Chapter

I

Installation

The application CrystalKit and its associated files are installed by double clicking on the installer package. After authorizing the installer with the administrator password, the installer will install CrystalKit into a directory in your applications folder. The driver for the hardware key will also be installed..

Installing the Hardware Protection Key

CrystalKit uses a hardware copy protection key which must be installed on your computer. If you already have installed a key for use with MacTempas, you do not need a second key to run CrystalKit and you can proceed to the next paragraph describing how to activate the key for running CrystalKit. Just plug the USB key into an open USB slot on your computer, keyboard or display.

Activating the Hardware Key and Personalizing the Program.

When CrystalKit is run for the first time it will put up its installation screen. Enter your name and affiliation as appropriate together with the installation code for the hardware key

Changing Hardware or Versions of the MacOS

If you have just changed your computer or installed a new clean version of the MacOS, you must ensure that the driver for the USB key is installed. Run the installation program for CrystalKit once more to install the driver. Without the driver in place, the program will not recognize the hardware key and CrystalKit will run in demonstration mode.

Chapter 1

Introduction

CrystalKit is a general purpose program for modelling atomistic defect and interface structures in crystalline material. The program works with either one or two crystals (A/B) which can be perfect crystals or “unit cells” defined by CrystalKit in previous sessions. CrystalKit accepts files created in MacTempas and also outputs files in the MacTempas file-format. Optionally, the program can also read and write files in the EMS supercell format. When creating precipitates or geometric interfaces/grain-boundaries, the program works with crystals A and B which may or may not be the same crystalline structure. In order to create point defects, voids, interstitials etc., it is necessary only to work with a single crystal. CrystalKit can be used to visualize crystal-structures and chemical bonds. Angles and distances are easily measured and planes can be identified. Atoms can be moved either single or in groups and can be cut from and pasted into the structure. New atoms are added by the click of the mouse. It is also possible to view the kinematical diffraction patterns for a given crystal.

Chapter 2

CRYSTALKIT MENUS

The File Menu

Unlike most Macintosh Applications, the File Menu has no Open... menuitem. The File Menu is not used to open existing CrystalKit files, but rather to store created defects as structure files or create Pict files from the display.

The first three menu-commands
Selection to Pict
Window to Pict
Mac Screen to Pict
are used to create a PICT file from either the current selection, (created by the selection tool), the CrystalKit Display Window or the entire Macintosh Screen.

Write U.Cell to file
is used to write a structure file ready for simulation in MacTempas using a unit cell that has been defined by the use of the “Define Unit Cell” tool.

Write Xtal A/B to File
writes a structure file using the currently defined data of either crystal A or Crystal B. This is useful for saving a structure that has been defined within CrystalKit and also for structures that have been modified since they were read in. Note: See General Info for use of the Option Key in conjunction with saving the structure.

Write U.Cell to EMS file
is for writing a unit cell defined with the “Define U.C. Tool” as an EMS compatible file for further manipulation.

Slice U.Cell to File

will instead of writing the defined unit cell out as a single structure file, write the structure out as n separate files where the z-direction has been divided into n equal slices.

Recreate Interface
When CrystalKit saves a unit cell defined with the Unit Cell Tool, it also saves information regarding the two crystals, their orientation relationship and other settings. Thus when the user opens a file through the “Recreate Interface...” command, the two crystals are loaded into crystal A and B and the display shows the interface identical to when the unit cell was defined.

Page Setup
is the normal Print Dialog for page setup.

Print...
will print either the content of the image window or the content of any selected region.

Quit
Exits CrystalKit

The Edit Menu

The Edit Menu
serves a dual function. First it provides for the normal cut, copy, etc. functions that allow all Macintosh applications to share data. Thus one can bring any picture displayed in CrystalKit into any other Macintosh application. However, by using the Option key in conjunction with Cut, Copy, Paste and Clear, the operation takes place on the atoms that are visible in the display.
It is important to remember that in order for the “special” version of Cut, Copy, etc. to work, the Keyboard equivalents can not be used, the menu commands must be invoked by selecting them with the mouse. The use will be further described in a working example.

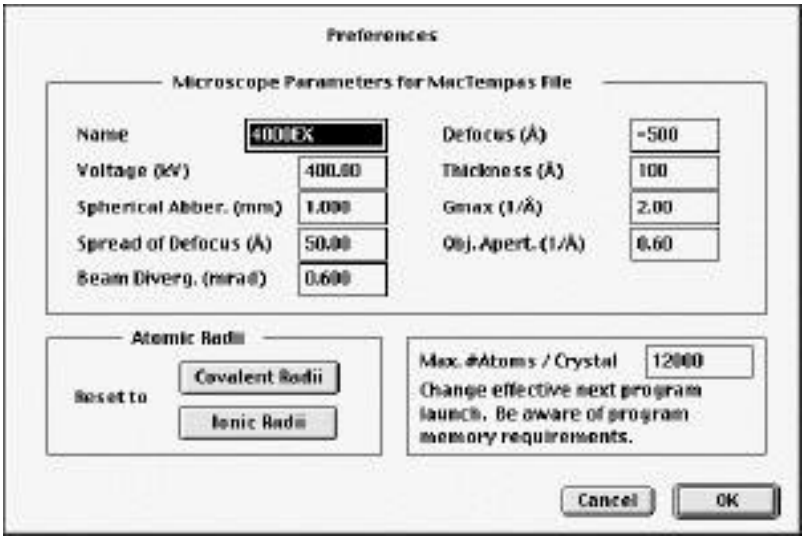
Undo

is not implemented.

Show Clipboard
shows the content of the cliboard in its own window.

Create A/B Precipitate
allows the user to create a precipitate of one of the crystals within the other. In order for this to work, the user defines two crystals, specifies the orientation relationship, an interface plane and a zone axis. The user then selects “Draw Penetrating Lattices” from the Display Menu. After the program draws the penetrating lattices the user creates a “selection” with one of the “Selection Tools” and chooses “Create A or B Precipitate” to keep A or B within the selection and B or A outside the selection.

Preferences...
is used to set the preferences associated with CrystalKit. One set of parameters determines the preference values for the microscope values and the crystal thickness to be used by MacTempas for doing an image simulation.

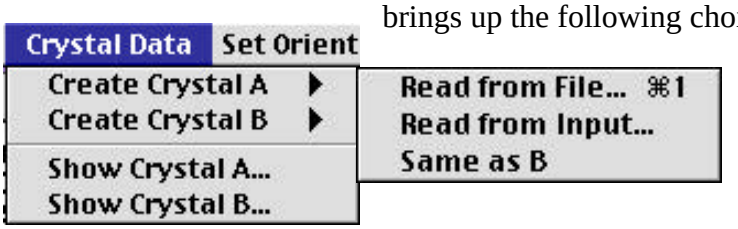


Atomic radii can be set to be either covalent or ionic by default. Individual atomic radii can always be changed manually by the

user at any time. The maximum number of atoms that the program can handle is set through the preference dialog. As is indicated, one also must make sure that adequate memory is allocated to the program by selecting the program in the finder and requesting “Get Info” from the menu and setting the amount of memory that is allocated to the program.

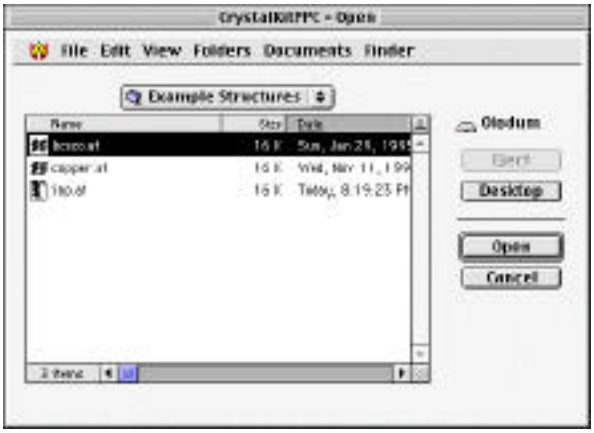
Crystal Data Menu

The Crystal Data Menu
is where the crystals A or B gets defined. Each crystal can be either read in from an existing file, entered manually or set equal to a structure that has already been read in.
Create Crystal A
Create Crystal B
brings up the following choice



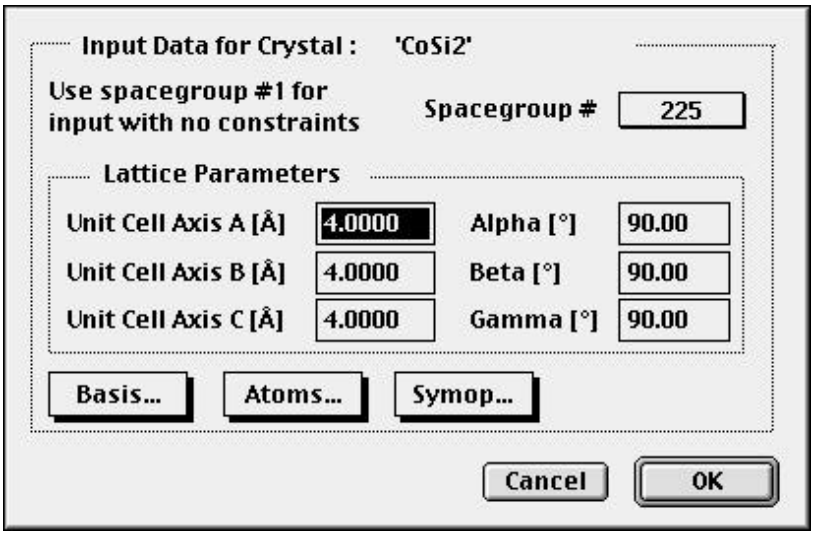
If the data is read from file, the normal Apple file-dialog appears, allowing the user to select an input file. If the **Option** key is held down when selecting “Read from File...” the program allows the user to choose an EMS file to be read in. No check on the filename is performed and the file must be a valid supercell EMS file.

The normal CrystalKit file shares the data format with the

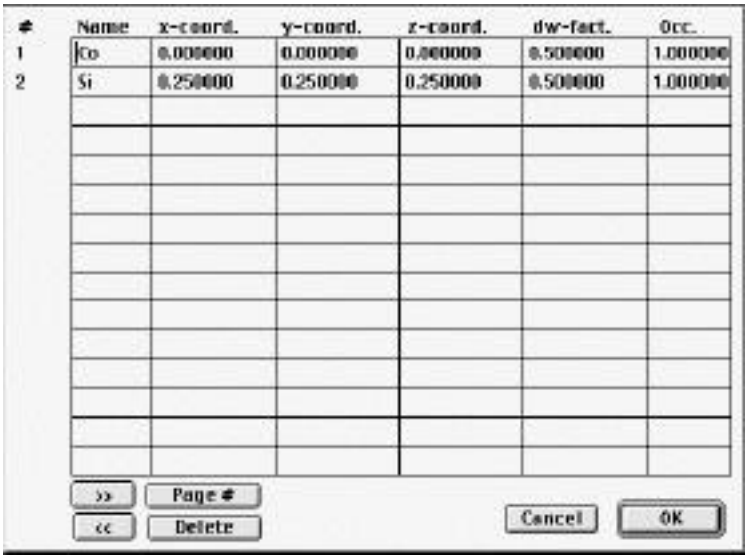


MacTempas program and has an extension of type ".at".
In addition, the resource fork can hold data about the two crystals that went into defining the unit cell if the structure was created by CrystalKit through the use of the “Unit Cell Tool”.

If the data is to be entered from within the program, the following dialog box appears, prompting for the relevant information.



If the crystal can be defined as one of the 230 spacegroups defined in the international table of crystallography, the user selects from the pop-up menu the type of crystal-structure (monoclinic, orthorhombic, cubic, etc.), and is presented with a choice of possible spacegroups for the selected crystal stucture. The number of symmetry operators associated with the crystal is automatically created by the program and the user only needs to fill out the data for the atoms in the basis (motif) after the data for the lattice parameters are entered.



Both the total set of atoms in the entire structure and the set of symmetry operators can be displayed by clicking on the two buttons "**Atoms**..." and "**Symop**..."

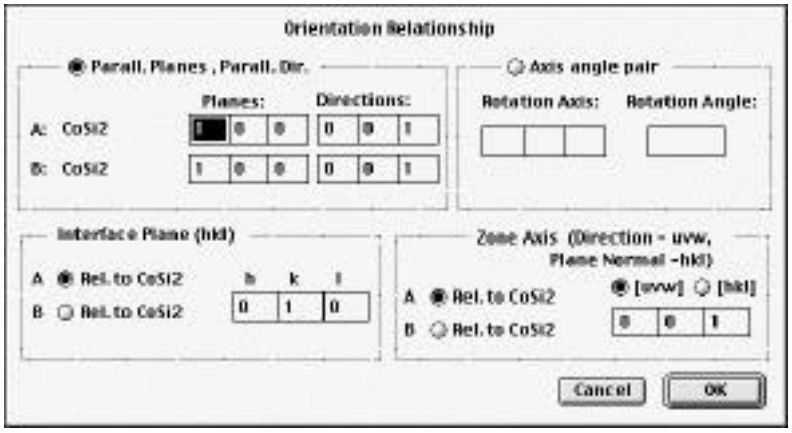
Show Crystal A
Show Crystal B
shows the user the data associated with the two crystals. The data is presented in the same fashion as when a new structure is created within the structure. The data can be edited to modify the structure.

Orientation Menu

has only one menu-command

Set Orientation...

which is used to specify the orientation relationship between the two crystals. The orientation relationship between the two crystals can be defined in two ways. The usual way to define the orientation relationship between two different crystals is to define two parallel planes and two parallel directions for the two crystals. It is also possible to define a common orientation axis and a rotation angle. Keep in mind that the axis/angle pair specification is only properly defined in the special case where the two crystals are identical. In this case, the two lattices are first oriented with their lattice parameters parallel to each other, before the rotation is performed about the common axis.

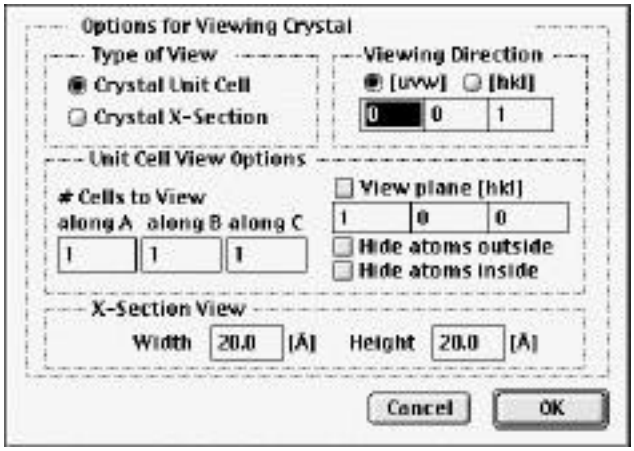


This allows for quickly defining a twin boundary in a crystal. In addition to defining the orientation relationship, the dialog is also used for defining the interface plane between the crystals and the zone axis. The interface plane cuts through the two lattices and crystal A is retained on one side of the plane and crystal B on the other side. This plane can be defined with respect to either crystal A or crystal B. The zone axis is used for defining the orientation for viewing direction and CrystalKit currently enforces the restriction that the zone axis must be perpendicular to the interface plane. Thus CrystalKit currently does not allow easily for the creation of inclined interfaces.

Display Menu

The Display Menu
is used to visually display the crystals or cross-section of crystals. In order to visually define a new unit cell with defects, interstitials etc., the user must first draw the crystal. In the case where the user whishes to define a unit cell containing an interface between two crystals, a cross-section showing the interface must first be drawn.

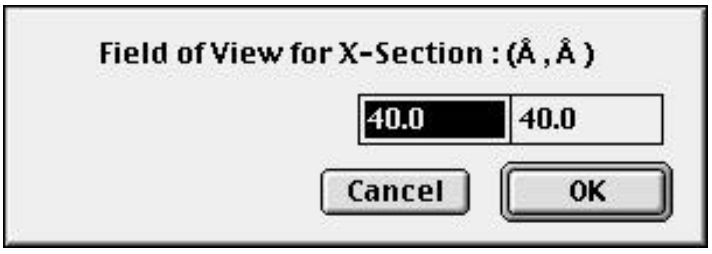
Draw Crystal A
Draw Crystal B
allow the user to display either a single unit cell or a cross-section of either crystal given a specified viewing direction.



The field of view and the specification of the zone axis are only associated with drawing a crystal cross-section and the zone-axis does not have an effect when displaying a single unit cell. When the display of a single unit cell is specified, the unit cell is always initially drawn in the [001] orientation. The crystal can be rotated into an arbitrary orientation with the Rotate Tool.

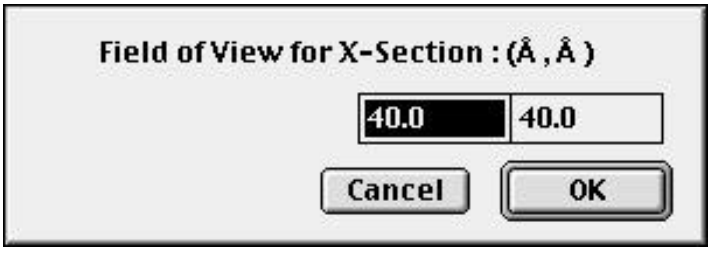
Draw X-Section
is used to display a cross-section of a defined interface. The command is only active after the user has defined two crystals,

their orientation relationship, interface plane and zone axis.



The specified zone axis defines the viewing direction. The values entered in the field of view is used to define the size of the crystalline material drawn. The interface plane is always drawn horizontally. It is important to remember when the interface is drawn, both crystals are allowed to "touch" the interface plane. This means that there are atoms from both crystals at the interface plane even though they may be obscured by other atoms or sit at the same site. By specifying how close either crystal A or B are allowed to come to the interface plane, this "double occupancy" can be resolved.

Draw Penetrating Lattices
uses the same information as draw cross-section, but allows both crystals to be drawn on either side of the interface plane. This way it is easy to see how the two crystals fit together and



one can visualize any coincidence lattice. This command is also used in order to define a precipitate of one of the crystals in a matrix of the other. Creating preciptates is done by first drawing inter-penetrating lattices and using the commands in the "**Edit**" menu for creating either an A or B precipitate.

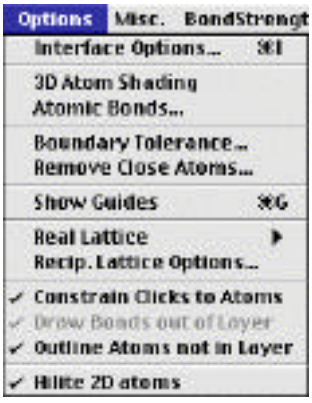
Redraw Display
redraws the view in case updating the display is required.

Make Movie
is used to create an animated sequence of either crystal A or B rotating 360 degrees. A selection rectangle must be defined which shows the size of the “Frame”.

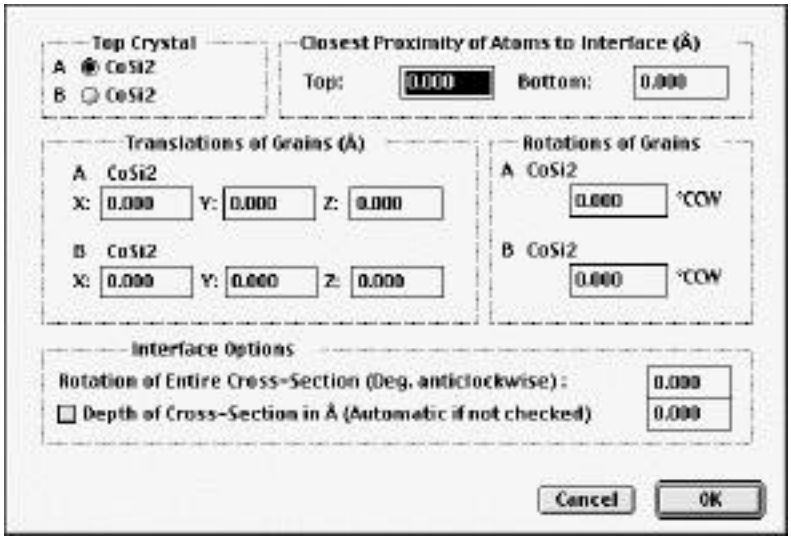
Play Movie
just plays back a movie created by Make Movie

Option Menu

The Option Menu
sets a number of optional parameters.



Interface Options...
brings up the following dialog box which controls many parameters determining the interface between two crystals.



Top Crystal
determines whether crystal A or crystal B is to be used towards the top of the display, above the interface plane.

Closest proximity of atoms to the interface
determines how close atoms from either crystal are allowed to be to the interface plane. Allowing both atoms to touch the interface will usually result in un-physical structures and also may obscure the fact that two atoms (one from each crystal) may occupy the same site without any visible indication thereof. This can easily happen when the same crystal is used for A and B and two atoms of the same type occupies the same position at the interface. The first indication that something is wrong may be during an image simulation where the interface plane shows wrong image contrast due to excess atoms at the interface plane. The value to be used is in Ångstrøm.

Translation of grains
allows the user to translate either of the two crystals with respect to the interface. These are rigid body translations. Units are in Ångstrøm.

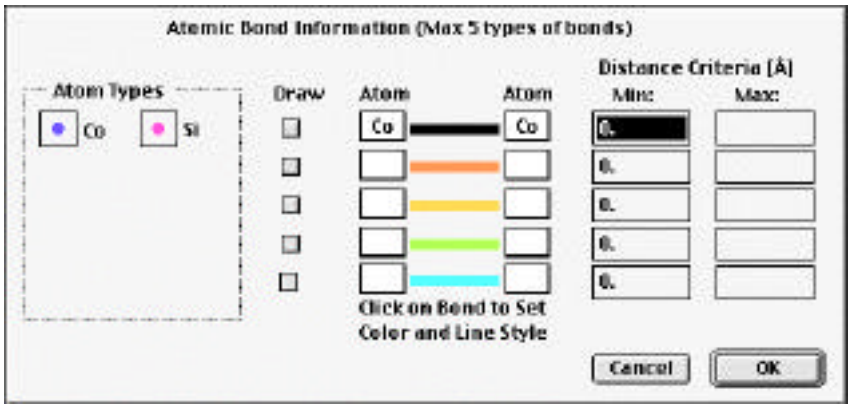
Rotations of grains
will rotate A and/or B with respect to the viewing (z) axis. The rotation is used in addition to the parameters set in the orientation dialog box. Thus the grains are first oriented as specified in "Set Orientation" and then additionally rotated by the angle specified.

Rotation of entire cross-section
is a rarely used option that allows for a slight rotation of the entire field of view to be rotated around the x-axis of the display. The x-axis is also the direction along the interface, going from horizontally from left to right in the middle of the display window.

Depth of cross-section
is used to set a specific value for the extent of a cross-section (using either one or two crystals). Normally the depth is automatically set by the program to be the length of the zone-axis for the crystal, that is one repeat distance in the z-direction of view. However, by checking the checkbox and inputting a value in Å, the depth will be set to the value entered by the user. Strictiy speaking the option for the depth of the view does not belong in this dialog since it is also used when displaying a cross-section view for a single crystal. Thus the depth is not necessarily related to an interface.

3D Atom Shading
will cause the atoms to be drawn as shaded spheres with lighting conditions specified by the “Lighting Tool”

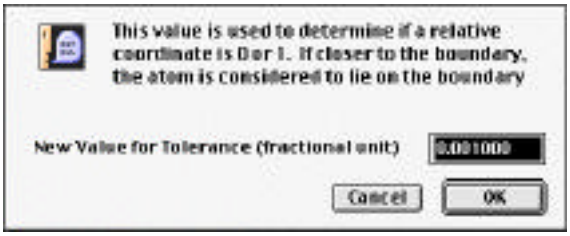
Atomic Bonds
allows the user to specify up to 5different types of bonds to be drawn between atoms. The user specifies the two atoms between which to draw a bond and the minimum and maximum distance between the two atoms for when to draw a bond.



By clicking on the line for the bond, it is possible to choose the

color for the bond the line-style and the width of the bond.

Boundary Toleranse
has been added to allow the user how close to zero or 1 a relative atomic coordinate can be without being considered to lie on the boundary (0 and 1). Default value is 0.001



Remove Close Atoms...
will initiate an attempt by the program to determine if two atoms are too close and to remove atoms that are within a specified distance.

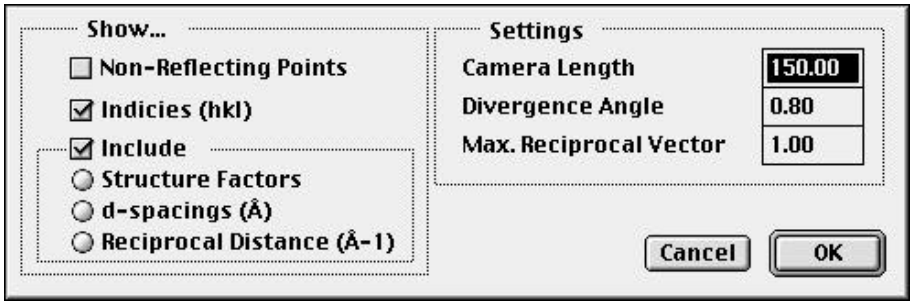
Show Guides
will turn grid lines on or off. The default gridlines appear as a vertcal and a horizontal line that can be positioned anywhere by dragging the line with the pointer tool. Additional vertical and horizontal lines can be added by dragging with the mouse from the “grayed” area at the edge of the image window into the win-

dow. These guides can be very useful to mark positions on the screen when creating interfaces.

Real Lattice
will cause the following pop-up menu to appear. The image

window can show the real lattice (default), the reciprocal lattice or both lattices at the same time.

Reciprocal Lattice Options
sets options related to the display of the reciprocal lattice. The camera length determines the scale of the pattern. The divergence angle sets the size of the diffraction spot which also is scaled by the structure factor.



The maximum reciprocal lattice vector is set through the dialog together with options for labelling the pattern. The options are i) indexing the pattern (hkl), ii) showing structure factors, iii) showing d-spacings and iv) showing length of reciprocal lattice vectors. If the “Show non-reflecting points” is checked, the program will also display points in the reciprocal lattice that are in non-reflecting positions.

Constrain Clicks to atoms.
Normally when using the mouse to select a point for defining a

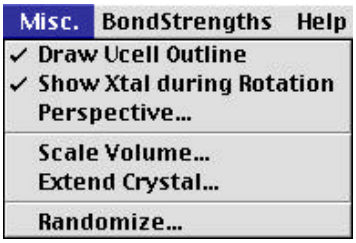
unit cell or to measure a distance, the program only allows click inside an atom. If this option is non-checked, it is possible to mark positions that are not associated with atom positions.

Draw Bonds out of Layer.
When a cross-section or an interface is being viewed it is possible to select which atomic layer to display through the pop-up menu in the lower left corner of the image window. If the “draw bonds out of layer” is unchecked, the program only will draw atomic bonds that fall within the displayed layer. If the option is checked the program will also draw bonds to atoms that do not lie in the displayed layer.

Outline Atoms not in Layer.
By default atoms that do not lie in the displayed layer are not drawn. If this option is checked, atoms that lie in other layers are outlined by a non-filled circle.

Miscellaneous Menu

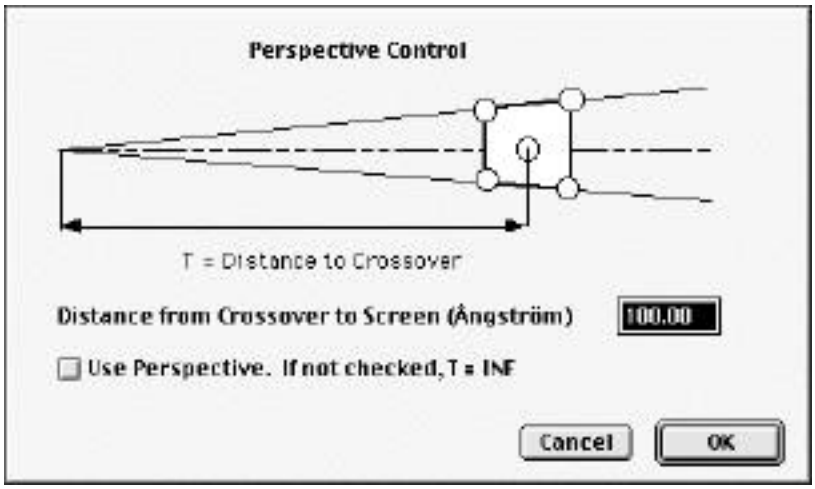
The "Miscellaneous Menu"
is a selection of commands outlined below.



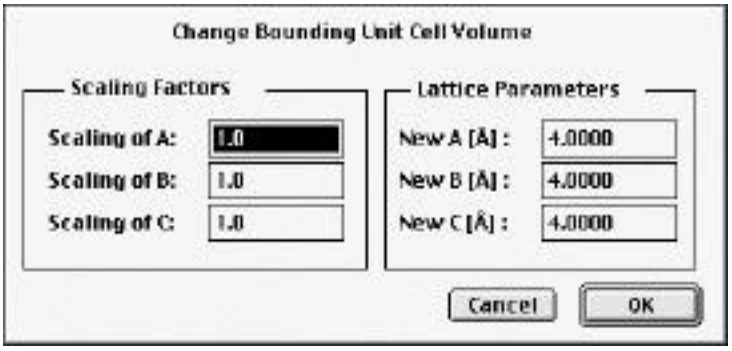
Draw Unit Cell Outline
determines whether the cystalline axes should be drawn when the crystal is drawn. By default the crystalline axes and the field of view boundaries are drawn.

Show Crystal during rotation
. By default the crystal is shown “real time” when the rotation tool is used. If this option is not used, the unit cell is only redrawn when the mouse is released and only an outline of the unit cell is shown during the rotation.

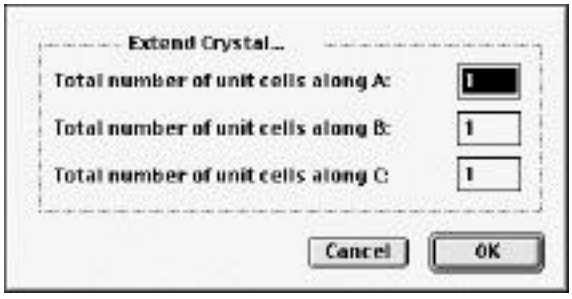
Perspective...
brings up the following dialog. If the option to use perspective is checked, the unit cell will be drawn in perspective with the distance to the cross-over indicated by the figure determined by the parameter set by the user.



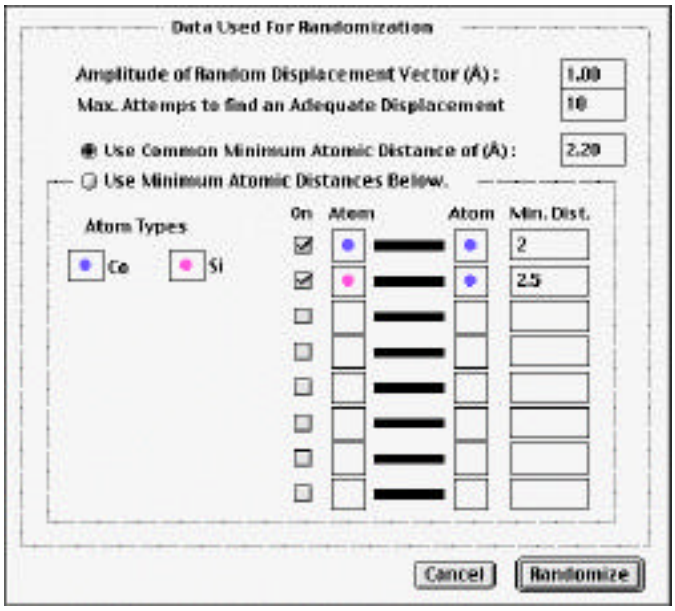
Scale Volume...
allows the user to scale the bounding volume of the defined unit cell such that the unit cell stays fixed and the bounding volume determined by **a**,**b** and **c** are scaled according to the input in the following dialog.



Extend Crystal...
will create a new unit cell by extending the previously defined unit cell by a given integral number of unit cells in each direction **a**,**b** and **c**.



Randomize.. b
rings up the following dialog.



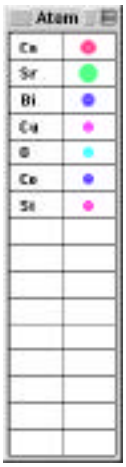
It is a fairly rude attempt to create an amorphous structure by displacing atoms in random directions according to the options set in the dialog above. By default, each atom is displaced by a specified displacement in a random direction and a displacement satisfying the criteria that two atoms are not closer than a specified distance is sought within a maximum number of attempts. If the distance criteria is not met for the maximum number of attempts, the program allows the last displacement and notifies the user at the end how many atomsdo not meet the

distance criteria. It is also possible to specifically give minimum distances for any specific two atoms. The atoms are specified by selecting the atom by clicking in the “Atom Type” and then clicking in the box for the “Atom” to deposit the selected atom. In order to create an amorphous structure of a given size, it is necessary to first display a cross-section of the required dimensions, marking a unit cell to set the boundaries and then randomizing. The unit cell can also be marked after randomizing, although it may be necessary to uncheck the “Constrain click to atoms” in order to mark the appropriate volume.

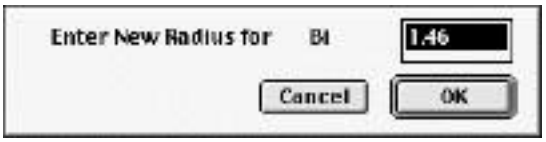
Chapter 3

CrystalKit Windows

CrystalKit has four main windows. These are the atom window, the info window, the tools window and the main drawing window. The windows are described in more detail below.



Atom Window
This window shows the different atom types in the crystal(s) that are defined. The relative radii of the atoms are represented by the size of the colored circles and the colors correspond to the ones used in drawing the atoms. By double-clicking on one of the circles, the atomic radius can be changed. When the

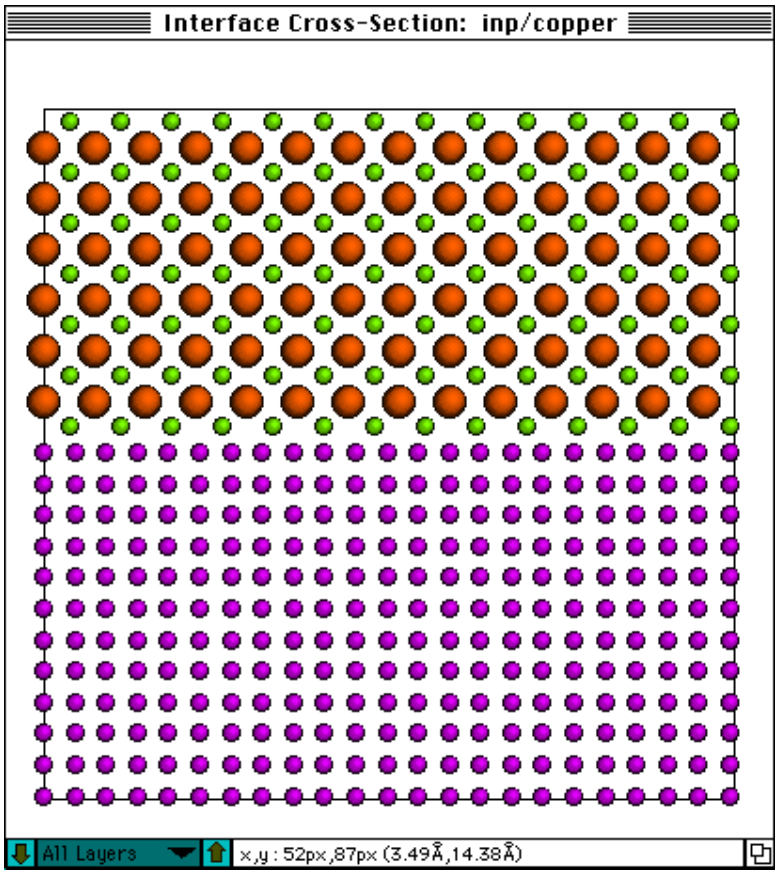


color-picker tool is active, the color of the atom can be changed by clicking on the circle and choosing a color from the pop-up window.

Info Window
This window is used for reporting information to the user. Information such as inter-atomic distances, angles and information regarding crystalline planes is written to this window. Additional information is also shown in the status line at the bottom of the main drawing window.

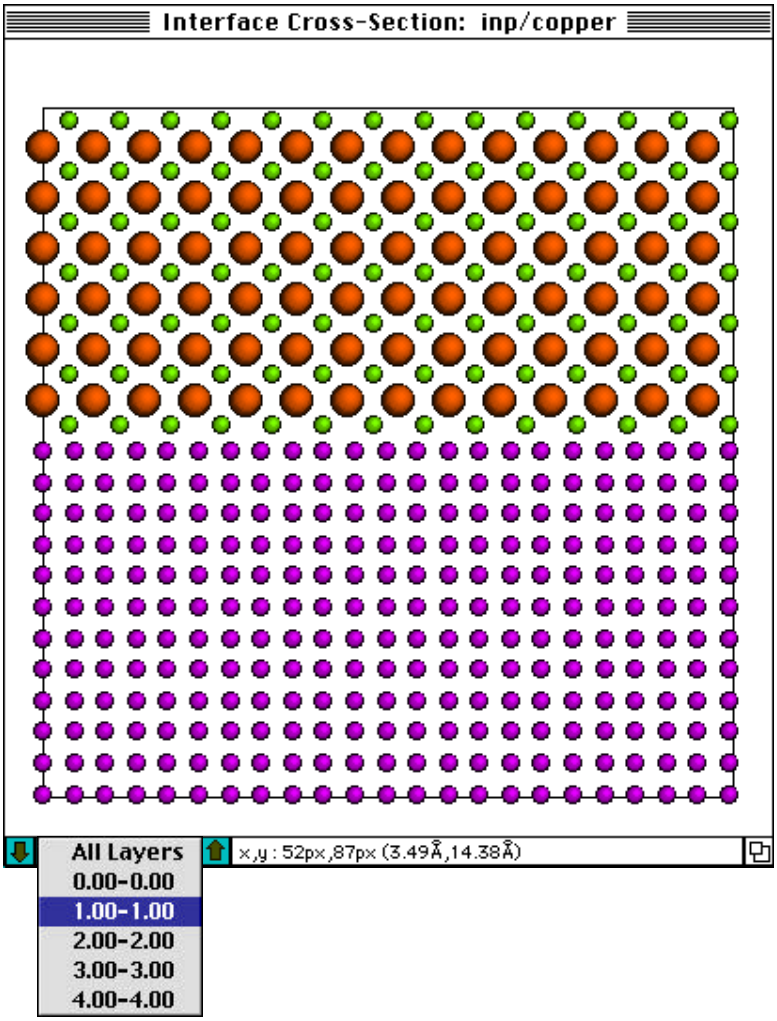
Tools Window
This window contains the various tools for controlling the actions of CrystalKit. The tools are described in further detail in the next chapter on the CrystalKit tools.

Main Drawing Window



This window is used for all drawing of unit cells etc.
When drawing a cross-section, the layer control at the bottom of the window can be used to display only atoms in specific layers. The control is a pop-up menu, displaying the various heights in

Ångstrom containing layers of atoms. By selecting one of these layers, only atoms in this layer is displayed. When operating on atoms, only atoms in the currently selected layer are effected.



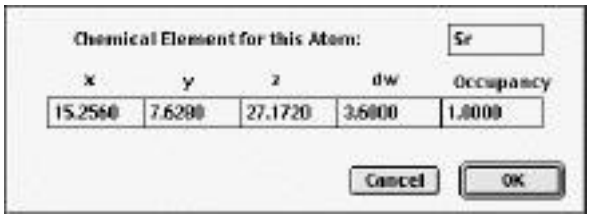
Chapter 4

CrystalKit Tools

All the tools that CrystalKit can use are defined here. The user selects a tool by clicking in the corresponding area. That tool is active until the user chooses another tool. The cursor will normally change to indicate which tool is currently active.

Pointer
The Pointer Tool is used only when the user wants no other tool to be active. It has no function except for insuring that no other tool is active. It should also be the active tool when creating and dragging grid lines

Info Tool
When this tool is active, clicking on an atom will bring up information regarding that particular atom. Normally a dialog box shows the data and these can be edited in the normal way.

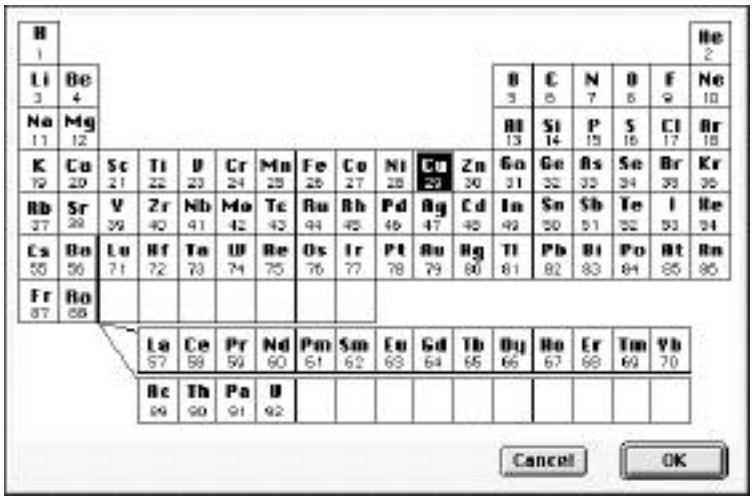


In the case when an interface is drawn, the data is displayed in the INFO window. By holding down the Option key, the normal dialog box is displayed.

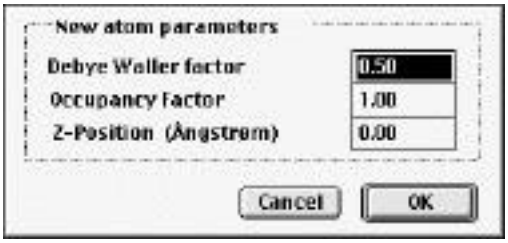
Move Atom Tool
Use this tool to move atoms around. It only works when an interface or a crystalline cross-section is drawn. It is important to note that with many of these tools, all changes are lost after redrawing.

Add Atom Tool

Add an atom at the location of the mouse click. At the time the-tool is activated, a dialog comes up to allow for specifying which atom to add.



A separate dialog appears allowing the specification of the Debye-Waller factor, the Occupancy factor and the height of the atom in the z-direction (perpendicular to theplane of viewing).



Delete Atom Tool

Deletes single atom. Does not work when viewing a single crystalline unit cell (displaying Crystal A or B).

Interface Tool

When a cross-section with an interface is drawn, use this tool to define an interface of arbitrary shape. Start to the left of the drawn crystalline section and mark points that defines the

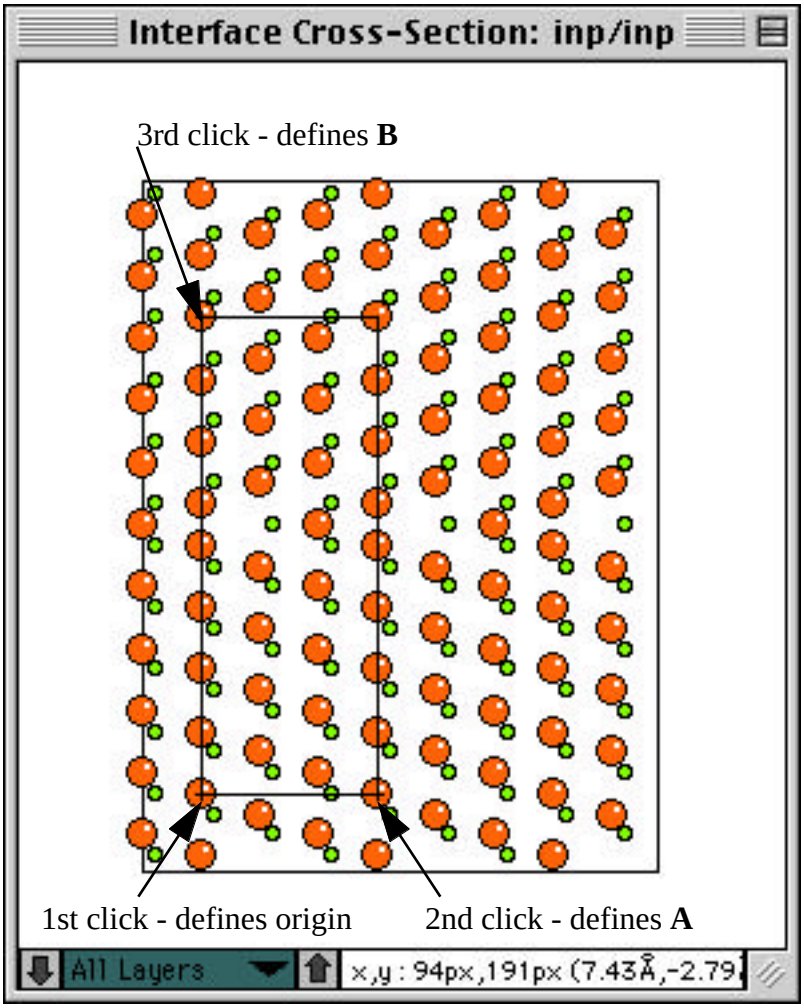
boundary until the other end is reached. Backtracking is not allowed. When the last point is specified, the interface will be redrawn with the specified path as the "interface plane".

Selection Tools
Use these tools to define a selection of various shapes for cutting, copying, defining a region for a precipitate etc.
When the “Shift” key is held down, a square or a circle will be drawn. When using the region tool, the path must be closed by ending up at the starting point.

Ruler Tool
Used to measure interatomic distances. Normally all clicks are constrained to atom positions and the program will sound a warning sound when an atom close to the mouse down position is not found. If the Option key is held down, the click is not constrained to atom positions.

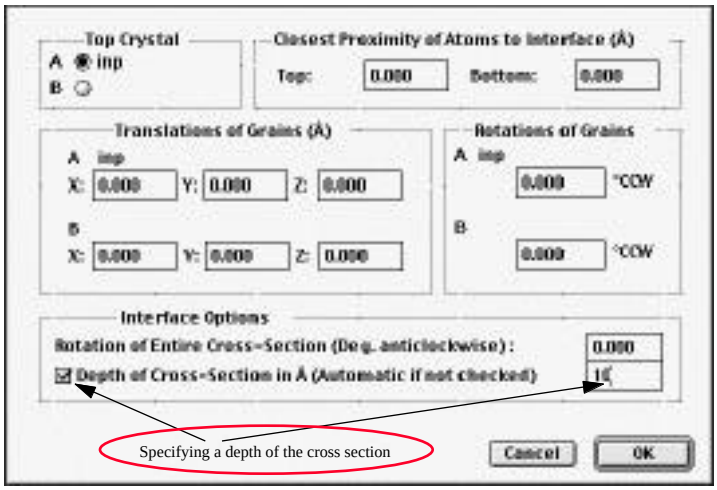
Define Unit Cell Tool
When a cross-section is drawn, either of a single crystal or an interface, this tool allows the creation of a unit cell for writing to a structure file. Mark first the origin, then one lattice vector (A) and then finally the second lattice vector (B). By using Write U.Cell To File, this unit cell is written to a structure file. One can continue defining unit cells, each one replacing the previous. All changes to the structure, such as moving atoms and deleting atoms will be reflected in the created structure file. If the cross-section is drawn once more, these changes are lost. Normally the cursor is constrained to fall on an atom. However, when the “Option” Key is held down when marking the unit

cell, the locations need not be on atomic sites.



Note: Often the repeat distance in the zone-axis orientation will not be the same for the two crystals A and B. The program will use the largest repeat distance as the C axis, but will fill the other crystal with atoms only to its repeat distance. The occupancy factor of the atoms within the “shorter” structure is modified to compensate for the larger c-axis. If the “shorter” Crystal was allowed to fill atoms up to the repeat distance of the other crystal, the “corresponding crystal would hold an incomplete number of unit cells and would cause forbidden reflections to show up in a diffraction calculation. The c-axis can be forced to

an arbitrary value by fixing the x-section depth (from the Option Menu).



Rotate Tool

When a crystalline unit cell is viewed (Display Crystal A/B), this tool is used to rotate the crystalline unit cell into any orientation. Click in the main window and hold down the mouse button while moving the mouse. If the “Shift” key is held down as the pointer is moved, the rotation is about the axis perpendicular to the screen.

Lighting Tool

When the 3D Option is used in drawing atoms, this tool is used to define the direction of light. Click in the center of main window and hold down the mouse button while moving the mouse to change the direction of the light. Because the circle showing

the shading is drawn at a distance from the location of the cursor, it may be necessary to press down the mouse with the cursor in the center of the screen.

Animate Tool
When a crystalline unit cell is viewed (Display Crystal A/B), this tool is used to continuously rotate the unit cell. The rotation starts by clicking in the main window. It stops when the mouse-button is pressed down a second time. It may be necessary to keep the mouse depressed for a short time to stop the rotation if the drawing of the unit cell takes a long time.

Angle Tool
Use this tool to measure the angle between two directions (3 atoms)

Plane Tool
Use this tool to determine the plane and the planar spacing by clicking on two atoms in the same plane.

Magnifying Glass
Clicking in the display magnifies a drawn unit cell by 10% per click. Holding down the Option Key demagnifies. By holding down the Shift Key the increments in magnification/reduction changes to 100%.

Color Picker Tool
Used to change the color associated with an atom species. When this tool is active, click in the colored circle in the atom window (actually anywhere in the rectangle) and choose any of the 16 different colors.

Chapter 5

General Information

Basis Atoms vs. Displayed atoms

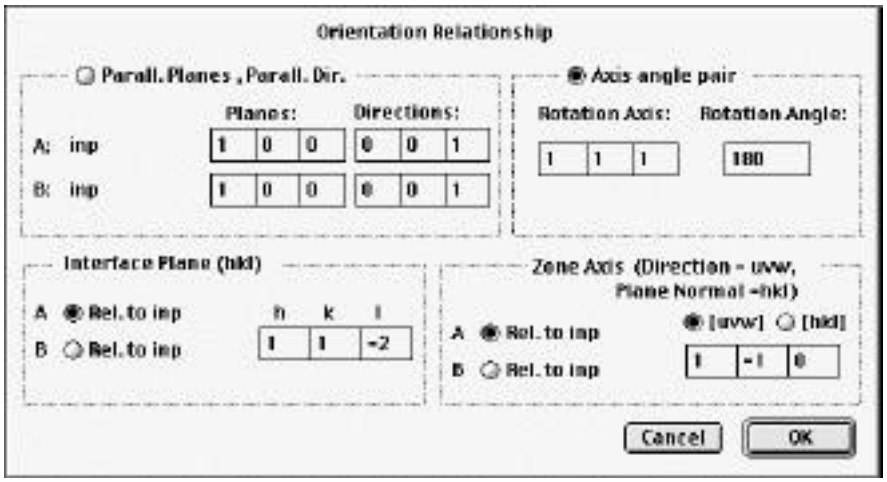
The structures referred to as Crystal A and B can be modified by the user and saved to a new file by the menu commands “Write Xtal A/B to File”. Normally this structure is associated with the list of “basis-atoms”. Thus if one displays the list of atoms (basis or atoms) in the dialog “Show Crystal A/B”, one can only modify the list of “basis-atoms”. This is because the “atom-list” is generated from the “basis-list” by the application of the symmetry operators. If the only symmetry operator is x,y,z (the identity operator), the “atom-list” and the “basis-list” are identical in content, but the program still maintains a separate list for the two. When one displays a single unit cell of a structure, as in “Display A”, the atoms drawn on the screen correspond to the “atom-list” plus the equivalent atoms drawn at corners and faces. For example in the list, one only has an atom at (x=0,y=0,z=0), but on the screen there will be additional atoms at (1,0,0), (1,1,0), (1,1,1), (0,1,0) etc... If one modifies the structure by typing in new information in the “basis-list”, this information will be reflected in the structure if one uses the command “Write Xtal A/B to File” to save the new structure. However, it is possible to modify the structure in a different way. When one draws a single unit cell on the screen and possible the rotate tool to view the structure from a convenient direction, one can get information on a single atom by clicking on it with the info tool (?) selected. This information can be modified by typing in new values for the coordinates, changing the atom type etc., and one will see the modifications on the screen. The information that is changed is maintained in the “atom-list”, not the “basis-list”. Thus if the structure is saved using the command “Write Xtal A/B to File”, these changes will not be reflected in the saved structure. However, if the Option Key is held down when invoking the saving of the structure, the “atom-list” will be saved, not the “basis-list” and your changes will be written to the file. It is important to realize that one could not

change the atom at (1,1,1) and have that change reflected in the new structure. The atom at (1,1,1) is not in either list and is only drawn to show the unit cell corners. One can either think of each the corner-atoms contributing 1/8th of an atom to the unit cell, or that the the atom at (0,0,0) is wholly within the unit cell and that the other corner atoms belong to neighboring unit cells. The latter convention is used in CrystalKit

Chapter 6

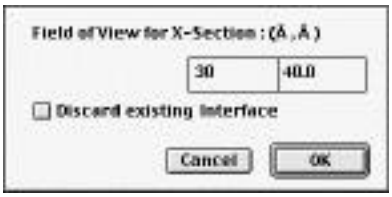
Example 1. Generating a twin boundary in Indium Phosphide

After starting up CrystalKit, go to the menu Crystal Data. Choose Create Crystal A (Read From File...) and select the file InP.at. Then proceed to define Crystal B (Create Crystal B -> Same As A). Now both crystals are defined and the orientation relationship must be defined. Choose the menuitem “Orient. Relations...” under Set Orientations and set the orientation relationship as shown below.
After you have filled out the dialog, click OK and go to the

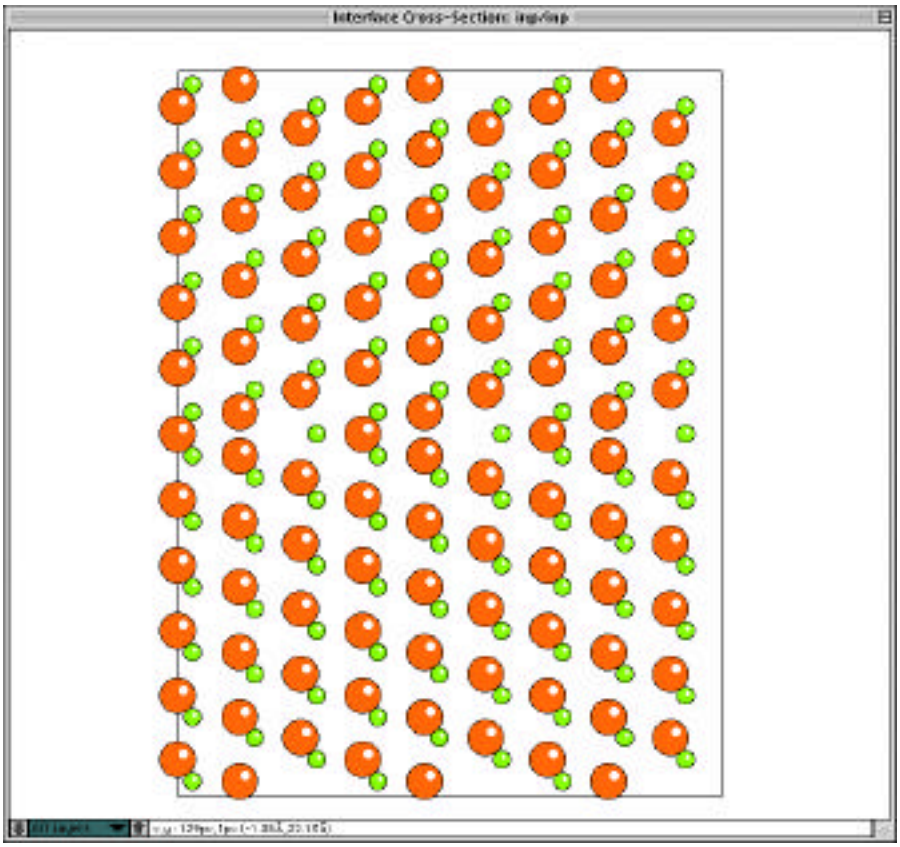


menu Display. Choose Draw XSection... and respond by setting

the field of view to 30 by 40. (Units are in Å). The result

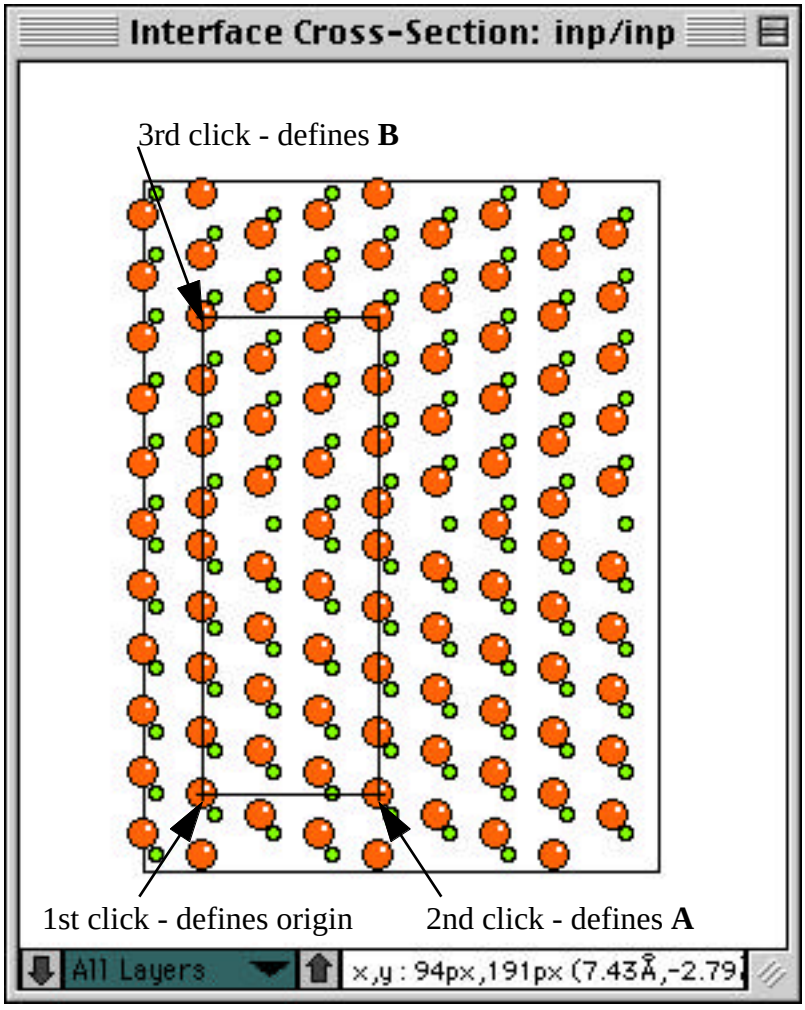


should be as shown below.



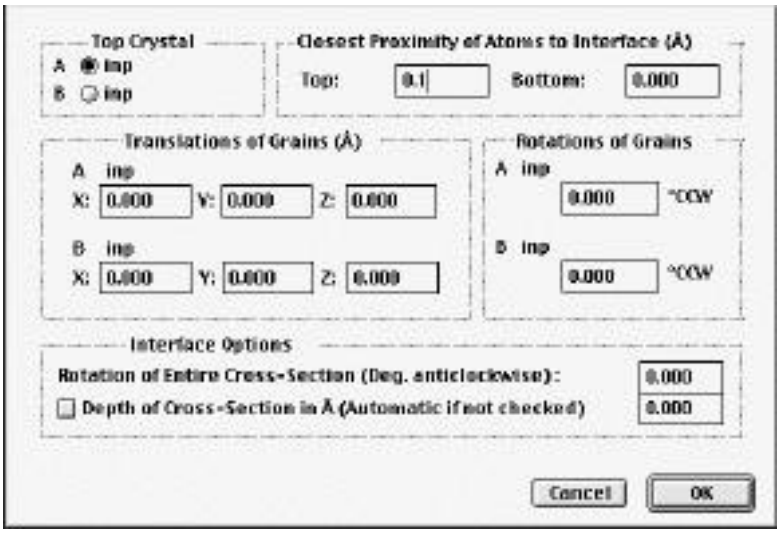
If you now want to define a unit cell, just use the “”Define Unit Cell” Tool and mark the Origin, A and B. At this point you will have a double set of atoms at the interface plane, because both

crystals are allowed to touch the interface.



In order to remove these atoms, choose Prox. of Top & IF in the Options Menu and set the value equal to 0.1.

The display will automatically redraw and only one set of atoms

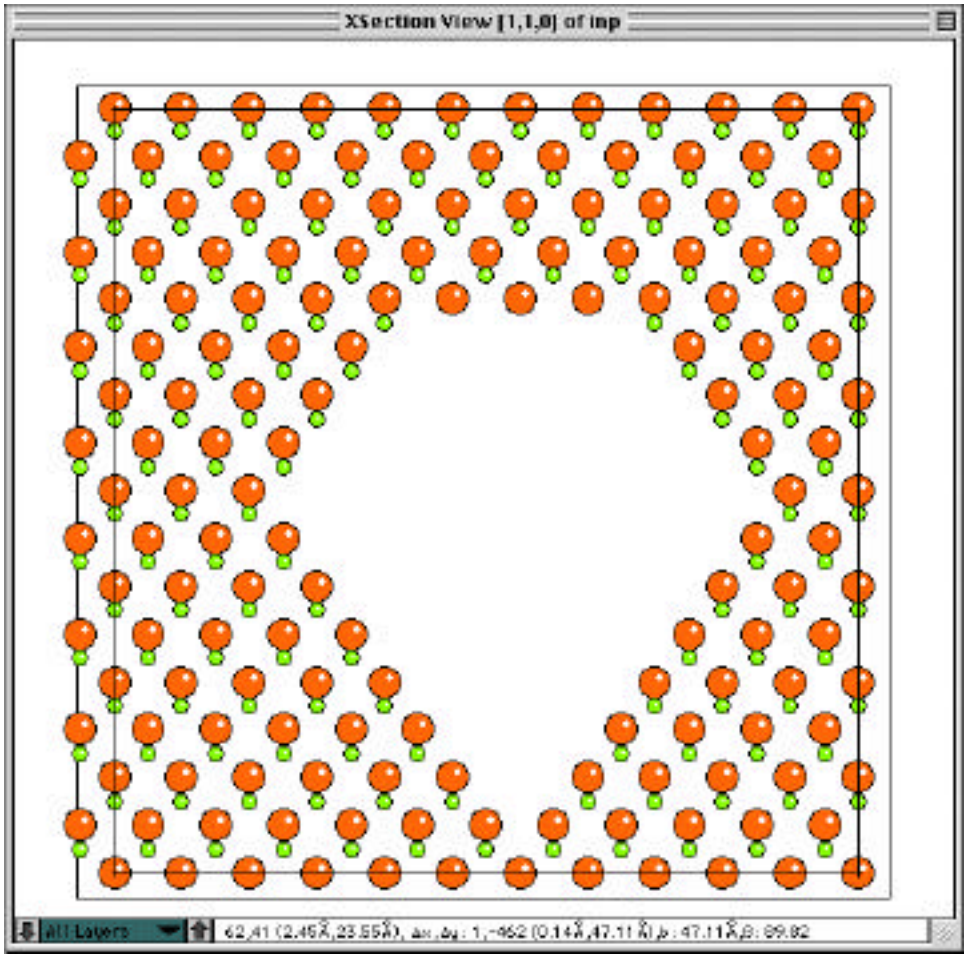


will be at the interface.

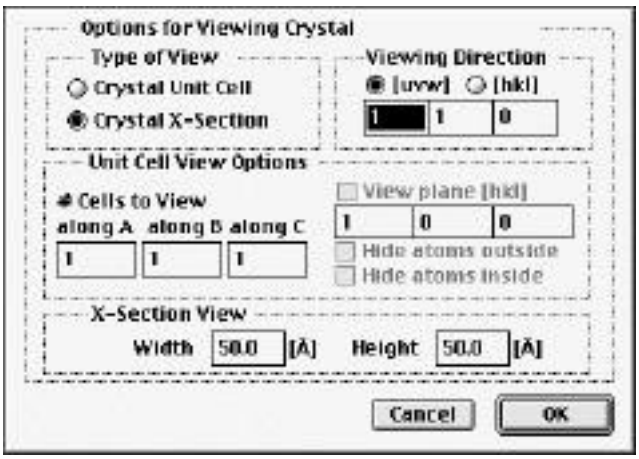
Chapter 7

Example 2. Creating a void in InP

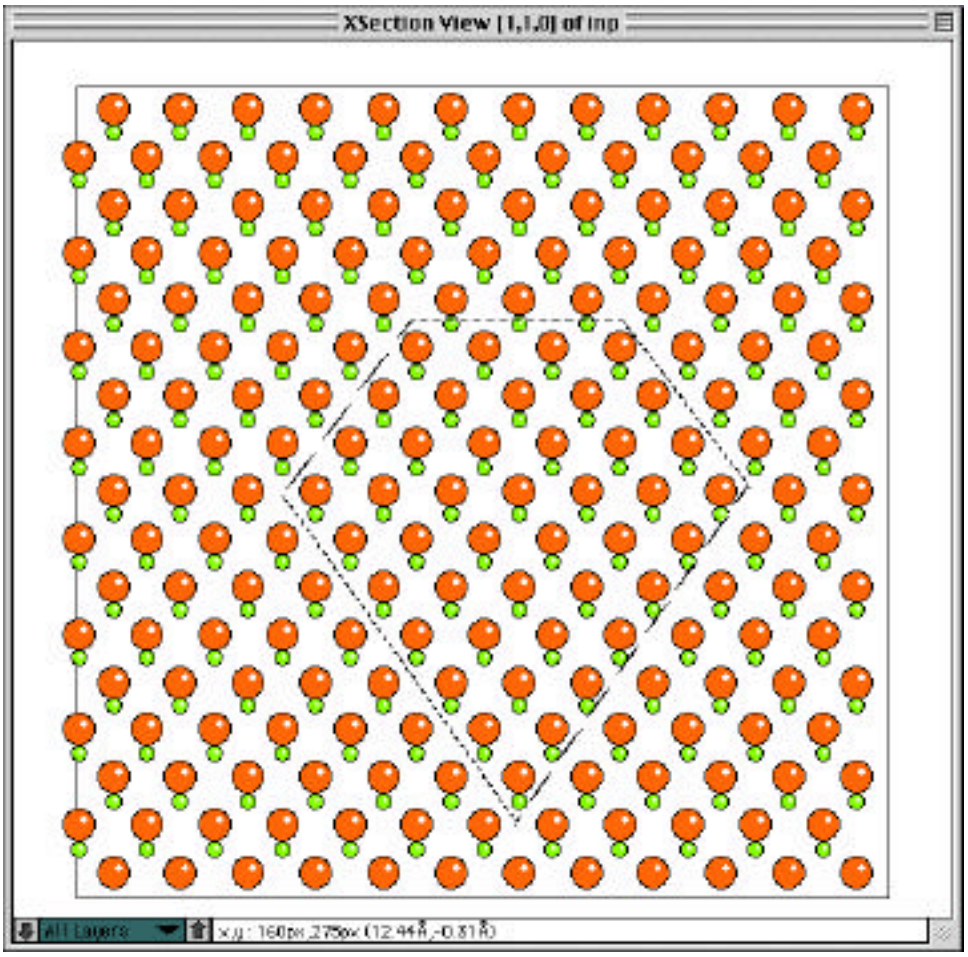
One picture



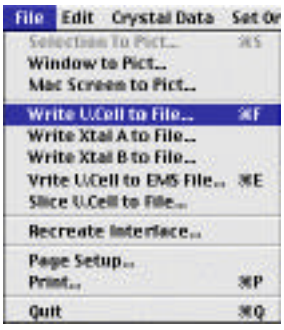
Two picture


Options for Viewing Crystal
Type of View
Crystal Unit Cell
Crystal X-Section
Viewing Direction
[uvw]
[hkl]
1
1
0
Unit Cell View Options
Cells to View
along A along B along C
1
1
1
View plane [hkl]
1
0
0
Hide atoms outside
Hide atoms inside
X-Section View
Width
50.0
[Å]
Height
50.0
[Å]
Cancel
OK

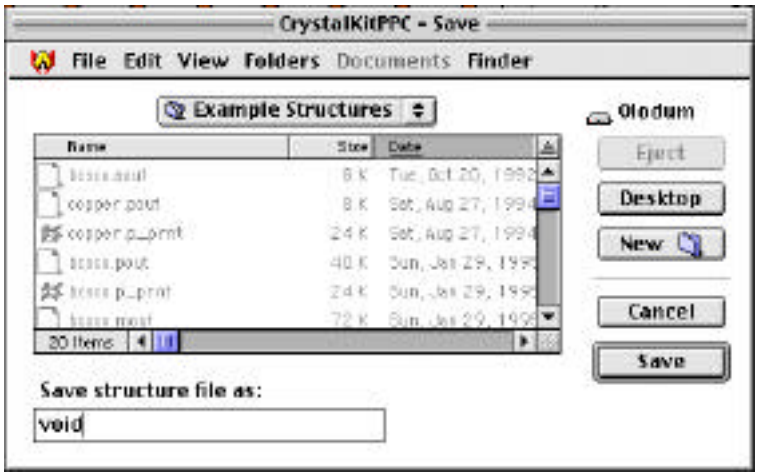
Three picture



Saving

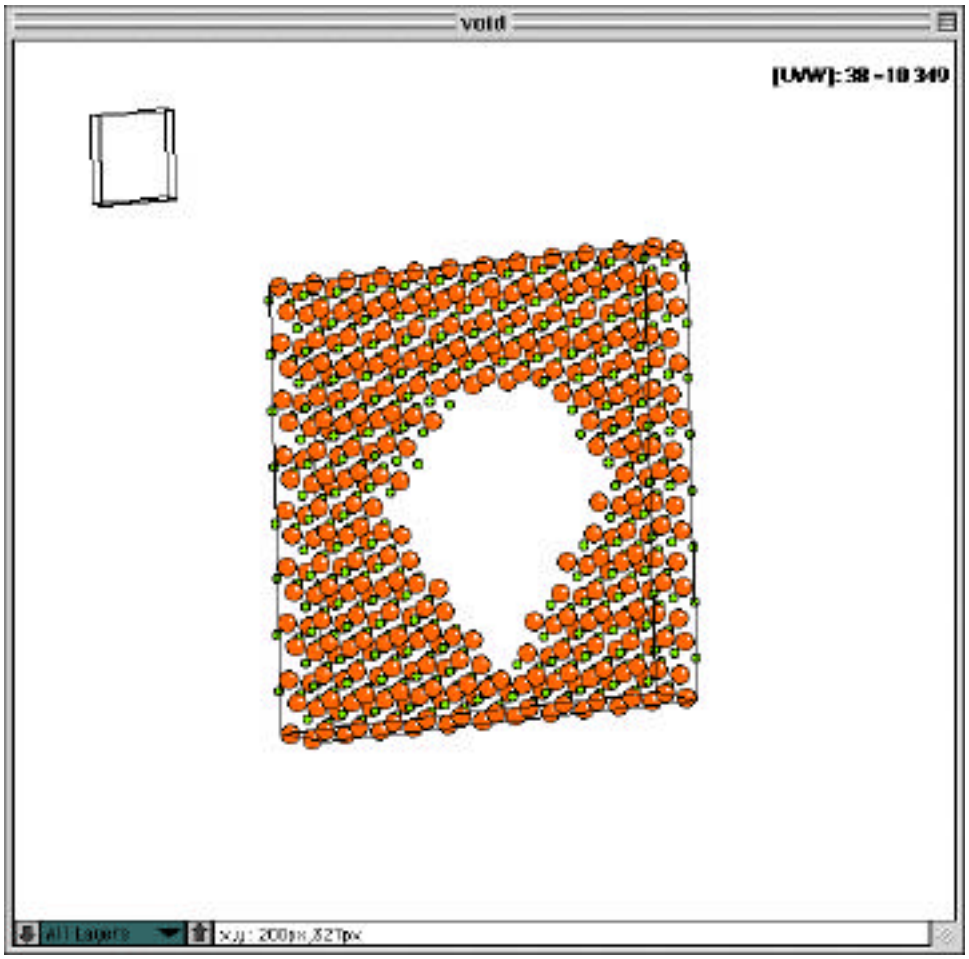


Further save

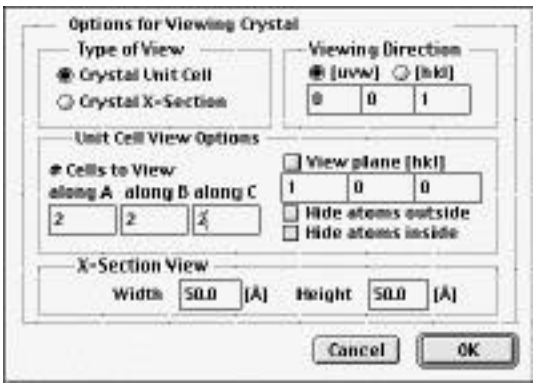


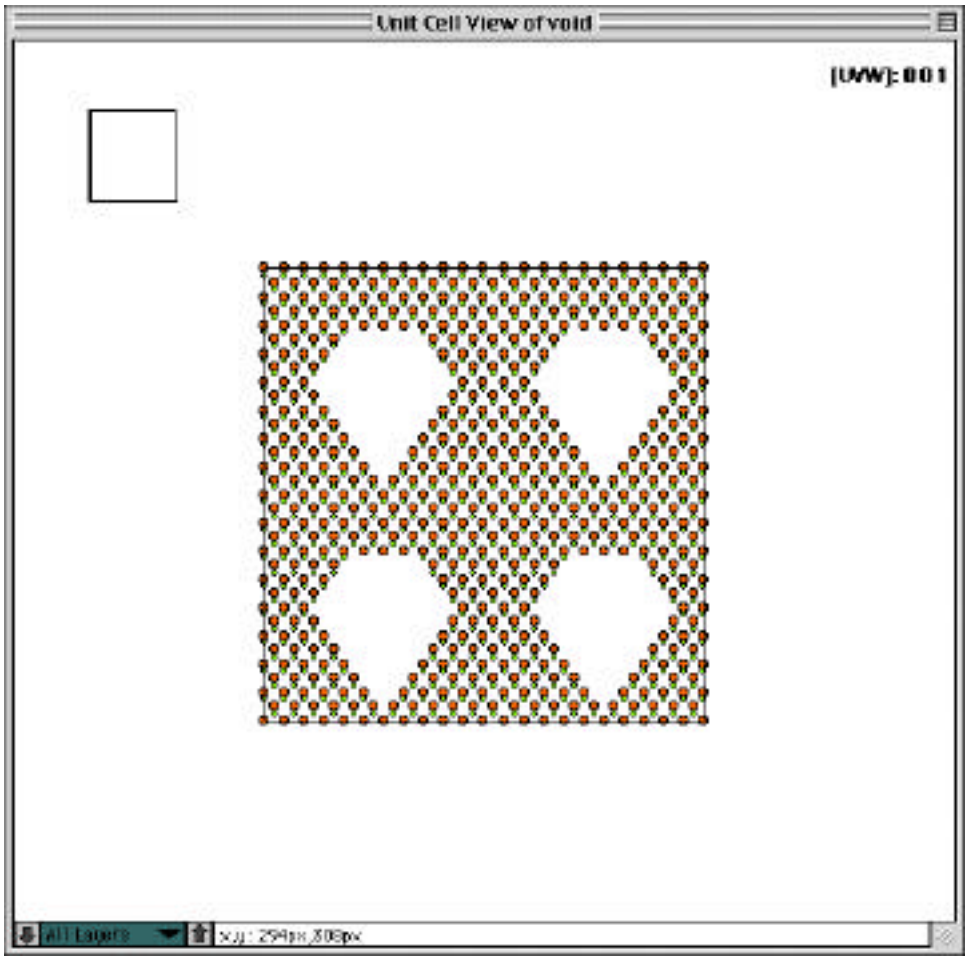
Opening and displaying

Displaying


void
[UVW]: 38 -18 349

Showing more than one unit cell




Unit Cell View of void
[UVW]: 001