.

File menu - This is a standard File menu which pertains *only* to the special files with extension .SHP used in the Text windows.

Edit menu - This menu has the normal text editing commands, which again pertain *only* to the special files with extension .SHP used in the Text windows.

Window menu - Use this menu to switch to the SHAPE graphic window for most operations on SHAPE data sets, and to set the font for the Text windows.

Help menu - Access to general help for SHAPE.

3.3.1 File menu (Text windows)

File Menu (Text Window)

The commands in this menu apply *only* to Text windows, which are opened by the List Results or Section Data (see Sections and Growth Zones) commands in the **File** menu of the Graphics window. See Types of Windows for further explanation.

Close - Closes the Text window, and the file associated with it.

Save - Saves the file associated with the window.

Save As - Saves the contents of the window to a specified file name.

Print - Prints the contents of the Text window.

Print Setup - Selects a printer and printer connection.

Exit - Exits SHAPE.

3.3.1.1 Save As (Text Windows)

Save As command [File menu, Text windows]

When called from Text windows, this saves the (text) contents of the current window in the file of your choice.

The standard SHAPE files RESULTS.SHP and SECTOUT.SHP are in the same directory as the SHAPE program (.EXE) file; if you want to save these files, you should probably give them new names and put them in the same directory as the crystal data (.SHP) file, if the data file is not in the SHAPE program directory. See Types of Windows.

To save a text file with its existing name and directory, use the Save command.

3.3.1.2 Save (Text Windows)

Save command [File menu**, Text windows]**

When called from Text windows, this saves the (text) contents of the current window in the file whose name is in the title bar. The standard RESULTS.SHP and SECTOUT.SHP are in the same directory as the SHAPE program (.EXE) file. They are overwritten each time you request a list of the corresponding type. Thus if you want to save these files, you should probably use the **Save As** command instead of **Save** , give the files new names and put them in the same directory as the crystal data (.SHP) file, if the data file is not in the SHAPE program directory. See Types of Windows.

3.3.1.3 Close (Text Windows)

Close command [File menu**, Text windows]**

Use this command to close the currently active Text window. SHAPE inquires if you want to save changes to your data file before you close it. If you close a data set without saving, you lose all changes made since the last time you saved it.

The standard SHAPE files RESULTS.SHP and SECTOUT.SHP are in the same directory as the SHAPE program (CPSHAPE.EXE file). They are overwritten each time you request a list of the corresponding type. Thus if you want to save these files, you should probably use the **Save As** command, give the files new names and put them in the same directory as the crystal data (.SHP) file, if the data file is not in the SHAPE program directory. See Types of Windows.

3.3.1.4 Page Setup

Page Setup command [File menu**]**

This allows setting of the paper type or size, the standard orientation (portrait or landscape) and the paper margins (except Macintosh). Margins will only be used in Text Windows.

---Macintosh only ------

Use the Page Margins dialog to set margins.

3.3.1.5 Page Margins

-----Macintosh only----

This dialog sets the margins for Text Windows. Use the Page Setup dialog to choose page size and orientation.

3.3.2 Edit Menu

Edit menu (Text Windows)

The Edit menu for Text windows offers the usual commands.

Undo Reverse previous editing operation.

Cut Deletes data from the document and moves it to the clipboard.

Copy Copies data from the document to the clipboard.

Paste Pastes data from the clipboard into the document.

3.3.2.1 Undo

Undo/Can't Undo command [Edit menu]

Use this command to reverse the last editing action, if possible. The name of the command changes, depending on what the last action was. The Undo command changes to Can't Undo on the menu if you cannot reverse your last action.

3.3.2.2 Cut

Cut command [Edit menu]

Use this command to remove the currently selected data from the document and put it on the clipboard. This command is unavailable if there is no data currently selected.

Cutting data to the clipboard replaces the contents previously stored there.

3.3.2.3 Copy

Copy command [Edit menu]

Use this command to copy selected data onto the clipboard. This command is unavailable if there is no data currently selected.

Copying data to the clipboard replaces the contents previously stored there.

3.3.2.4 Paste

Paste command [Edit menu]

Use this command to insert a copy of the clipboard contents at the insertion point. This command is unavailable if the clipboard is empty.

3.4 Non-Menu Dialogs

The Face at Cursor dialog is called up when you click on a face in the Identification cursor mode.

The colors dialog is used for selecting colors in several places.

3.4.1 Face at Cursor

Dialog box: Face at Cursor

This dialog comes up when you click the mouse pointer on a face, if the Cursor Mode (Cursor menu) is set on **indexing** rather than **resizing** or **rotation**. It lists the face indices, the form indices and the crystal number, if there is more than one crystal. It also gives the interfacial angle (angle between face poles or normal) between the current faces and the one last identified.

You can change the **Central distance** for the form - to put this into effect, you must **Recalculate.**

You can also use this dialog to set up a color or pattern fill of a face or form, or to delete one. See Face/Form Fills in the **Input1** menu for more details on fills.

In Direct3D Drawing Mode, fullscreen, there is no atom identification - the only function of the mouse cursor is to rotate the structure, or to stop rotation or vibration by a click anywhere.

3.4.2 Select Color

Dialog Box: Select Color [various dialogs].

This dialog allows color selection from the current 16-color palette, and also allows selection of a custom color. The **Custom** button calls up a system standard color-picking dialog.

The red, green and blue values are given below each color box, to the right of the radio button. These values are on a scale of 0-255, as used by Windows.

It is usually best to use one of the 16 colors in the palette, because 1) the 256-color or 8-bit display palette is derived from these colors, and faces of shaded crystals will be forced to one of these colors anyway at plot time; and 2) display and output are usually more satisfactory when simple colors, such as those in the default palette, are used.

The default colors selectable in this dialog may be changed in the Palette dialog (Settings menu).

4 Reference

Reference - General Topics

4.1 Cartesian (QSHAPE) Operating Mode

The normal operating mode, called SHAPE mode, is restricted to the symmetry of the 32 crystallographic point groups. The QSHAPE mode avoids this restriction by using Cartesian reference axes and Cartesian symmetry matrices. The choice is made in the **Modes** menu.

Solids which show external morphology, X-ray and/or electron diffraction patterns of apparent symmetry not belonging to one of the 32 crystal classes have been termed *quasi-crystals*; hence the name Quasi-SHAPE or QSHAPE. Crystals cannot have symmetry axes of order five, or higher than six, so that quasi-crystals cannot truly have this symmetry (or else they cannot be true crystals). Nevertheless their external form often shows apparent icosahedral or other non-crystallographic symmetry. Polyhedra with non-crystallographic symmetry are also of interest from a purely geometric standpoint; the icosahedron and pentagonal dodecadron are among the five Platonic solids.

Since reference axes based on lattice translations are not applicable to quasi-crystals (this term will be used here for all solids with faces like crystals, but which have non-crystallographic symmetry), the QSHAPE mode always uses a Cartesian axis system. Whereas the SHAPE operating mode, in order to find all the symmetry equivalents of a face, uses a simplified system of transformation of the indices in integral form, the QSHAPE mode must multiply the indices by Cartesian symmetry matrices, one for each symmetry operation in the point group. The sets of symmetry matrices are in separate files, which must be generated beforehand with the auxiliary program SYMGRP, described in the next section. The symmetry files for the pentagonal and icosahedral groups have already been generated and are provided on the SHAPE disk(s).

In calculating the locations of corners, the SHAPE mode makes use of sectors defined by mirror planes (see I-3). Since the orientations of mirror planes cannot be fixed beforehand in the general case of non-crystallographic symmetry, this method cannot be used in the QSHAPE mode, and calculations may be much slower. Because of the

necessity of generating the symmetry files beforehand, and the usually slower execution for crystals with mirror planes, the QSHAPE mode is not recommended for use with true crystals, although it is perfectly capable of drawing any crystal.

Operation in the QSHAPE mode differs from that in the SHAPE mode in only a few respects: otherwise, everything in the instructions pertains to both modes.

1) In entering a crystal using the **Title/Axes** and **Symmetry** dialogs (**Input1** menu) you do not supply the axis lengths and angles and crystal class. Rather, the axes are always Cartesian and in the **Symmetry** dialog you must give the name of a file containing the symmetry matrices. Normally such a file will have been generated by the auxiliary program SYMGRP (next section), and will have the extension .SYM.

2) The indices for forms, faces and vectors are decimals, rather than integers (whole numbers). You do not need to enter a decimal point, and you can enter integral indices of any size, but once entered the indices will be normalized to a length of one ($h^2 + k^2 + l^2 = 1.0$). QSHAPE uses a threshold value of 0.0001 to test whether numbers are the same; thus five significant figures are usually sufficient.

3) Because of the necessity of storing all the symmetry matrices, the number of epitaxial crystals allowed in the QSHAPE mode is smaller than that in the SHAPE mode: see the README file for current limits.

4) If you are in normal mode and you read a data file written with QSHAPE mode, you will be switched automatically (with your approval) to the QSHAPE mode, and vice versa. However, files written by V4.1 or earlier SHAPE for DOS must be converted to the current format with the DOS program FILEUP.

4.2 Central distance

central distance. The central distance for a face or form (set of symmetry-equivalent faces) is the perpendicular distance in arbitrary unit of the user's choice (often referred to as central distance units) from the center of the crystal coordinates to the face in question. Generally, the larger the central distance the less prominent (smaller) the face is.

SHAPE uses finite tolerances in many parts of the calculations, for example to test whether corners formed by the intersection of three faces are coincident with existing corners, whether faces are parallel, etc. Usually these tests work best when the central distances are approximately 1.0 or smaller. However, if the results are obviously incorrect, changing all the central distances by a factor of 10 up or down with the Factor button in the Forms List Dialog may improve things.

4.3 Colors and Palettes

This section applies to true colors - see Dot Patterns for the nature of "colors" or shades in black-and-white display and output.

In principle, Macintosh and Windows allow full freedom to specify colors for lines and fills in color display or output. In practice, it is advisable to select colors carefully to take best advantage of a wide range of display and output devices. For 8-bit or 256 color screen displays, it is also necessary to supply a palette of the desired colors to the system to avoid unnecessary color mixing or dithering.

SHAPE uses a primary palette of 16 colors to assist in color selection, and from which a 256-color palette is derived.

Display or screen devices in the past were most easily or directly able to produce colors which have the simplest combinations of components red, green and blue. The binary combinations of red, green and blue are cyan(green+blue), magenta or violet (red+blue) and yellow (red+green). On the other hand, the primary colors for printing are cyan, magenta and yellow. Screen devices such as VGA and super-VGA can now produce any color, but it is still best to select the six colors red, green, blue, cyan, magenta and yellow, plus black and white, as first choices for colors of lines and fills in SHAPE. These are the first 8 colors in the SHAPE palette. Actually, black is not a good color for fills, since it cannot be shaded. The next-best group of full-intensity colors consists of the six colors which are binary combinations of the six mentioned above. These 6, plus two shades of gray, are the second 8 colors in the SHAPE palette.

At this time, 8-bit color, allowing a total of 256 separate colors, is still sometimes used for screen display and is often convenient for raster files. SHAPE generates a color palette for 8-bit display and output as follows. If the number of shading zones selected in the Shading dialog in the **Input2** menu is 16 or less, 15 colors are derived from each of the colors in the primary 16-color palette, except for black, ranging from the pure or full-intensity color to near black. There are thus 15 gradations of red, for example, with rgb values of (255,0,0), (238,0,0), down to (17,0,0). Including black (0,0,0), this allows a different shade for each of the 16 zones.

If the number of shading zones selected in the Shading dialog in the **Input2** menu is 32, only the first eight colors in the palette, excluding black, are used to derive the shaded colors, and there are 31 gradations of each. (Note that this is different from the DOS versions of SHAPE, in which the *second* 8 colors were used for the 32-zone palette; however, the colors used, namely red, green, blue, cyan, magenta, yellow and white are the same, and there should be no problem with SHAPE-DOS files).

To summarize, colors used in SHAPE should be as simple as possible for best success on a wide range of display and output devices. Choose colors first from the first eight colors

in the standard SHAPE palette, then from the second eight.

You do have the freedom to define any color as desired, specifying the RGB components. You can also redefine or rearrange the SHAPE 16-color palette with the Palette dialog in the **Settings** menu, and this will give correct results for 8-bit (256-color) screen display. However, it is probable that more complex colors will not be rendered very satisfactorily on color hard-copy devices (depending, of course, on the sophistication of the device).

4.4 Colors/Patterns/Pens for Input

In color display or output, lines may be drawn with different colors, and faces or forms may be filled or shaded with different colors (except in pen plots). In black-and-white display or output, various dot-patterns, simulating shades of gray, are normally used for fills, and for lines if they are wide enough.

This section discusses the common aspects of color/shade input for lines and fills, as occurs in many input dialogs in SHAPE. Depending on the type of display and output involved, any of three different sets of colors or patterns/shades may be used.

(a) For color screen displays, printer, raster or Metafile output, actual colors are used. The RGB components, which are numbers ranging from zero to 255 can be directly entered in the edit boxes, but the color is most easily and reliably selected with the **Select...Color** buttons. These bring up the Choose

Color dialog, presenting the colors of the current 16-color palette. If the color is being selected for shading (Shading dialog in the **Input1** menu), the color chosen here is that at maximum (perpendicular) illumination.

For 16-, 24-, and 32-bit color screen displays you have complete freedom to choose colors. For 8- or 4-bitcolor the colors for fills and shading may be forced at plot time to one of a limited number of allowed colors. For 8-bit color the number of colors allowed depends on the number of shading zones selected in the Shading dialog in the **Input2** menu. See the general section Colors and Palettes for further information on palettes for the 8-bit color mode.

For best results on a wide range of display and output devices, chose the simplest colors, which are firstly colors 0-7 in the default 16-color palette, and secondly colors 8-15

(b) For black-and-white screen displays and dot-matrix output, either true grays or dot patterns of various densities are used. The codes for these shades or patterns range from 0 for white to 15 for solid black. See Dot Patterns for details on the nature of these patterns.

The selected pattern is used for lines only if the width of the line is greater than one dot.

The width of various types of lines is set in the Line Attributes dialog in the **Input2** menu. Note that rendering of gray-scale for lines in black-and-white printed output is determined by the printer driver, not SHAPE. Many printer drivers do not support gray lines, and pattern numbers other than 15 may give either white or black lines.

(c) For pen-plotters the number requested refers to the pen number used in drawing the lines. There are no fills or shading in pen plots. These numbers are not used if the single-pen mode is selected in the Pen Plotter Settings dialog in the **Settings** menu.

When changing the red, green and blue values directly in the edit boxes which appear in many dialogs in SHAPE, the rectangle showing the actual color does not change until the focus shifts from the current edit field, that is until the mouse is clicked in another place in the dialog.

4.5 Coordinate Systems

Three types of coordinate system are used frequently in SHAPE: the observer Cartesian system; the natural crystal system; and a clinographic system.

The *observer system* is fixed with respect to the display screen or paper of dot-matrix or pen-plotter copy. The origin is at the center of the screen or paper, and the x axis points directly toward the observer. The y axis points to the observer's right and the z axis vertically, both in the plane of the screen or paper.

The parameters of crystal faces are given in terms of the natural crystal axis system, although in the QSHAPE or Cartesian mode this is itself a Cartesian system. Once all the faces have been generated by symmetry, their coefficients are converted to Cartesian coefficients. Except for crystals using rhombohedral axes, the natural c axis is originally placed parallel to the observer z axis, and the natural b axis is aligned in the y-z plane (or in crystallographic terminology the a^* axis is parallel to x). If rhombohedral crystal axes are chosen, the three-fold symmetry axis is parallel to z , and the the vertical plane containing the first rhombohedral axis is aligned in the x-z plane.

This conversion defines the "original" orientation of the crystal. After the location of corners etc., and before the initial display, the orientation may optionally be modified by the rotations in the Initial Orientation dialog in the **Input2** menu, and by clinographic rotation, defined in the next paragraph.
Clinographic Viewing . One of the standard methods of drawing crystals is clinographic projection, in which the crystal is in effect viewed from above and slightly to the right of the a axis, or to be more precise, in towards the center along the vector [621]. If the option for clinographic viewing is chosen, after the faces, corners etc. are found, the crystal and its associated Cartesian system are rotated -18.4 degrees on the z axis, then 9.5 degrees on the y axis. This is not true clinographic projection, but the results are almost the same.

After the drawing appears, additional rotations may be made either on (1) specified vectors in the natural crystal system; (2) the observer Cartesian axes; or (3) if clinographic viewing is on, the rotated Cartesian axes, or *clinographic system.* The clinographic system does not rotate with the crystal; it is always related to the observer system by the two rotations given above.

If clinographic viewing is not on, the clinographic and observer systems have the same orientation, and if the natural crystal system is Cartesian or cubic all three systems have the same orientation.
Stereonet Viewing. When this display mode is selected **(Modes** menu) the crystal is viewed directly down the c axis, if in standard or original orientation. The a* axis is downward. Rotations made in standard mode are carried into this mode, but the clinographic rotations are not used.

Summary of axial systems:

1) *Observer Cartesian system* . Reference system, fixed with respect to the display screen or paper.

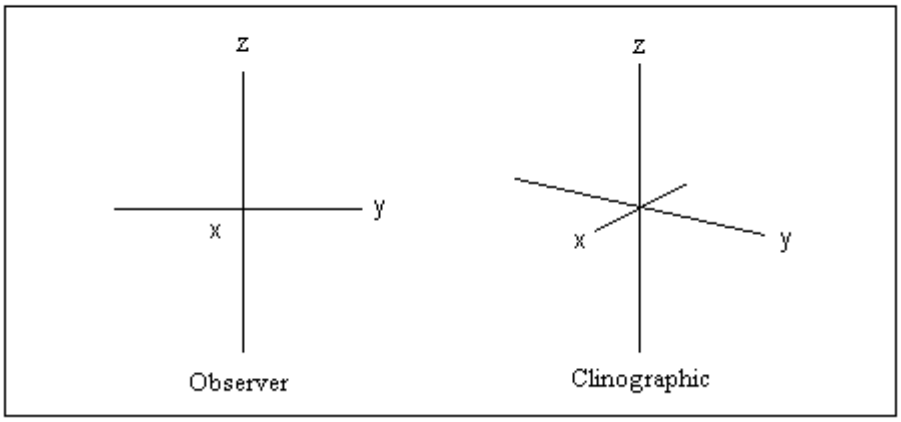
2) *Natural or crystal system* . The axes are the unit-cell edges. Axes may have unequal lengths and may be at angles of other than 90 degrees.

3) *Clinographic system.* Only applies when clinographic projection or viewing is on. Axes are those of the observer Cartesian system, but rotated in a certain manner to avoid a straight-on view of the crystal.

If Perspective viewing is not selected, the drawing is a direct projection in the *x* axis direction (observer system). If perspective viewing is selected, the corners are projected onto the *y*-*z* plane from a point on the *x*- axis at the specified distance in the positive direction (toward the observer).

In SHAPE, *a, b* and *c* (or A, B and C) refer to the natural crystal axes. The three axes will always have these names or *a*1, *a*2 and *a*3 if the axes are equal by symmetry. The letters *x, y* and *z* usually refer to the observer Cartesian axes. If it is necessary to refer to the clinographic system, this is mentioned explicitly.

Coordinate Systems for Rotations



4.6 Direct Modification of Files

Data Files. The .shp files written for each structure are of the standard ASCII type. Direct modification of these files is no longer recommended. However, occasion may arise for repairing a damaged file, which can be done with any word- or text-processor or other program which handles ASCII files.

SCRPTR Setup File. There is now only one type of data in the SCRPTR file which should be modified; the dot-patterns. The SCRPTR file will be replaced after the first startup by a user- and platform-specific file.

There are two sets of 32 dot-patterns (fine and coarse), each consisting of 32 lines of 8 numbers each. Each number can range from 0 to 255, with a binary 1 bit representing a black dot and 0 representing white (or color in the case of 4-bit raster files). Note that earlier versions of SHAPE may have had either 14 (V1.0) or 16 patterns in each series. The fine series, which is first, contains duplicate lines so that there are only 16 patterns for shading, even if the number of shading zones is greater than 16. These patterns could be modified to give 32 distinct shades, although it is doubtful if this would greatly improve the quality of the image.

Patterns can also be modified to give striations, hachures or other patterns for use in face fills. For example, the sequence "1 1 1 1 1 1 1 1" will give vertical striations, and the sequence "255 0 0 0 0 0 0 0" will give horizontal striations. Such patterns should not be used when shading is in effect.

The patterns in the SCRPTR file or user- and platform-specific file are only used for raster-file output, and for standard printer output when SHAPE patterns are selected; they are not used for the screen.

Although the data for the 16-color palette are also in the SCRPTR file or user- and platform-specific file, it is easiest to modify the palette with the **Palette** dialog in the **Settings** menu, or to prepare files to be read in with these dialogs.

4.7 Directories and Files

SHAPE looks for files in two folders or directories: (1) the *home* directory, which is the one containing the SHAPE program or application, CPSHAPE.EXE; and (2) the *data* directory, containing data files.

The home directory should contain, in addition to the SHAPE application itself, the setup files (SCRPTR and DEFAULTS), the pen-plotter information file (PPLOT) the help file (CPSHAPE.HLP), the space-group symmetry file (HALL.DAT) and palette (.pal) files. The SCRPTR and DEFAULTS files will be replaced after the first startup by a user- and platform-specific file.

The data directory should contain the crystal data files (.shp) and cartesian symmmetry files (.sym), and will contain any output files (raster, metafiles, EPS and pen-plotter files). Output files can be quite large.

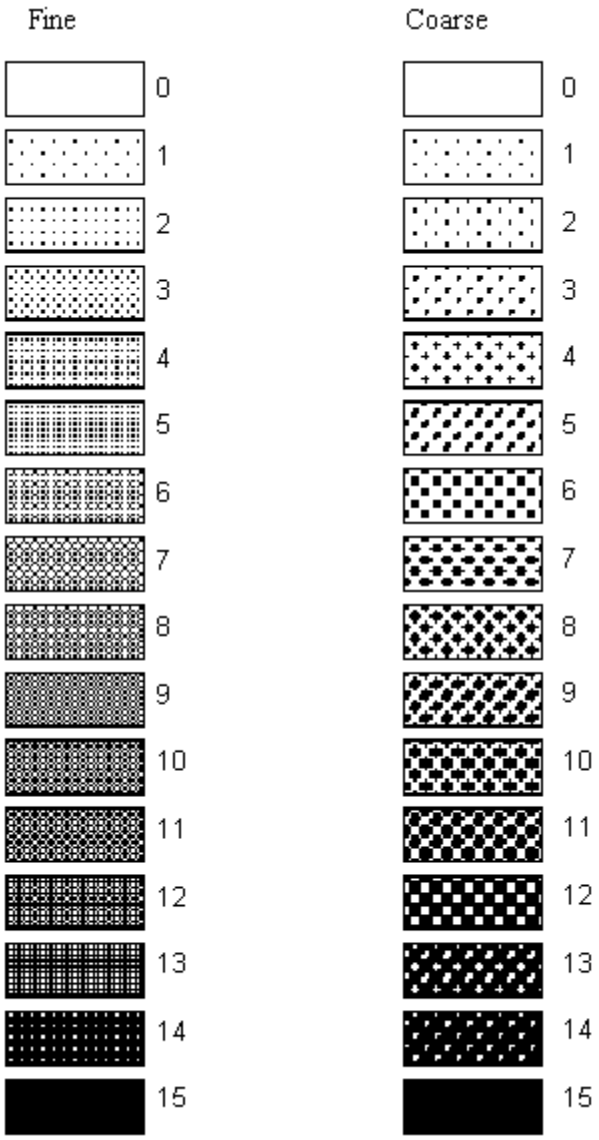
The files RESULTS.SHD, containing the output from the **List Results** command in the **File** menu, and SECTOUT.SHD, containing data on sections and growth zones (**Sections and Growth Zones** dialog in the **Input1** menu), are written to the home directory.

The data directory is initially the same as the home directory - it is reset whenever a data file (.shp) is read in with the **Open** option or a file is written with **Save as**.

4.8 Dot Patterns

The dot-patterns which are the "colors" for face fills, for shading, and for wide lines in black-and-white printer and raster output (if SHAPE patterns are selected in preference to those supplied by the printer driver), are shown below. The patterns comprise two series of dot-patterns of increasing density with shade numbers 0-15; the choice between them is made in the **Print** or **Raster File** dialogs (**File** menu).

The fine series is recommended for 9-pin or other low resolution dot-matrix plotting, for very small drawings done at high resolution, or for raster files which will be shown on a low-resolution screen. The coarse series contains patterns more like the half-tone screening used in printing. It is appropriate for gray tones and shading in high-resolution dot-matrix plotting. Actually, for shading with 32 zones, there are 32 patterns in the coarse series, only half of which are shown in Figure IV-1. The fine series has only 16 unique patterns even if the number of shading zones is 32, although this could be changed in the SCRPTR file (see Direct Modification of Files).



4.9 File Types

SHAPE uses several different types of auxiliary files, with different extensions. When reading files, the extensions are not mandatory, and you can usually choose a different extension when saving a file, or specify "all files" when browsing or searching for a file.

Crystal data files (.shp). These hold the information on individual crystals and intergrowths. The **Open, Save** and **Save As** commands in the **File** menu of the Graphics window pertain to these files.

Internal files. These are for SHAPE internal use and should not normally be modified by

the user (but see section IV-8 of instructions for special cases) . SCRPTR is the main start-up file which saves current settings. DEFAULTS saves default display variables for use with the New command. PPLOT contains data on pen plotters. CPSHAPE.HLP is the help file, which is in condensed format and not modifiable by the user. SCRPTR and DEFAULTS are replaced after the first startup with a user- and platform-specific file.

Cartesian symmetry files (.sym). These contain Cartesian point-symmetry matrices generated by the auxiliary program SYMGRP. They are for input only.

Palette files (.pal). These contain RGB values for the 16-color palette which forms the basis for 8-bit (256-color) palettes, and which is used to simplify color selection. They can be modified, read and written with the Palette commands in the **Settings** menu.

Text output files (.shd). These are (1) RESULTS.SHD, containing the output from the List Results command in the **File** menu, which gives most of the input data and results for normal views of crystals and intergrowths; and (2) SECTOUT.SHD, containing corner coordinates and other information on sectors and growth zones if this type of output is selected in the Sections and Growth Zones dialog (**Input1** menu).

Graphics output files. SHAPE can write graphics output files of various types: raster files (.bmp, .pcx, .tif); encapsulated PostScript files (.eps); HPGL vector files (.pgl) and Windows metafiles (.wmf).

Import files . SHAPE can obtain crystallographic information from a number of database and structure-refinement file types - see Import Files for further information.

File Locations

SHAPE expects to find certain files in the "home" directory, which is the directory containing the SHAPE program file (wxShape.exe). These files are SCRPTR, DEFAULTS, PPLOT, HALL.DAT and palette (.pal) files.

The "data" directory is the directory containing the crystal data (.SHP) file. The data directory is reset whenever you read or write a crystal data file. If you are using Cartesian symmetry files (.sym), they should be in the data directory. Most output files, including EPS, raster, HPGL and metafiles, will be written to the data directory. However, the data output files (.shd) are written to the home directory, to avoid cluttering the disks. To save these files permanently, use **Save As** to give them new names in the directory of your choice.

4.10 Frames

With most types of hard-copy output, you have a choice of using the full page, or confining the output to a *frame* . For Raster Files and Metafiles (both in the **Output**

menu) output always goes to a frame.

If you are using the **Universal** or **Maximize Each View** scale modes (Scaling dialog in the **Input2** menu), the image is scaled to fit in the frame. Note that starting with V6.0, there is a rescale factor which is applied to this scaling. If you are using the **Fixed** scale mode, the image is clipped to the frame.

In hard-copy output, the frame can be positioned on the page; the offset gives the displacement of the upper left corner of the frame from the upper left corner of the page.

In some cases, you can choose the units for the size and offset of the window; either inches, centimeters or dots (pixels), and you may also be able to specify the nominal dots per inch or centimeter. The units setting is independent of the overall choice of inches or centimeters in the Preferences dialog in the **Settings** menu.

4.11 Free-Form Input Files

Files of this type are read and written by ATOMS and CRYSCON (Shape Software). Such files have atomic-coordinate information, but this is ignored by SHAPE.

All information needed for a SHAPE calculation can be entered with these files, and they should be easy to write with other software. The **SPGP** , **HALL** , **SYMM** AND **LATT** lines are used only in the **Donnay-Harker Morphology** option.

The required information is entered in lines which begin with one of the 4-letter keywords shown in boldface type below. Information follows the keywords in numeric or character fields - fields do not contain spaces (may contain underscores), and are separated from each other by spaces.

TITL line. Up to 76 characters (may contain spaces).

CELL line. The unit-cell lengths in Angstroms and the interaxial angles in degrees (6 floating-point values).

SPGP line. The Hermann-Maughin or standard International symbol for the space group. There should be no spaces in the symbol, although there may be underscores (which are ignored when the symbol is interpreted).

HALL line. The Hall symbol for the space group. There should be no spaces in the symbol, although there may be underscores (which are ignored when the symbol is interpreted. If this line comes after the SPGP line (or that line is absent), the Hall symbol will be used.

SYMM lines. These give symmetry operators in "xyz" form, that is in the form in which

the coordinates of the general position are listed in the *International Tables for X-Ray Crystallography* . Fractions must be given as integers separated by a slash ("1/2", "2/3"), rather than decimals ("0.5", "0.333"). The x, y and z positions must be separated by commas and there should be no spaces in the operator. There should be one line for each operator. If the space group is centrosymmetric, only half the operators need be given, if the origin is on a center of inversion. If the origin is not on a center, all operators must be given and the space group should be denoted non-centric in the LATT line.

LATT line. This gives the Bravais lattice type (single capital character), followed by a space and 0 if the space group is centrosymmetric or 1 if it is non-centric.

Generally, the **SYMM/LATT** combination supercedes **SPGP** or **HALL** lines - if **SYMM** lines are present, SHAPE will attempt to determine the space group from them, and if successful will replace any H-M or Hall symbols which have been read in.

FORM lines. These lines contain the three indices and the central distance for each form. The indices may be floating point for entry in the Cartesian (QSHAPE) operating mode - be sure to set this mode before reading the file.

4.12 Lighting Equation (3D)

In the 3D display mode the material properties of objects determine the way the objects interact with the light sources.

The color observed at a given point is a resultant of the light source(s) and the Material Properties; that is, the RGB coefficients of the **Ambient** , **Diffuse** and **Specular** components of the light source(s) are multiplied by the specified colors of the objects, and by the material coefficients in this dialog, then the results are limited to the range 0.0-1.0.

```
Itotal  =  Ke C                          ;emissive
        +  Ia Ka C                       ;ambient
        + Sum(i) [  ( NdotVi ) Ii Kd C ]   ;diffuse
        + Sum(i) [ ( NdotSi )^ns Ii Ks ]   ;specular
```

Where Itotal is the total intensity as an RGB triplet at any point on an object;

Ia is the intensity (RGB triplet) of the ambient light source (1.0 for the simple light model used in SHAPE);

Ii is the incident intensity (RGB triplet) at the object of directional or positional light source i (1.0 for the simple light model used in SHAPE);

C is the assigned color (RGB triplet) of the object (crystal edge, crystal face, symmetry

axis or mirror plane color);

Ke is the emissive material coefficient of the object (Material Parameters dialog);

Ka is the ambient material coefficient of the object (Material Parameters dialog);

Ks is the specular material coefficient of the object (Material Parameters dialog);

ns is the specular exponent or shininess coefficient of the object (Material Parameters dialog);

N (a vector) is the normal to the surface at the point in question;

Vi (a vector) is the direction of the incident directional or positional light i at the point;

S (a vector) is the bisector of the angle between the light-surface vector (or Vi) and the eye-surface vector;

"dot" signifies the vector dot product.

Ambient light has no direction or origin and is considered to bathe all objects uniformly. Having a significant ambient component causes non-illuminated parts of objects to be other than black. It thus "softens" the illumination in a somewhat similar way to the **Darkest Shade** and **Darkness Angle** parameters (Shading dialog) in the **Standard** display mode.

Diffuse color is usually the main component of the appearance of objects. The intensity of the color is dependent on the angle between the light ray and the normal to the surface in question.

Specular reflection only occurs when the normal to the surface in question is close to bisecting the angle between the incident light and the vector from the point on the surface to the eye. It produces bright highlights on a curved surface. The larger the **Specular** material coefficient, the smaller will be the bright specular highlight on a curved surface. The shininess coefficient has a maximum of 128 because of computational restrictions, but values on the order of 5-30 are usually realistic. In SHAPE, specular reflection is always white, that is it does not depend on the color of the object, only the color of the light source(s). For directional lights, specular reflection may not work well for polyhedra because faces at certain angles will give a solid white appearance.

Emission is similar to ambient, except that there is no dependence on the color of any light source. A high value of emission makes an object look like is is glowing.

This equation ignores translucency, which causes colors objects lying at different depths to be blended.

4.13 Precision, Tolerances and Errors in Corner, Edge and Face Identification.

Many calculations in SHAPE depend on finite absolute tolerances to decide whether corners are outside of any face, whether a corner derived from one triplet of faces is coincident with another, etc. Sometimes there are errors, for example extra corners, missing edges, or missing faces (in the Shading or Face Fill options, or in 3D mode). Errors may occur either in the calculation of corners and edges, or during actual plotting
Situations which can cause problems:

1) **Multiple edge/face intersections** . When more than three edges (or more than three faces) intersect or nearly intersect at a point, the identification of the number of corners involved may be arbitrary. In some cases more than three faces intersect at a point and form a single true corner by symmetry - for example 3, 4, 6 or more faces in a pyramid in trigonal, tetragonal or hexagonal crystals. Tolerances must be large enough to identify these intersections correctly. In other cases the intersection of edges is fortuitous.

2) **Low-angle face intersections** . When faces are nearly parallel, the precision of locating intersections decreases.

3) **Junctions of twin or epitaxial intergrowths** . Special situations may arise in multiple crystals which do not occur for single crystals. There may be problems either during the calculation of corners and edges or during drawing.

Possible remedies:

1) The **Remove Hidden Lines** option in the Display menu controls the plotting of edges on one crystal which are hidden by another crystal.

2) **Rotation** . Missing lines of type 3) above can sometimes be restored by rotating a small amount, on the order of a degree or less.

3) **Change of individual central distances** . Problems of type 1) may often be cleared up by slightly changing the central distance of one of the forms involved, rather than all forms.

4) **Change of all central distances** . Since most of the tolerances are absolute (not relative), increasing all central distances by a common factor has the effect of reducing all tolerances by the inverse of this factor. There is an option for this in the Forms List dialog.

5) **Change of criteria for showing edges in twins and epitaxial intergrowths.** Certain types of edge may or may not be desirable to draw in intergrowths. The **Edges in faces** and **Always show composition-plane edges** options in the Preferences dialog control some such cases. Trial-and-error change of these parameters may give a more correct or more pleasing appearance.

6) **Change of perspective distance** . Increasing the Perspective distance sometimes clears up problems.

Note on units . Most distances used in SHAPE are in arbitrary units called central distance units (abbreviated cdu). These may be considered to correspond to any desired units on a real crystal, such as millimeters, centimeters, inches, etc. When fixed scale factors are used (Scaling dialog), it is necessary to specify the ratio of these units to the units (inches, centimeters or pixels) which are used to describe the screen or paper. Growth rate equations must be given in the appropriate units per time unit (also an arbitrary unit). Otherwise the absolute values of central distances have no effect - it is the relative values which determine crystal shape.

4.14 Palettes

Although Windows programs can specify colors made up of any admixture of red, green and blue components, it is generally a good idea to use simple colors whenever possible, to increase the chances of faithful reproduction on a variety of display and output devices.

16-Color Palette. SHAPE uses a primary palette composed of 16 colors for two reasons: to aid in the consistent selection of simple colors; and to form a basis for the 256-color palette used for 8-bit displays or other devices. The first eight colors in the default 16-color palette are black, white, red, green and blue, and then the binary combinations of red, green and blue which are cyan, magenta (violet) and yellow. The second eight colors are two shades of gray, then the binary combinations of red, green, blue, cyan, magenta and yellow (these six have no universally-recognized names). The colors in this palette are the same as those in the Alternate palette which is used in the DOS versions of SHAPE, but in a different order.

The RGB values in the 16-color palette can be changed with the **Palette** dialog in the **Settings** menu. You can also save and re-read palette (.pal) files.

256-Color Palettes. The palettes which are used in 256-color screen-display modes are primarily designed for shading. There are two distinct palettes; the first has 15 principal colors, each with 16 gradations from full intensity to almost black, and is used when the number of shading zones (**Shading** dialog in the **Input1** menu) is 16 or fewer; the second has only 7 principal colors, each with 32 gradations from full intensity to almost black, and is used when the number of shading zones is 32.

The first or "16-zone" palette is made up as follows. The first 15 colors (0-14) start with full-intensity color number 1 (white), and grade with decreasing intensity to near black; the second 15 colors (15-29) start with full intensity color number 2, grading to near black, and so on. When shading is in effect, SHAPE finds the nearest color in the 16-color palette to the crystal color selected in the **Shading** dialog (**Input1** menu). Any face receiving full illumination is given this full-intensity color and faces at angles to the illumination vector are given colors in the series of 15 colors derived from that principal color. The palette defined in this way actually contains only 225 colors. Windows reserves 20 colors for its own use, including black which therefore does not have to be defined in the SHAPE palette.

In the second or "32-zone" palette, the first 31 colors (0-30) grade from full-intensity color 1 to near black, the next 31 from full-intensity color 2 to near black and so on, through color number 7 and its derivatives. When shading is in effect, SHAPE again "forces" the color to one of those in the 16-color palette, but the choices this time are only colors 0-7. As the colors are arranged in the default palette, this results in changing colors 8-15 to 0-7 respectively. Actually, colors 0-7 can be regarded as "simplified" or more basic versions of colors 8-15. The above shaded colors add up to only 217, so colors 8-15 are also added to the palette to be usable for lines and unshaded fills.

Again, if shading is in effect and you are using more than 16 shading zones (**Shading** dialog in the **Input2** menu), any fill colors or shading colors in the range 8-15 will be automatically "downgraded" to colors 0-7.

All these complexities and restrictions pertain *only* to 8-bit or 256-color display or raster files. For standard VGA (4-bit) display, the RGB values are sent to the display driver, which determines in its own way what combination of pixels to mix to represent a given color. This is likewise true for printer and PostScript output. The RGB values are also sent directly to 24-bit screen displays, which can presumably render any color without dithering.

4.15 Settings, Preferences or Configuration Files

SHAPE has in the past saved various settings in two files, SCRPTR and DEFAULTS, both of which are in the same folder or directory as the wxSHAPE program or executable file. SCRPTR saves general settings which may be used for all data, such as frame sizes for printing and graphics file output and is always saved before exiting the program. DEFAULTS saves settings which are more particular for each data set - these may be used as the initial or default values for a new data set. The DEFAULTS file could be read or written through options in the Settings Menu, and at other times when starting a new data set or importing a file.

Starting with V6.3, this information is saved in a standard type of file which is specific to the platform (Windows, Mac or Linux), and this file is in a location specific to each user.

Thus each user will have his or her settings preserved, even if only one copy of the SHAPE folder/directory and executable file is present. Further, these settings will be carried on as new versions of SHAPE are installed.

Specifically the new settings files will be in the following locations:

Windows: \Documents and Settings*username*\SHAPE.ini

Macintosh: :Users:*username*:Library:Preferences:SHAPE Preferences

Linux: /home/*username*/.SHAPE (note the period - this is a hidden file)

where *username* is the name of the current user logged in.

The .ini, Preferences or config file has separate sections containing the SCRPTR information and the DEFAULTS information.

The SCRPTR and DEFAULTS files still exist. On startup, SHAPE looks first for the user-specific file, and if this is not present it reads the values from the SCRPTR and DEFAULTS files in the folder or directory containing the SHAPE executable file. Thereafter the user-specific file is written and used.

The Windows and Linux versions have separate Help server programs, and these write their own user-specific preferences files. These files will be in the above locations, and the program name is "wxHTMLHelpController" instead of "SHAPE". In the Macintosh version, there is no separate Help server program and the data for the Help windows (window sizes and location and fonts) is in the SHAPE Preferences file.

In the Settings menu, there are now options to read and write the "archive" SCRPTR and DEFAULTS files - this writes the values currently used by SHAPE. If there are multiple users of SHAPE, these files should probably be written only the the system administrator. All users may read the files to get the "standard" or archive values.

4.16 Shortcut Keys

Since several viewing or drawing modes have been added for V6.4, and since stereo images may require full-screen viewing in which menus are not available, the keyboard shortcuts for modifying or animating the images have been revised and extended.

In the full-screen modes accessed with the Fullscreen button in the Dialog Bar - Left or the menu option, the left mouse button always performs the identification function, identifying either atoms or crystal faces, and the right button performs the rotation

function. Clicking outside the crystal faces or structure (not on an atom) brings up a dialog giving most of the options, which can be selected with buttons. If the structure is in motion, clicking with either mouse button will stop it. Exit from Fullscreen mode either with this dialog, or with the Esc(ape) key.

The displacement function with the right mouse button which was available in earlier fullscreen viewing has been discontinued.

In the Direct3D fullscreen mode, the mouse buttons only cause rotation (click and drag), not crystal-face identification and no dialog is called up by clicking. When the crystal is in automatic rotation clicking anywhere will stop the motion. The same keyboard shortcuts are available, and exit from fullscreen is with the Esc(ape) key.

The shortcut key combinations:

SHIFT-X Rotate on the x axis (horizontal in screen). Stop rotation on x, y or z with a mouse click or SHIFT-Q, and change the speed with the SHIFT-F (faster) and SHIFT-G (slower) keys.

SHIFT-Y Rotate on the y axis (up in screen)

SHIFT-Z Rotate on the z axis (out of screen)

SHIFT-O This restores the original or standard orientation.

SHIFT-I This restores the initial orientation

SHIFT-P This decreases the perspective distance, increasing the 3-D effect.

SHIFT-[This increases the perspective distance (the [key is the one to the right of the P key on U.S. keyboards, but it may be elsewhere on other keyboards).

SHIFT-plus This will change the rescale factor upwards.This factor can be set in the Scaling dialog (Input2 menu SHAPE). The plus and minus keys are those in the regular alphanumeric part of the keyboard, not the number pad.

SHIFT-minus This will change the rescale factor downwards.

SHIFT-A Increase the stereo rotation angle between the two images, or increase the effective interocular distance. In the the Direct3D stereo mode the amount of rotation may be limited because the stereo relations are handled differently, in terms of interocular distance instead of rotation angle.

SHIFT-S Decrease the stereo rotation angle between the two images.

SHIFT-F Speed up motion. The SHIFT-F and SHIFT-G keys only apply when there is continuous rotation. They permanently affect the angular rotation increment in the Continuous Rotation dialog (Rotation menu).

SHIFT-G Slow down motion.

4.17 Stereoscopic Display

Improved technology has made stereoscopic viewing, that is viewing stills and movies with separate left- and right-eye images to give apparent depth, better quality and and more common on computers and televisions. As far as SHAPE is concerned, there are two separate kinds of stereo-enabled video cards of the most recent types. At present, software stereoscopic drivers for these cards appear to be available only for Windows.

Direct3D stereo in Windows (only) is supported by the nVidia GeForce series of graphics cards,with their 3D Vision package, and perhaps some others. The GeForce series only supports Direct3D in stereo (not any kind of OpenGL).

The 3D Quad Stereo Drawing Mode is available only for graphics cards supporting OpenGL quad-buffered stereo. It is potentially supported for Macintosh and Linux as well as Windows, though driver software does not seem to be available yet for them. The Quadro series of cards from nVidia actually supports either Direct3D or quad-buffered OpenGL stereo.

With either type of video card there are basically two types of viewing hardware.

1) **Shutter glasses**. The images are drawn independently and flashed alternately on the screen at a high rate - 120 times per second in the latest computer implementations, for example those supported by both the nVidia Quadro and GeForce series of display cards. A 120 Hz monitor or projector is required, and it must be viewed with special shutter glasses which blank out the left and right eyes alternately in synch with the images on the screen. Projectors and projection TVs are also available.

2) **Polarizing monitors or projectors.** The monitor or projector simultaneously or alternately (very rapidly) generates two images which are view with glasses with the two lenses polarized at 90 degrees to each other, or with different circular polarizations. Movie theater 3D (stereo) systems use a more elaborate variant of this method. It does not require expensive shutter glasses, only relatively inexpensive polarizing glasses for each viewer.

These types of hardware stereo viewing are full-color and should not be confused with the old two-color (red-green) anaglyph technology which really only shows monochrome or bi-chrome images. SHAPE has always supported stereo viewing using two spatially separated images combined with the naked eye or an optical viewer - this type of technology goes back to the 19th century.

The terminology for stereo viewing can be somewhat confusing. In movie theaters and television, the term 3D means stereoscopic viewing, that is separate images for left and right eyes. In computer and video-game graphics, the term 3D has been applied to several kinds of software techniques, at present primarily OpenGL and Direct3D, which keep track, pixel-by-pixel, of the third dimension in drawings and thus typically produce more realistic images than 2D line and space-fill drawings, though they are not necessarily stereoscopic (no separate images for left and right eyes). This is the way the term 3D is used in all SHAPE literature. OpenGL and Direct3D may be used in SHAPE for single non-stereo images as well as stereo (2D images may also be shown as stereopairs with SHAPE, although this is usually inferior to using a 3D method).

SHAPE in the past has used only OpenGL, which is available for Windows, Macintosh and Linux . A special, full-screen Direct3D mode has been added to SHAPE for Windows to support stereo viewing with GeForce cards and any others which require Direct3D. This is selected only in the Display menu, or with a button in the Dialog Bar - Left, not in the Drawing Mode drop-down. SHAPE also supports stereo viewing using the quad-buffered OpenGL method, which is currently available on the Quadro series of video cards from nVidia and some other video cards.

Older Shutter-Glasses Systems

Older stereo display drivers from nVidia, which worked only on Cathode-Ray-Tube monitors, not flat-screen LCD monitors, supported Direct3D and OpenGL without quad-buffering. This system works with inexpensive shutter glasses, but if the refresh rate of the monitor is less than 100 Hz or so the flicker tends to be excessive. Such systems are basically outmoded and may not be supported by manufacturers.

Changes in operation of SHAPE

In order to keep the total number of options to a minimum, what were formerly Display Modes have now been separated into Model Modes and Drawing Modes. The Model Mode specifies the type of model which represents the crystal, and includes Standard, Ellipsoid, Cavities and Protein. The Drawing Mode specifies which computer technique and viewing mode is used, and includes 2D single, 2D stereopair, 3D single, 3D stereopair and 3D quad stereo. The 2D modes use essentially line and fill drawing, which is suitable for schematic drawings for publication, for example, though shading is available in SHAPE. The 3D modes use generally more realistic lighting and superior interpenetration relations, and usually look better on screen or in full-color high-

resolution printed images. The OpenGL 3D system software is available on Windows, Macintosh and Linux.

An additional 3D mode, Direct3D, which is available only on Windows, is selected with a separate button or menu option. This is the Drawing Mode which is required for stereo viewing with nVidia GeForce display cards or any others which support Direct3D only. It is full-screen only (not windowed)

Selection of Stereo Viewing Methods

Simple stereo methods. These allow stereo viewing using no aids or inexpensive glasses or optical viewers. The stereopair modes allow stereo viewing with or without optical aids, but these modes have limitations; the stereopair modes halve the size of the image and the other image is always visible, giving three images (unless some special type of viewer is used).

Hardware stereo methods. In these methods a single image drawn by SHAPE is split into left- and right-eye images by the display hardware, or actually its resident software. Then the two images are displayed on screen, either alternating rapidly in synchrony with shutter glass, or as two differently polarized images. Any of several SHAPE Drawing Modes may need to be used, depending on your video card and monitor.

1) *nVidia GeForce cards* which support their 3D Vision system, and any other display cards which support only Microsoft Direct3D. Click on the Direct3D button in the Dialog Bar - Left or the Direct3D option in the Display menu. These cards will also display in anaglyph (red-green glasses) mode without shutter glasses or a special monitor. In this stereo mode, or any other except quad-buffered OpenGL, the program sends only a single drawing (or really, a 3D object) to the video card, which then rotates the image one way for the left-eye image and the other way for the right-eye image. nVidia drivers and most others have their own control for this rotation, which may be referred to as the depth or stereo separation adjustment. There is usually a "hot key" or combination for this, and there may be another which controls the actual physical separation of the images on the screen. The perspective distance, which controls the degree of nearness and also influences the stereo effect, is set by SHAPE and can be changed even in fullscreen mode with the SHIFT-P and SHIFT-[keys (see below).

Setting up nVidia 3D Vision for Direct3D (DirectX). Some setup in the nVidia control panel may be required to enable adjustment of the convergence, which can be critical for satisfactory viewing. In the Control Panel, select Set up stereoscopic 3D in Stereoscopic 3D. Click on the button "Set Keyboard Shortcuts". If necessary click on "Show advanced in-game settings" and then check the box for "Enable advanced in-game settings". Instead of using the Increase and Decrease convergence hot keys, you can also change convergence by holding down the green-lit on-off button on the front of the nVidia IR emitter while rotating the adjustment wheel on the back of the emitter, but this is not

enable unless the hot keys are enable here.

Adjusting perspective distance, convergence and depth. The nVidia parameter "convergence", adjusted with hot keys as in the previous paragraph, can have the effect of moving the object viewed forward or backward so that is in front of or behind the plane of the screen. However, for SHAPE it is usually best to have the center of the image roughly in the plane of the screen - this minimizes eye-strain and the prominence of "ghost" images. Thus the convergence hot keys should be used to cause the two images to coincide at the approximate center of the object. This is best done without wearing the glasses. Once this is done the convergence can be saved with a hot key (CTRL-F7). A convergence value is appropriate for a given value of perspective distance, so if you always use the same perspective distance (say 100 Angstrom), it should not be necessary to adjust convergence again. Once convergence is adjusted, the depth, which corresponds to the SHAPE parameter stereopair rotation angle, can be adjusted with hot keys to change the stereo effect. However, the perspective distance and convergence settings probably have more effect on the perceived depth. The SHAPE stereopair rotation angle is ignored in Direct3D.

2) *Cards which support OpenGL quad-buffering*, such as the nVidia Quadro series: Select the 3D quad stereo option in the Drawing Mode drop-down box in the Dialog Bar - Left or in the Display menu. Stereo can be shown either in a window or full-screen. The program itself sends the two completed images or objects to two separate buffers, so both the perspective distance and the stereo rotation angle (= depth or stereo separation) are controlled by SHAPE; perspective distance is changed onscreen with the SHIFT-P and SHIFT-[keys and the rotation angle with the SHIFT-A and SHIFT-S keys.

Setting up nVidia 3D Vision for quad-buffered OpenGL. In the nVidia control panel, select Manage 3D Settings in 3D Settings. In the Global Settings tabe, the Global presets option can be set to "3D OpenGL Stereo". It may then be necessary to select the particular setting Stereo - Display Mode and set it to "Generic active stereo (with NVIDIA 3D Vision)".

For full-color operation these options will also require either the nVidia 3D Vision shutter-glass kit and a compatible 120 Hz monitor, or a stereo polarizing monitor and polarizing glasses. Other hardware combinations may also be available.

3) *Older nVidia cards* or some other card with stereo driver software, a CRT monitor and shutter glasses. These may work with the Direct3D option as in 1) and/or with the 3D single option in the Drawing Mode drop-down box in the Dialog Bar - Left or the Display menu. This will only work in full-screen. Like Direct3D in 1) above, SHAPE sets the perspective distance but the stereo rotation is controlled by the video driver.

Shortcut keys for controlling SHAPE images. Since stereo images may require full-screen viewing in which menus are not available, the keyboard shortcuts for modifying or

animating the images have been revised and extended.

Additional Details

The stereoscopic option for the video card may use additional shortcut keys to turn stereo on or off; to increase the counter-rotation of the left- and right-eye images; to change the separation of the two images; or to change other settings

It seems that nVidia cards, at least, produce a stereo effect only by rotation of the two images, rather than by themselves changing the perspective distance. SHAPE has a stereopair rotation angle settings, but these are used only in the quad-buffered OpenGL stereo mode, not the Direct3D mode (these angles are also used in the separate stereopair Drawing Modes, 2D stereopair and 3D stereopair). The physical separation of the two images may also be adjusted independently or in combination with the rotation. Thus in practice it may be necessary to adjust the rotation (which may be called depth or separation) with the video-card control, and the perspective distance with the SHAPE controls, by trial and error to get the optimum amount of stereo effect. The physical separation of the two images on screen, if that is an independent control, primarily affects comfort - if the separation is too large, the eyes may not be able to merge the two images. The controls supplied by the video card may have different names; depth, separation and/or convergence and the action of each may involve both translation of the image on screen and rotation. Considerable adjustment of these controls may be required to get the desired stereo effect and an acceptable level of comfort.

The major market for stereo viewing is for video games and movies, and the scenes viewed may extend to infinite distance and do not really have a center, as do the objects viewed in SHAPE. Thus the approach used for adjustment of the stereo parameters is somewhat different from what would ideally be used for SHAPE, and the settings for video games and movies may be considerably different from the ideal ones for SHAPE.

If the perspective distance is small in SHAPE, the projection of spherical atoms will be elliptical on the screen, and while this may actually be what the eye would see at a short distance, such a projected image is usually unsatisfactory in practice. Thus the perspective distance should usually not be decreased beyond the point at which atoms begin to look non-spherical.
Although the nVidia cards do not themselves change the perspective distance, there is no stereo rotation or stereo effect at all in Direct3D if the projection is orthographic rather than perspective - that is if Perspective is not selected in the Input 2 menu. Therefore, SHAPE always uses perspective projection in the Direct3D mode, with the perspective distance entered in the Perspective dialog (Input2 menu). If that distance is zero, a plausible value is entered based on the dimensions of the crystal.

In real life, viewing real objects with the two naked eyes, the stereo rotation angle is fixed by the perspective distance because the distance between the two eyes is fixed

(approximately). Although the macroscopic crystals drawn by SHAPE may be viewed in the real world, the scaling is arbitrary, and it is generally easier to change the stereo parameter(s) than all the central distances. Changing the stereo rotation angle is equivalent to changing the interocular distance. Thus it is necessary to adjust the two parameters stereo rotation angle and perspective distance independently. SHAPE rotates structures about their own centers (at least if you choose automatic centering), so the physical separation of the images should not need to be adjusted in the quad-buffered OpenGL mode.

In real life when attention is directed to a near object, not only is each eye directed towards that object, but the focus is adjusted; viewing a near object causes distant objects to go out of focus or become blurred and vice versa. This enhances perception of depth. On a computer or movie screen the focus cannot be changed, and this may interfere with depth perception for some people. Of course everything drawn by SHAPE is always in focus, unlike a non-animated movie which is recorded by cameras which change focus like the eye. In SHAPE, you may select fog, which only fades out the colors from front to back and does not change the focus.

To review:

In Direct3D stereo viewing, you may need to make three adjustments; the perspective distance, in SHAPE; and the stereo rotation angle and image separation, with controls supplied by the video card. The terms used for the latter two may differ, and there may be interdependence of all three controls. With nVIDIA systems the convergence setting is closely related to the SHAPE perspective distance; keeping the perspective distance constant may make it unnecessary to readjust the convergence for every problem.

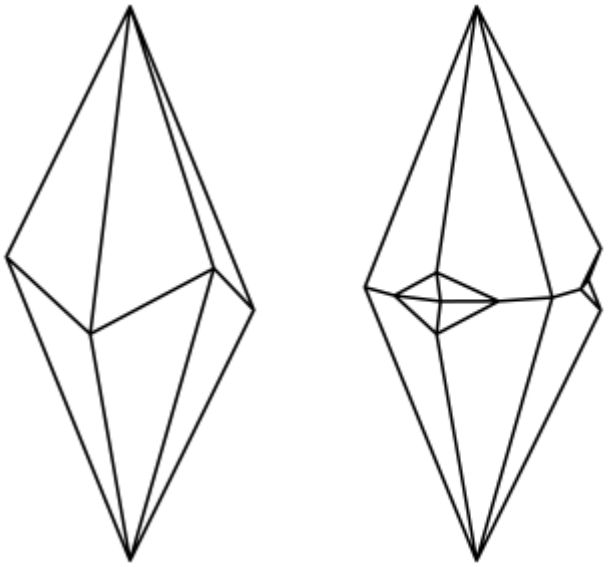
In quad-buffered OpenGL stereo, as well as the stereopair modes of SHAPE, both the perspective distance and stereo rotation angle are set in SHAPE. If Automatic Centering is selected (Input2 menu), the objects will be rotated about their own centers and it is not necessary to change the separation (separation of the two images in stereopair modes is determined by the size of the window or the screen).

5 Examples

This section gives instructions for entering data for the examples in the Sample sub-directory

Note on form/face/vector notation: for typographical reasons, negative signs in front of the indices are used instead of bars over the indices.

5.1 Calcite Scalenohedron - Simple Contact Twin



(TUTORIAL).

Double click on the SHAPE icon. From the **File** menu, select **New**. A dialog asks if you want to read default display variables. This is not necessary, as they are read in at start-up, so click on **No**. This brings up the **Title/Axes** dialog first. For a title "Calcite scalenohedron" will be sufficient, since other information will be supplied in the printout. From the **Crystal System** pull-down, select **trigonal hexagonal**. In the **a** and **c** boxes, enter 1.0 and 0.8543 respectively. This is for the morphological axes, which are most often used in designating faces (the true or X-ray axes are different).

Click on **OK**, and the next dialog, **Symmetry,** will come up. Click on the radio button to the left of **B3m**, and then on **OK**.

The **Forms List** dialog is next. Click on **Add Forms**, which will bring up the **Add/Revise Forms** dialog.

The indices of the common scalenohedron are {21-31}. The third index, -3, is superfluous, and you should enter only 2 , 1 and 1 in the boxes under **h**, **k** and **l**. Since there is only one form, the **Central distance** can be 1.0. The remainder of the items in the dialog do not need to be changed or filled in. Click on **OK** in this dialog, and on **OK** again in the **Forms List** dialog to complete data entry.

In the message box "New input completed - calculate now?", click on **Yes**. In a short time the computation will be complete, and the drawing will appear in the Graphics window.

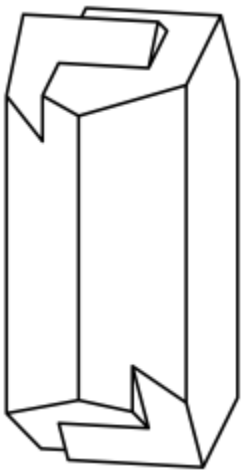
Now select **Twins** from the Input1 menu. From the set of radio buttons labelled "Type..." select **Contact with composition planes**. Now click on the **Add** button, which brings up the **Twin Operator** dialog. For the choice of reflection or rotation, select **Reflection**. Next enter the indices of the twin plane, (001). Click on **OK** to return to the **Twins** dialog.

Now click on the **Composition Planes** button, bringing up the **Composition Planes** list, then on the **Add** button in that dialog. Select **Indexed plane**, with indices (001).

This completes data entry for the twin. Click on **OK** in each dialog to remove them all. In order to put the changes into effect, you must select **Calculate** from the **File** menu.

To calculate exactly the same thing using rhombohedral axes, select trigonal rhombohedral for the **Crystal system** in the **Title/Axes** dialog, and enter 1.0 for *a* and 101.9 for alpha - this is again for morphological indices. The rhombohedral indices of the scalenohedron are {20-1}, and the indices of the basal twin plane are (111) - otherwise the input is the same.

5.2 Orthoclase - Carlsbad Twin



Data entry in this example follows almost exactly the same sequence as the last example, except that multiple forms are entered in the **Add/Revise Form** dialog. Use the **Next/New** button when finished with each form.

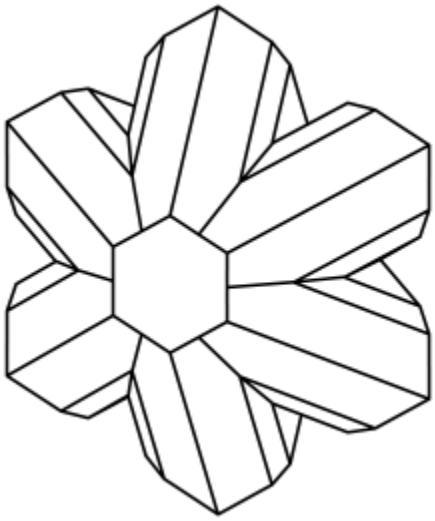
The **Crystal system** is **monoclinic**, and you can use the true axes, which are A=8.56, B=12.96, C=7.21 and BETA=115.83. This type of twin is usually drawn in a distorted habit, so it is not possible to use the full point group symmetry, which is "2/M" - instead enter "2". The forms present (indices followed by central distance) are:

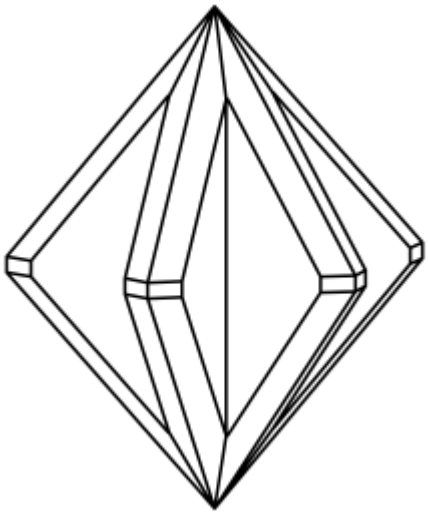
1) {110} 1.0
2) {1-10} 1.0

3) {001} 1.6
4) {20-1} 1.3
5) {010} 0.8
6) {0-10} 0.4

The twin is type I**nterpenetration with intertwin edges**: the operation is rotation by 180 degrees on axis [001]. Select **Remove Hidden Lines** from the **Display** menu to remove extra lines. It does no harm to leave this option on - it is ignored for single crystals.

5.3 Chrysoberyl and Aragonite/Cerussite Sixlings





In reality these twins are interpenetration twins by reflection, with three individuals per twin. They can be computed in this way, but it is slower in terms of computer time, and in both cases gives a number of small extra faces which appear rather messy. Therefore these twins are most satisfactorily done with a pseudo-twin operation, which is actually the pseudo-symmetry of the twin aggregate.

Both crystals have point group MMM, orthorhombic.

For chrysoberyl, the axial lengths or ratios are 0.58 : 1 : 0.47 and the forms are:

1) {111} 1.0
2) {001} 1.0
3) {121} 0.97
4) {010} 0.5

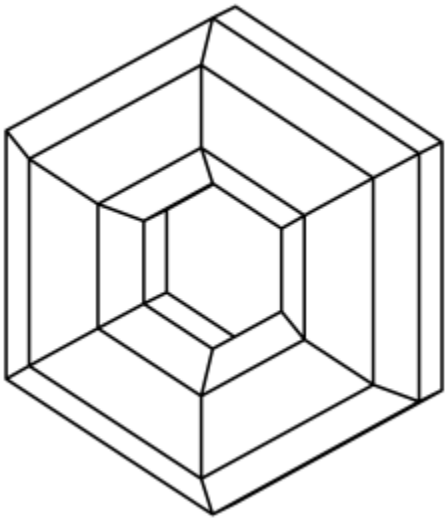
The twin type is **Contact with composition planes** and there are five twins, each by rotation on axis [001], by angles of 60, 120, 180, -60 and -120 degrees. The two composition planes are (130) and (1-30) which are the true twin operators.

When completed, the twin will be lying on its back, so to speak. Select **Cartesian Axes** from the Rotation Menu. The **axis** is *y* and the rotation angle is 90 degrees. You must click on the **Rotate** button before you click on **Done**.
For aragonite/cerussite the axes are 0.62 : 1 : 0.72 and the forms are:

1) {111} 1.0
2) {010} 0.2
3) {110} 1.2

There are again five twins by successive rotation of 60 degrees about the axis [001]; however, only three of these are visible (60, 120 and -60 degrees), and no subsequent rotation is required. Although the true twin operator is reflection on 110, in the sixlings the contact plane is quite different, approximating to (-130) - for the drawing use composition planes (-8,23,0) and (-8,-23,0). These indices were chosen so that the twin individuals almost touch, and do not overlap; if they overlap, the intertwin edges will not be drawn if **Remove Hidden Lines** (Display menu) is selected (although removal of hidden lines is actually not necessary for this view). An alternative would be to use composition planes (-130) and (-1-30) and adjust the axial ratios. This sort of problem does not arise in real contact or interpenetration twins, only in those constructed with pseudo-operators.

5.4 Rutile Doughnut Sixling

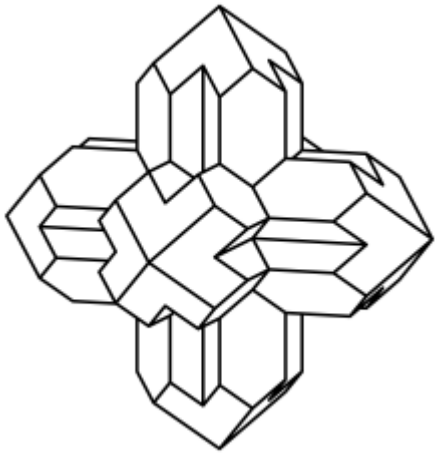


This "crystal" makes use of several tricks. Use point group "2", monoclinic, and axes 1 : 1 : 0.577, with BETA=90. This is not the true axial ratio of rutile, but is chosen so that the individuals just touch and do not overlap. The real forms which will be shown are {100} and {110}, but you must enter:

1) {100} 1.0
2) {010} -1.0
3) {0-10} 3.0
4) {1-10} 2.4749
5) {110} -0.3536
6) {001} 2.5

Note that the distances for forms 2) and 5) are negative - this causes the crystal to be drawn to the left of the center. The twins are type **Contact**, five successive rotations by 60 degrees about axis [100], with composition planes (011) and (01-1).

5.5 Phillipsite Twenty-fourling Pseudo-dodecahedron

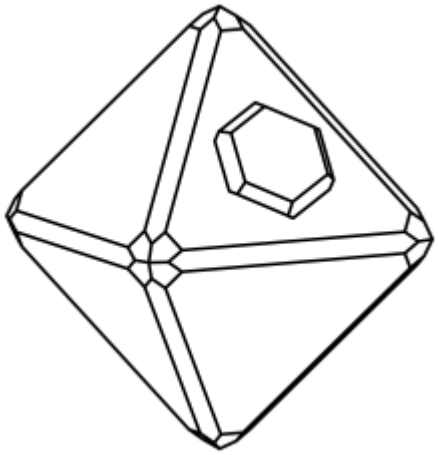


Phillipsite is really monoclinic and the true forms shown in this twin are {001}, {010} and {110}. It would take twenty-four individuals if it were done as contact twins - in this case it is easier to do it as penetration twins, and things are greatly simplified by using the cell dimensions and indices of the cubic twin pseudo-symmetry. Use crystal class B1, triclinic, with axes of length 1.0 and angles of 90 degrees, and input the following forms:

1) {110} 2.0
2) {1-10} 1.0
3) {101} 4.3
4) {-101} 4.3
5) {011} 4.3
6) {0-11} 4.3

Use twin suboption **Interpenetration - intercrystal edges**. There are 5 twins, by rotations of 120 and 240 degrees about axes [111] and [11-1], and 90 degrees about [001].
Try reducing the central distance of the forms 3) through 6) gradually, to see the transition to a pseudo-dodecahedron with complete faces.

5.6 Hematite on Magnetite (Contact Epitaxial Intergrowth)



First, generate the host magnetite crystal, in group M3M, cubic. The forms used on this crystal were:

1) {111} 1.0
2) {110} 1.17
3) {211} 1.3

Now select **Epitaxial crystals** (Input1 menu). Click on the **Add** button. Now enter the data for the guest hematite crystal.

For the **Type**, enter **Contact**.

Next enter the orientation. Fill in the indices in the boxes in the center of the **Epitaxial Relations** dialog; the epitaxial face of the host, (1 1 1); the alignment vector in that plane, [-1 -1 2] (this vector points directly toward the apex): the epitaxial face of the guest hematite crystal, (0 0 -1); and the alignment vector in that face, [1 1 0] (this may not be correct, but it looks good).

For the **Distance**, which in the case of contact intergrowths is the central distance of the epitaxial face on the epitaxial crystal, enter 0.06 (actually, anything less than the central distance of the normal (001) face, 0.1, would do). The **Translations** should be zero, although you can later move the epitaxial crystal around with these items.

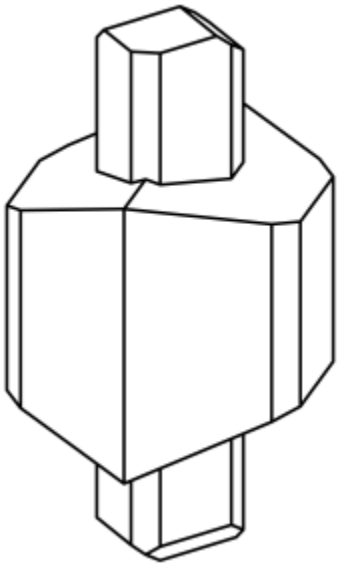
The data on the epitaxial crystal itself are entered with the **Revise Title/Axes**, **Revise Symmetry** and **Revise Forms** buttons towards the bottom of the **Epitaxial Relations** dialog, which bring up the same dialogs as for the main crystal. These buttons are the only way to enter or revise data for epitaxial crystals, and you must enter appropriate values in each dialog.

The crystal class is B3M, trigonal hexagonal, and the axes are 1.0 and 1.3. The forms are:

1) {2-23} 0.31
2) {101} 0.33
3) {001} 0.1

Note that these central distances fix the relative sizes of the two crystals, although you can change the size of the epitaxial crystal with the **Rescale** button.

5.7 Augite Enclosed by Hornblende (Epitaxial Interpenetration)



Generate the augite crystal first, although the order actually doesn't matter in this case. Crystal class is 2/M, monoclinic, and the axes are A=9.8, B=9.0, C=5.25, BETA=105. Forms are:

1) {110} 1.0
2) {100} 1.2
3) {010} 1.1
4) {001} 4.0
5) {11-1} 3.7

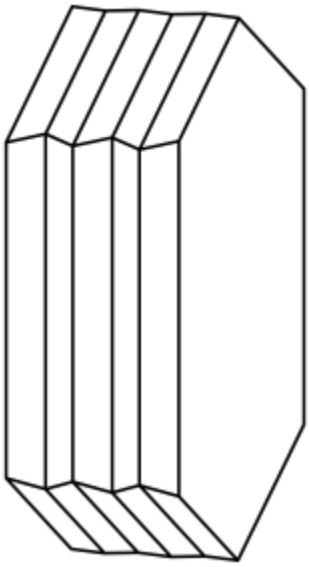
Go to the **Epitaxial Crystals** dialog in the **Input1** menu and enter the data for hornblende: the crystal class is also 2/M, axes are A=9.9, B=18.0, C=5.3 and BETA=105.5. Forms are:

1) {110} 2.0
2) {010} 2.4

3) {011} 2.0
4) {120} 2.3

Specify (100) and [001] as the face and vector of the host, and (-100) and [001] as the face and vector of the guest hornblende. Specify the type as **Interpenetration**, and center-center **Distance** of zero. **Intercrystal edges** should be checked, and you will need to **Remove Hidden Lines** (**Display** menu).

5.8 Lamellar Albite Twins



This intergrowth consists of two different orientations of albite crystals, but the input for the crystals themselves is exactly the same. The crystal class is B1 and the axes are a=0.63 b=1.0, c=0.56, ALPHA=94, BETA=116 and GAMMA=88. The forms are:

1) {110} 1.0
2) {001} 1.4
3) {-101} 1.4
4) {010} 0.1

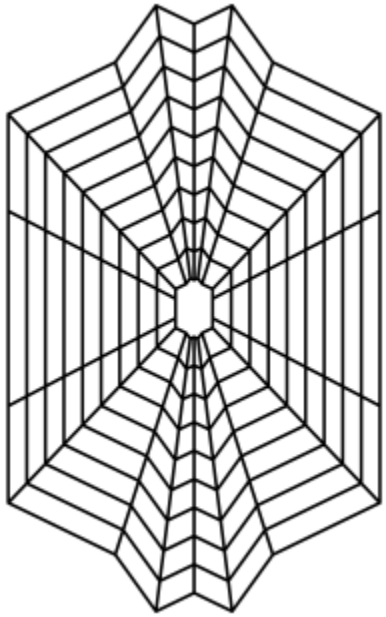
After entering the first or main crystal, select **Epitaxial Crystals**, and in this case you can simply click on the **Duplicate** button. After the new entry appears in the list, select that entry and click on **Revise**. For orientation, specify face (010), vector [001] for the host and face (0-10), vector [00-1] for the guest. Choose type **Interpenetration**, and give 0.2 for the center-center **Distance**. Note that the vector for the guest is the negative of that for the host; this results in a 180 degree rotation about the normal to the common face, which is the definition of a "normal" twin, and exactly equivalent to reflection in the face. It is not necessary to revise any of the data for the epitaxial crystal itself (**Revise...** buttons).

Returning to the dialog with the list of epitaxial crystals you can again just duplicate the last crystal and **Revise** the new crystal. This time, use face (0-10) for the host and (010) for the guest (the vectors remain the same), so that the new crystal will be on the back side of the host. The center-center distance is the same, 0.2.

Next, add another pair of epitaxial crystals on front and back - (010) and (0-10) of the host - at distance 0.4. However, for this pair, use the same vector, [001], for the guest and the host; this pair is thus in parallel, not twin, orientation with the original crystal. This could go on forever, but the intergrowth shown has just one more crystal, with the twin orientation, at distance 0.6.

Intercrystal edges may be left unchecked, but you must **Remove Hidden Lines** (**Display** menu).

5.9 Growth Zones in Carlbad Twin



This illustrates modelling of growth sectors in an intergrowth.

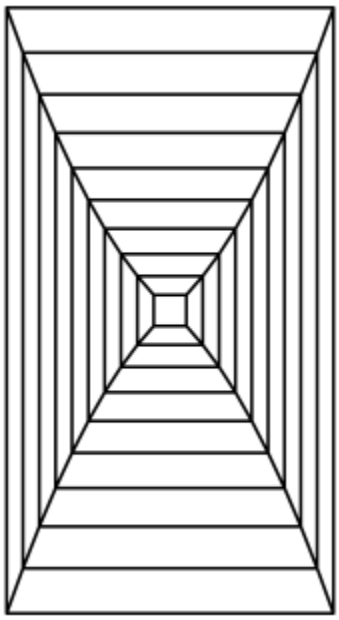
After generating the Carlsbad twin in example 2, select **Save/Recover Orientation** in the Rotation menu, and select the **Recover original orientation** button. Then select **Cartesian Axes** in the Rotation menu to rotate 90 degrees on *z*. This should give a view down the *b* axis.

Now select **Sections/Growth Zones** from the Input1 menu. Click on the **Growth Zones** radio button, and then on the **Zone Settings** button. In the **Growth-Zone Settings** dialog, click on the **Linear** button, and enter 10 in the **number of zones** box. Check the **Sector boundaries** box.

Remove the dialogs by clicking on **OK**, then select **Display** from the **Modes** menu, and set the display mode to **Sections/Zones.** The drawing will be replotted automatically.

Most of the growth sectors can be assigned to one face or two faces belonging to one or the other of the two individuals in the twin. The exception is the middle sector of the three bounded by 110 faces - actually, what is shown in this plot is the boundary between the (110) and (1-10) sectors of one individual and the (-110) and (-1-10) sectors of the other. There are thus four "combined" sectors, in which (110) of one individual is coincident with (-110) of the other, etc. These combined sectors may be illustrated more clearly in the normal three-dimensional view of the twin by switching **Edges in faces** in the **Preferences** dialog (**Settings** menu) on. Although the two coincident faces in each sector belong to the same form, they are not in the same orientation, so these "combined" sectors can not exist in reality. Presumably in a real twin the non-combined sectors above and below are extended to squeeze out the combined sectors, forming an irrational line of junction across the 110 faces.

5.10 Hourglass Zoning



This illustrates exponential growth rates in section. Enter a simple crystal with MMM symmetry, orthorhombic, A, B and C axes of length one, and forms 100, 010 and 001, all

with central distance one. Remove the orthographic rotation, if present.

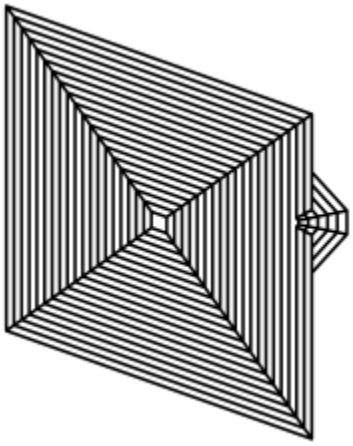
Now select **Sections/Growth Zones** from the Input1 menu. Click on the **Growth Zones** radio button, and then on the **Zone Settings** button. In the **Growth-Zone Settings** dialog, click on the **Exponential** button. In the Non-linear group, the **Total time** should be 1.0 and the **Interval** 0.1.

Now click on the **Rate Constants** button. This brings up the **Forms List...** dialog - you must set or reset the rate constants for each of the forms listed.

The equations for all three forms by default have non-zero *a* coefficients only for the first term, giving constant rates. Leave the first two forms alone, and select the third form, 001. Set a_1 to 0.75 and a_2 to 2.0. This gives a dependence on time to the power one, since b_2 is one by default.

Remove the dialogs by clicking on **OK**, then select **Display** from the **Modes** menu, and set the display mode to **Sections/Zones.** The drawing will be replotted automatically. On the first calculation, the plot will probably go off-scale; simply select **Replot** from the Display menu and the results of the first plot will be used to scale the second.

5.11 Hematite on Magnetite - True Epitaxy



This illustrates a crystal nucleating on another, with the two continuing to grow together for a period of time.
Enter the hematite on magnetite example number 6, with the following changes: 1) for simplicity, use only the form {111} for magnetite; 2) for the hematite epitaxial crystal, select interpenetration, at a distance 0.85, instead of a contact relation; 3) use the central distance 0.36, instead of 0.1 for the {001} form of hematite.

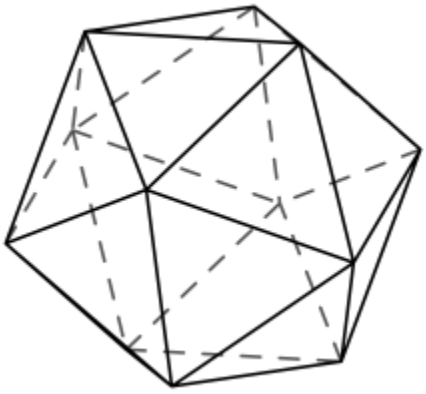
After the crystal has generated, select **Align Face/Vector** from the Rotation menu and

rotate the face (111) parallel to the screen, using alignment vector [11-2]. Then select **Cartesian Axes** and rotate 90 degrees on z. This gives a view down the epitaxial plane, showing the hematite to be partially buried in the magnetite.

Now select **Sections/Growth Zones** from the Input1 menu. Click on the **Growth Zones** radio button, and then on the **Zone Settings** button. In the **Growth-Zone Settings** dialog, click on the **Linear** button, and enter 20 in the **number of zones** box. At the bottom of the dialog, click on the **Times** button, which brings up the **Start and End Times...** dialog. Set the start and end times for crystal 2, the first epitaxial crystal to 0.8 and 1.15 respectively. Exit the dialogs and reset the display mode, if necessary, as for the previous examples.

The start time of 0.85 causes the hematite to start to grow just as the host magnetite reaches its center, simulating epitaxial nucleation. The two crystals grow together in the time interval 0.85 to 1.0 (host growth time), forming the small "root", and the epitaxial hematite grows alone in the interval 1.0 to 1.15.

5.12 Icosahedron - Quasi-Crystal



You must switch to the QSHAPE mode of operation with the **Operate** command in the **Modes** menu - see section IV-6 for principles and details of operation in this mode.

In the **Symmetry** dialog, you must supply the name of a Cartesian symmetry file - this is "Ih_example.sym", which is the file for icosahedral symmetry, as derived in the Cartesian (QSHAPE) Operating Mode section. You may need to Browse to the Samples folder to get the full pathname of this file. As the only form, enter {0 0 1} or {0.0, 0.0, 1.0} at a distance of one.

To get a pentagonal dodecahedron, enter {5.23607,0,1} as the only form. You can also try {010}, a rhombic triacontahedron.

As given above this example uses the orientation for the icosahedral groups from the trial-and-error example for SYMGR (see Help for SYMGRP). The symmetry file Ih_std.sym has the standard orientation for the groups, which is similar to that of cubic crystals, with the 3-fold axes (some of them) in the [111] position. Some simple forms for this orientation:

icosahedron: {1,1,1}
pentagonal dodecahedron: {0.525727, 0.850653, 0}
rhombic triacontahedron: {100}

5.13 General Comments on Twins and Epitaxial Crystals

As may be seen from these examples, a great variety of twins may be drawn. The only serious restrictions on twins drawn with **Twins** are that they must all be derived from a single original individual, composition planes must pass through the center, and contact and interpenetration twins may not be intermingled. One may draw multiple interpenetration twins in which the individuals turn out to be different, but in contact twins, the composition planes are applied to all individuals, and all the individuals are exactly the same or enantiomorphic.

In the **Twins** option, composition planes must go through the center of the crystal, but it is certainly possible to simulate off-center contact twins with the **Epitaxial Crystals** option.

For moderately complicated twins, such as fivelings, sixlings, etc. in which the individuals are all identical it usually saves computer time to treat them as contact twins and use for a twin operator the pseudo-symmetry operator of the twin. On the other hand using interpenetration twins usually requires fewer twin individuals and less operator time. For very complex cases like the phillipsite twenty-fourling (example 5) it may be necessary to use interpenetration twins. In all cases it may be easier, and the results simpler and aesthetically more satisfactory (if not strictly correct), if the pseudo-symmetry of the twin aggregate is used as twin operator instead of the true twin operators.

Interpenetration twins in high-symmetry systems, especially the cubic system, can give some complex and interesting shapes, based on fairly simple forms and twin operations. Try for example the spinel law - reflection on (111) or rotation by 180 or 60 degrees on [111] - on various isometric shapes such as cubes, tetrahedra, dodecahedra, distorted octahedra (unequal tetrahedra), and general and special forms of the lower-symmetry groups of the cubic system.

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