CrystalKit User Manual

Total Resolution LLC

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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..

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.

When CrystalKit is run for the first time it will put up its installation screen. Enter your name and affiliation as appropriate together. If you are using a purple USB hardware key, also enter the supplied installation code.

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.

Introduction

CrystalKit is a general purpose program for modelling atomistic defect and interface structures in crystalline material. CrystalKit accepts files created in MacTempas and also outputs files in the MacTempas file format (files with the extension "at"). MacTempas input files (.at) are normal text files which can be read with any text editor. CrystalKit will also read and write files in the CIF (Crystallographic Interchange Format, extension "cif") and files written in the XYZ format (extension "xyz"). The program can also read and write files in the EMS supercell format (extension "ems").

Apart from reading existing crystal files, CrystalKit can also create crystals on its own. Any crystal can be created from a set of atoms belonging to a set of Basis (Motif) atoms, together with a set of symmetry operators belonging to one of the 230 3D space groups. In addition, CrystalKit can readily create such structures as single or many walled Carbon nanotubes, Icosahedral and CubeOctahedral particles.

When creating precipitates or geometric interfaces/grain-boundaries, the program works with two crystalline structures (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 using one of the tools from the tools window and planes are identified in the same way. 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 different types of kinematical diffraction patterns for any given crystal, as well as viewing the reciprocal lattices for the two crystals making up an interface. CrystalKit can also assist in visualizing diffraction patterns in a Matrix/Precipitate (up to 3 precipitates) condition.

There are a number of options and visualization possibilities that are not covered in this user manual. These will probably be added with time. The one thing to keep in mind is that most windows have contex-

tual menus that are shown when Right-Clicking (ControlKey+Click if the Right Click is not available) in the window. Similarly many objects have contextual menus associated with them when they are selected. Thus it is important to keep this in mind as you are using CrystalKit.

CrystalKit Tools

Pointer Tool

Used to select objects and manipulate size of selections. The pointer tool is also used to translate objects. Some translations, such as moving atoms, shifts of grains, etc. are accomplished by using the pointer tool in conjunction with the Option Key. The use of the Option Key changes both the function of the translation tool (pointer) and the rotation tool

Rotate Tool

For rotating crystals, cross-sections, interfaces, diffraction patterns and so on. Some rotations are done while holding down the Option Key. Double clicking in the window will usually reset the view or rotate a crystal to the nearest major zone axis.

Zoom Tool

Used for zooming in/out on objects. Normal zoom is zooming in (enlarging) while holding down the Option key will turn the function into zooming out. Zooming is also performed by using the scroll wheel, track-pad or the scrolling action on the mouse.

Hand Tool

Used for translation of objects

Angle Tool

The angle tool is used for measuring angles between three atoms.

Plane Tool

The plane tool operates differently depending on the type of object that is being displayed. When displaying a single unit cell of crystalline material, clicking on successive atoms will define a plane whose properties such as color and transparency can be independently adjusted. When displaying a cross-section or an interface between two materials, the plane tool is used to inquire about the plane defined by the atoms being

selected.

Move Atom Tool

The "Move Atom Tool" is used to move atoms when displaying cross-sections or interfaces.

Add Atom Tool

The "Add Atom Tool" is used to add atoms to a cross-sections or an interface. When selecting the tool, a periodic table pops up such that the element of the atom to be added can be chosen.

Animate Tool

When clicking the "Animate Tool" in a window showing a crystalline unit cell, cross-section or an interface, the object will start rotating in the window. Default rotation axis is the y-axis ("up" in the plane of the screen). Holding down the Option Key will change the rotation axis to the x-axis ("horizontal" with respect to the plane of the screen), while holding down the Shift Key, changes the rotation axis to the z-axis (towards the viewer, out of the plane of the screen).

Line Tool

The "Line Tool" is used to add lines between atoms, which also can be expanded to appear as cylindrical "surfaces" connecting a group of atoms (molecules). Click in an atom to start the sequence of connected atoms. Click in successive atoms while holding down the Shift key to add atoms to the "chain". When OpenGL is the drawing mode, the contextual menu for the window will add menu items for controlling the appearance of the connected group of atoms. The color of the connecting lines / cylinders is taken from the color of the atoms making up the group.

Box Selection Tool

Creates a 3D box selection that can be modified in 3D by using the Pointer Tool on the various anchor points of the box. When right-clicking on an active selection, a pop-up menu will appear such that further actions can be taken.

Cylinder Selection Tool

Creates a circular (Shift Key down) or an oval cylindrical selection. When right-clicking on an active selection, a pop-up menu will appear such that further actions can be taken.

Ellipsoid Selection Tool

This creates a 3D ellipsoid selection. Holding down the Shift Key will cause the selection to be spherical. Again, right clicking an active selection will bring up a contextual menu.

Polygon Selection Tool

Creates a 3D polygonal selection which can be modified in 3D by using the pointer tool (as with all the types of selections). Right-clicking will as usual bring up a contextual menu. With Pointer tool, Option+Click will add a vertex. Option+Shift+Click in a vertex will remove it. The selection needs to be active.

Ruler Tool

The "Ruler Tool" will measure distances between selected atoms.

Define Unit Cell Tool

The "Define Unit Cell Tool" is used to define a unit cell that can be extracted such that it can be used as a "crystalline unit cell" in simulation and/or modeling. Clicking three points will define in succession, the Origin, the A-Axis, followed by the B-axis. C is towards the viewer. By default, clicks are constrained to atoms. Holding down the Shift Key, will remove the constraint, which can also be done through a menu-command. The use of the Shift Key will cause the axes to be in either the horizontal or the vertical direction.

Define Interface Tool

When an interface is defined between two structures and it is displayed as intersecting lattices, the actual interface can defined by clicking successive points, starting from to the left of the structure and finishing to the right. The points need to be in monotonically increasing distance (x) from the left side.

Delete Atom Tool

By clicking on displayed atoms in a cross-section or interface, atoms can be deleted. If the Option Key is pressed, the entire column being clicked is removed.

Info Tool

When clicking on an atom in any structure, the information belonging to the atom is shown. If the Option Key is held down while clicking the atom, a dialog box is shown such that the information cam be edited.

Picker Tool

The Picker tool is used to quickly change the color associated with an atom type. Clicking in an atom brings up a Color Dialog through which to change the current color of the atom type. For a Crystal Unit Cell, all the atoms of the particular type is changed while for a cross-section or interface, only the color of that particular atom is changed. Use "Edit Site Properties" to have more control of the display properties of the atoms.

CrystalKit Menus

File Menu

New
Open...   ⌘O
Open Recent   ▶

Close   ⌘W
Save
Save As...
Save As CIF File...
Save As XYZ File...

Save Window As Image...

Revert to Saved

Print...   ⌘P

New (Command+N)

Creates a new crystal structure based on a simple template. The template unit cell is a cubic structure with a single Copper atom (Cu) in the corner of the unit cell. The unit cell lengths are all 4.0 Å, There is one symmetry operator, namely the identity operator x,y,z.

In order to create the desired structure, one needs to specify the correct spacegroup (if it is known) and replace the single copper atom with the desired atoms in the basis of the unit cell.

The total number of atoms in the unit cell is given by operating the symmetry operators on the atoms in the basis. Thus specifying the number of atoms in the basis (referred interchangeably to as the Motif) and the spacegroup is generally much more efficient than specifying all the atoms in the unit cell.

Open... (Command + O)

This will open the standard "Open Dialog" and prompt for the structure to be opened. CrystalKit will recognize the standard structure file format used in MacTempas, the CIF file format and files in the XYZ format.

Open Recent

CrystalKit will remember the last 5 structures that were opened and place these in the Open Recent menu for quick access.

Close (Command + W)

Closes the foremost front window.

Save (Command + S)

If the file associated with the front structure window, the file will be rewritten with the updated information.

Save As...(Command + Shift + S)
Save As CIF File
Save As XYZ File

These commands are used to save the structure file in one of the specified formats.

Save Window As Image...

Use this command to create an image of the front window in the .png format.

Revert to Saved

If the front most window is associated with a structure that has been modified, "Revert to Saved" will restore the information in the structure by reading it back from the file saved on disk,

Print... (Command + P)

Prints (draws) the content of front window

Edit Menu

Undo Last Annotation	⌘Z
Redo	⇧⌘Z
Cut	⌘X
Paste	⌘V
Copy Crystal	⌘C
Delete	
Duplicate Crystal	⌘D
Cut Atoms inside of Selection	⌥⌘X
Copy Atoms	⌥⌘C
Paste Atoms	⌥⌘V
Create A Precipitate	
Create B Precipitate	
Load Background Image	
Remove Background Image	
Scale Background Image to model/calculation	
Deselect All Atoms	
Select All	⌘A

The function of each of the menuitems in the Edit Menu will be clarified later as it is easier to show their use through some examples. Some of the functionality is fairly self-evident such as the Copy and Paste commands. The Copy command generally is used to make a copy of the object in the front most window. The Paste command will most of the time create a new instance of the object in a new window of the same type. Thus the Paste command will at times function as a "Paste New" command while at other times function as a Paste Into command depending on the type of window (window object) that is the front most window. Some commands such as "Create A/B Precipitate" only have meaning when the front window is an "Interface" window. Similarly commands relating to a Background Image, only are valid for certain types of windows.

View Menu

Real Lattice
Reciprocal Lattice
✓ Real / Reciprocal Lattice

Reciprocal Lattice Options...

Show Grid   ⇧⌘G
Edit Grid
Show Guides   ⌘G

Remove Annotations

The first three commands relate to the type of view for a "Crystal Window", a "Cross-Section Window" and an "Interface Window". "Real Lattice" refers to a view of the atoms in the structure while "Reciprocal Lattice" refers to depicting the reciprocal lattice points with relative size of each point, mimicking what one expects to see in a Diffraction Pattern". Selecting "Real / Reciprocal Lattice" results in showing both the atom positions in the structure and the simulated "Diffraction pattern" (Reciprocal Lattice) overlaid on the atom positions.
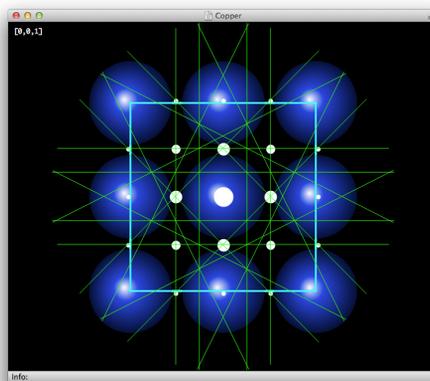
When the Reciprocal Lattice is drawn, the menu command to specify the "Reciprocal Lattice Options..." is active. This would bring up the following dialog box.
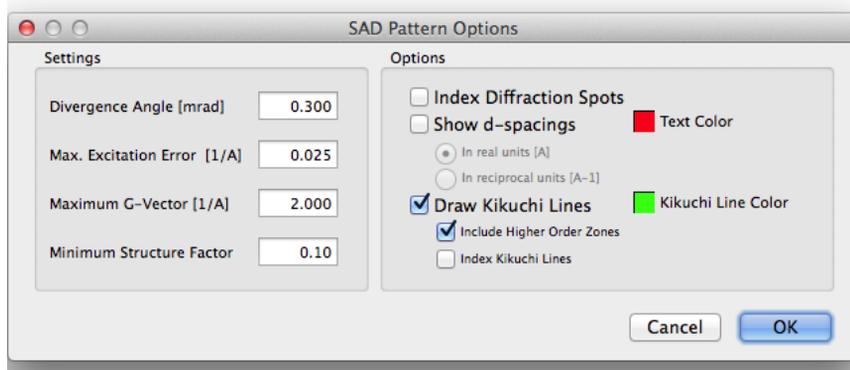
The Grid and Guides options are only active for a Cross-Section and an Interface Window. "Remove Annotations" is active when an annotation has been placed in the window, such as a Distance Measurement (Ruler), an Angle Measurement or a different type of an annotation.

Commands Menu

The Commands Menu contains the following entries:
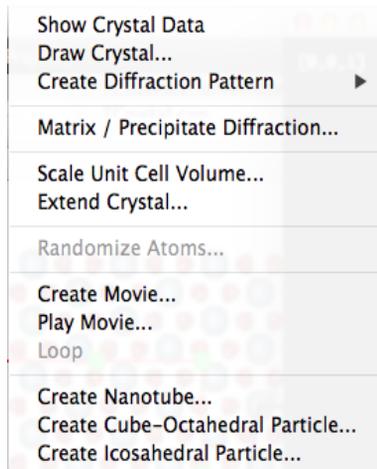
Show Crystal Data

This command brings up the data associated with the crystalline structure displayed in the front most window. From the following Dialog the structure can be edited if needed.

Show Crystal Data
Draw Crystal...
Create Diffraction Pattern ▶

Matrix / Precipitate Diffraction...

Scale Unit Cell Volume...
Extend Crystal...

Randomize Atoms...

Create Movie...
Play Movie...
Loop

Create Nanotube...
Create Cube–Octahedral Particle...
Create Icosahedral Particle...

Crystal Data

Spacegroup # 123   Tetragonal... ↕

Lattice Parameters

Unit Cell Axis A [A] 3.9000   Alpha [°] 90.00
Unit Cell Axis B [A] 3.9000   Beta [°] 90.00
Unit Cell Axis C [A] 4.1000   Gamma [°] 90.00

Number of Atoms in the Basis: 4
Number of Atoms in the Unit Cell: 5
Number of Symmetry Operators: 16

Basis...   Symmetry Operators...   Atoms...

Cancel   OK

Using the "Crystal Data" Dialog, the basis, spacegroup (symmetry operators) and lattice parameters are all easily modified.

Draw Crystal...

is used to display the crystal structure from a given direction, drawing a specified number of unit cells in the three directions.

The Display Dialog looks like:
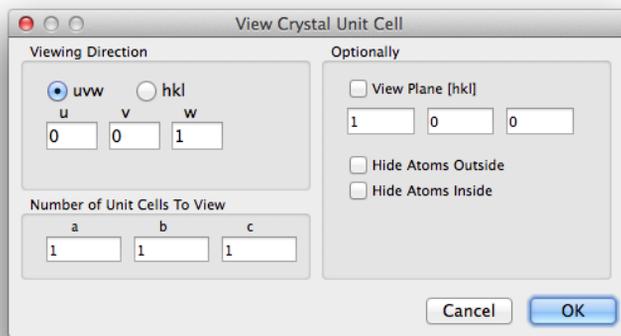
Optionally a crystallographic plane can be drawn and atoms on either side of the plane can be drawn or not. The color and transparency of the plane can be adjusted from the Display Option Menu or the equivalent Contextual Menu displayed by Right-Clicking (or Control+Click) the mouse in the active Crystal Window.
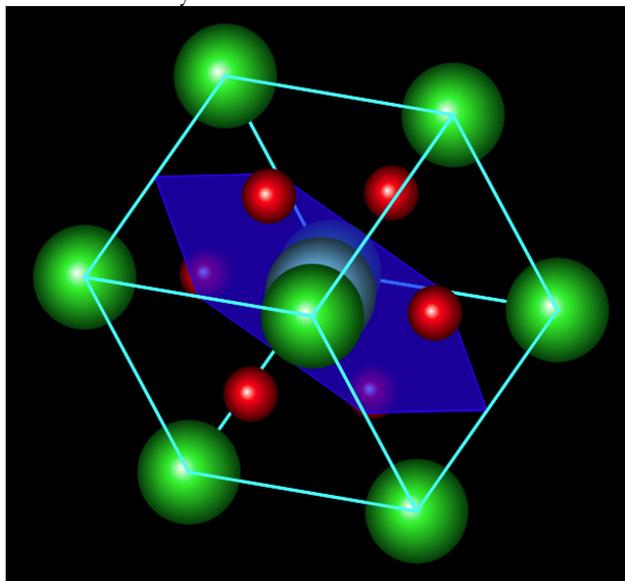
The Hierarchical Menu "Create Diffraction Pattern" gives access to the three menus for creating three different types of kinematical diffraction patterns

Create Diffraction Pattern ▶	Kinematical SAD Pattern...
Matrix / Precipitate Diffraction...	Powder Diffraction Pattern...
	Kinematical CBED Pattern...
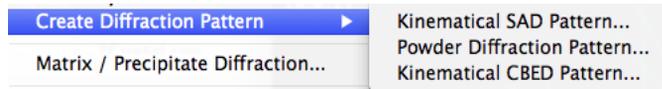
Examples of the patterns are:

Kinematical Selected Area Diffraction (SAD) Pattern
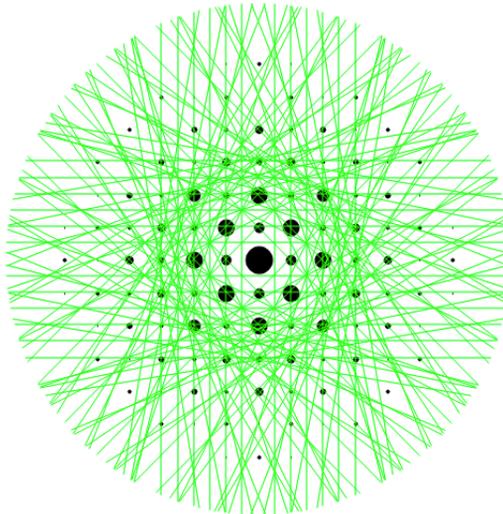
Powder Diffraction Pattern:
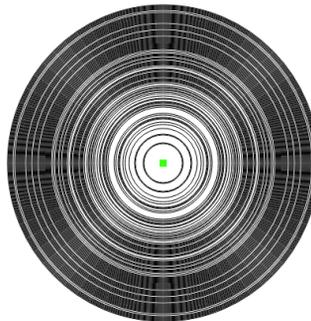
Kinematical Convergent Beam Electron Diffraction (CBED) Pattern:
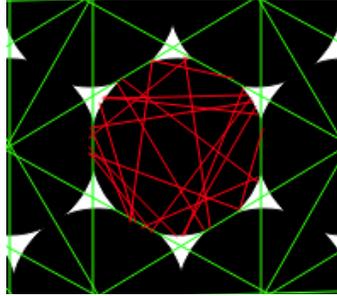
Each pattern has its own Create Pattern Dialog with a number of options relevant for the pattern. Control-Clicking (Right-Click) in the pattern will also bring up an option to edit the pattern after it is created such that the adjustable parameters can be modified.

Dragging the outer radius (pointer tool)of the central spot will change the size of all diffraction spots. Dragging one of the other diffraction spots will change the camera length.

Matrix / Precipitate Diffraction...

Allows you to define the orientation relationship between a matrix and a precipitate, up to 3 precipitates. The resulting window gives the diffraction pattern relationships for the precipitate(s) with respect to the matrix..
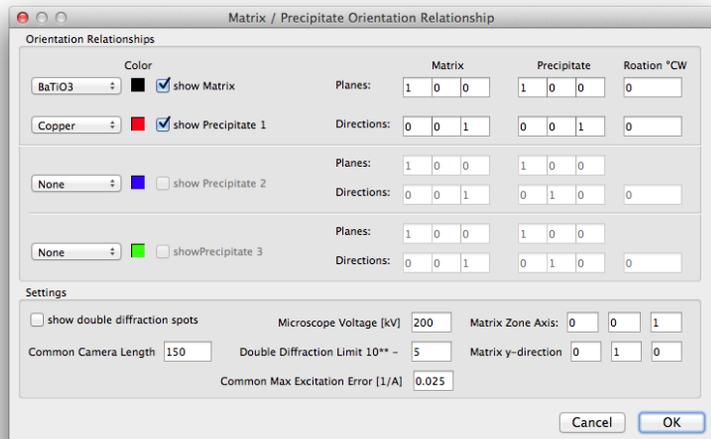
Resulting Matrix / Precipitate Diffraction Pattern Relationship Window:
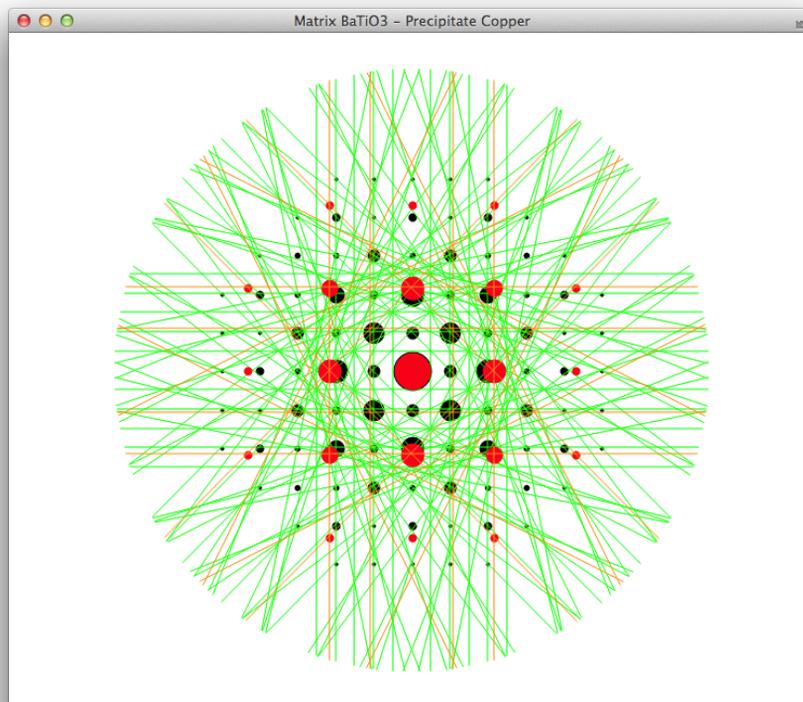
Randomize Atoms...

is used to randomize (create pseudo-amorphous) atoms within the entire field of view or within the selection if there is one. This action only works when displaying a cross-section of a material or an interface between crystals.

Create Movie...
Play Movie...

The Create Movie Command is active when displaying a single crystalline structure, a cross-section of a crystal or an interface. The only input

parameter is the axis of rotation.
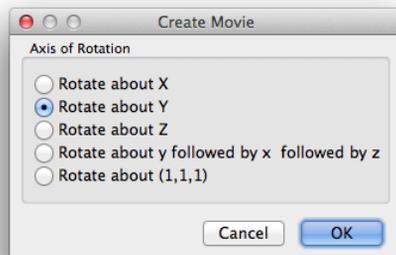
The output is a mpeg movie which can be played back via the "Play Movie... command.

Create Nanotube...

Create Cube-Octahedral Particle...

Create Icosahedral Particle...

are three commands for quickly creating the structures the names clearly are referring to.

The three actions are described later under "Creating Other Predefined Structures" in the chapter *Using CrystalKit*.
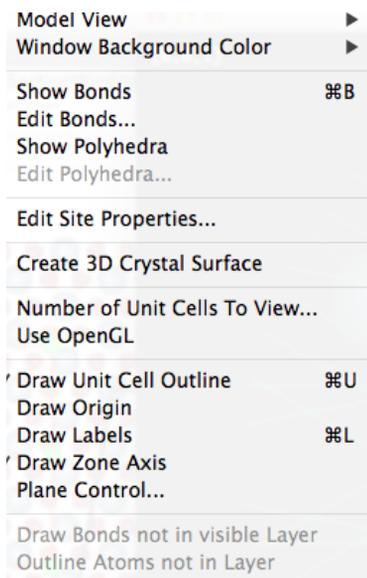
Display Options Menu

The Display Options Menu is the main menu for controlling the appearance of the crystalline structures.

The first two entries are hierarchical menus, with the first of the two being.
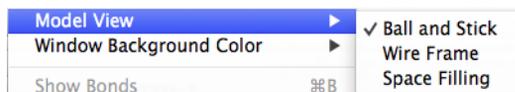
The Ball and Stick is the default view of the display of the structure. Atoms are drawn with a scale of half of the atomic radius. The Wire Frame options show the structure with "rods" drawn between atoms as in the figure below.
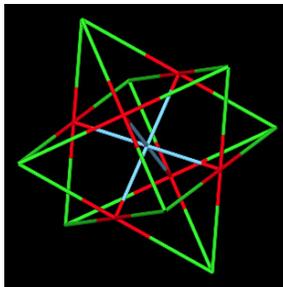
Space Filling draws the atom large enough to fill the space between them.

Window Background Color gives the user the choice of the window background color.

Most of the menuitems in the Display Options Menu are self-evident with respect to their meaning.

Show Bonds

Edit Bonds...

control the display of atomic bonds. The first turns the display of bonds on or off, while the second gives more control over which bonds are being drawn.

The following shows the structure Fe3O4 being drawn with bonds and the option Use OpenGL checked.
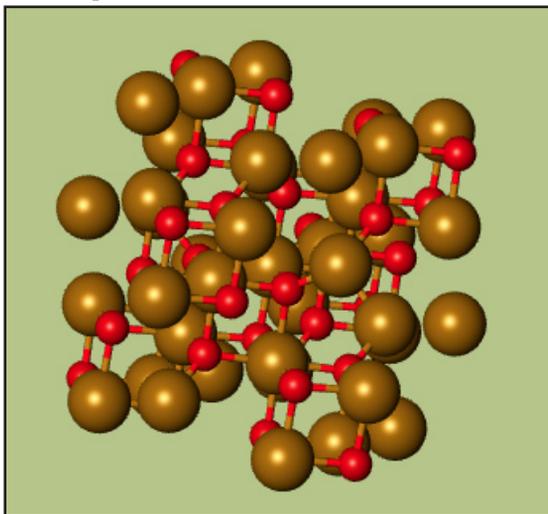
The **Edit Bonds**. menu item brings up the following dialog which gives further control over the drawing of the bonds.
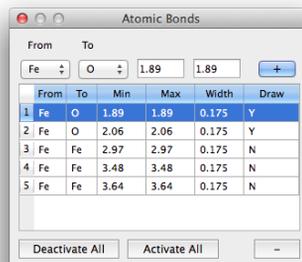
Show Polyhedra

Edit Polyhedra...

Show Polyhedra will attempt to locate atoms forming the center of polyhedra and if successful draw these.
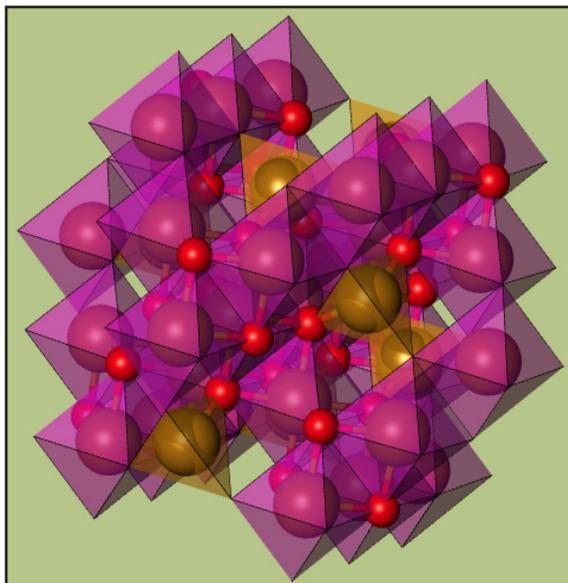
Edit Polyhedra will let you tailor the appearance of the polyhedra to your liking. Besides specifying which polyhedra to draw, the color of
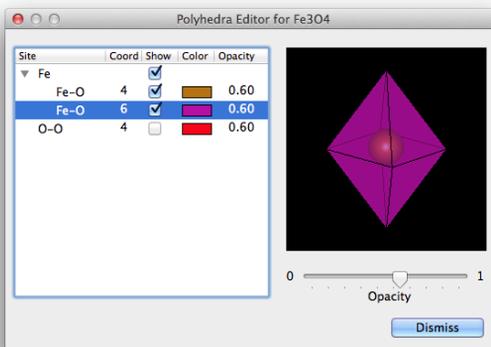
each type of polyhedra and its transparency can be set.

Edit Site Properties...

will bring up the following window which allow further control over which atoms are drawn and their appearance.
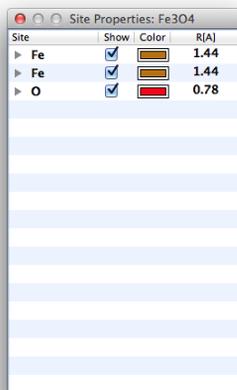
Create 3D Crystal Surface...

This command will attempt to draw a surface around a particle or some structure with a specified 3D extent. An example of this is illustrated for the following crystal structure.
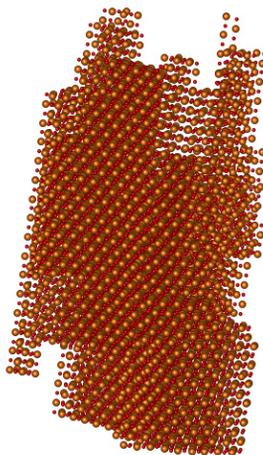
Selecting "Create 3D Crystal Surface..." menu item will bring up the

following dialog
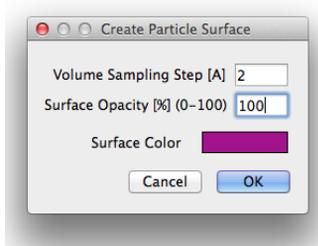
which in turn produces the following surface
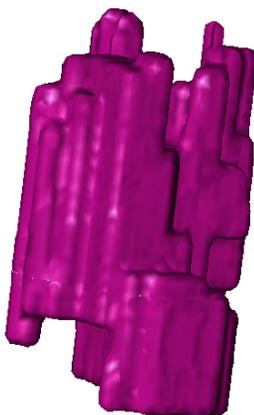
Right-clicking in the window brings up a contextual menu with additional options
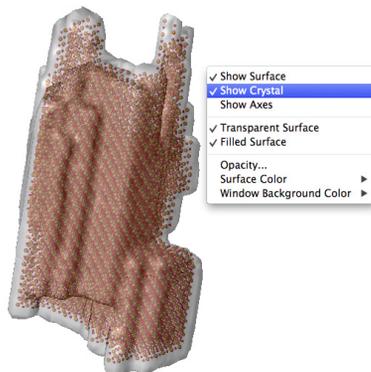
Number of Unit Cells to View...

brings up a dialog such that the number of unit cells in the a, b, and c directions can be set.
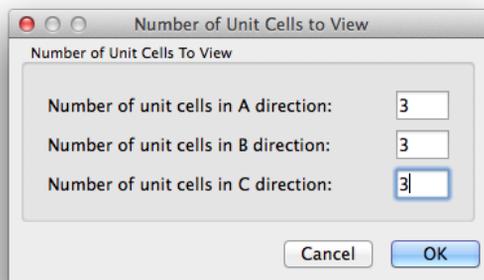
3 x 3 x 3 unit cells of BaTiO3
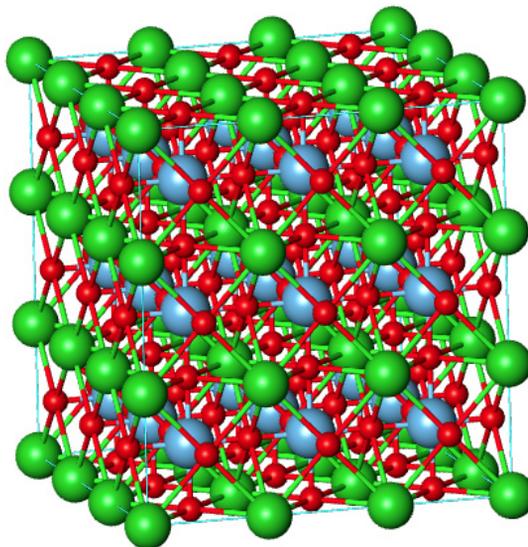
Use OpenGL

Normally all the models are drawn not using OpenGL, but rather the native 2D graphics routines. Switching to Open GL will allow for improved 3D rendering of the structures. Open GL is only active

for Crystal windows and not Cross-Section and Interface Windows. There are some differences in what can be drawn while using OpenGL compared to not. It is hoped that everything drawn will eventually be available in the using OpenGL mode.

Example drawing with/without OpenGL
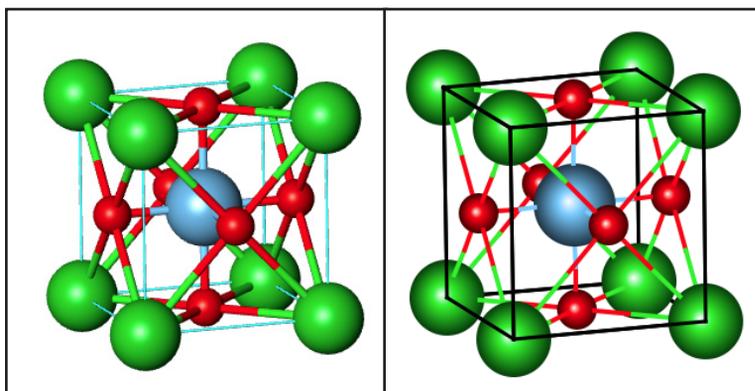
Draw Unit Cell Outline
Draw Origin
Draw Labels
Draw Zone Axis

are fairly self evident to their meaning. The first two are relevant when drawing a crystalline unit cell and turn on and off the drawing of the outline of the unit cell (the boundary of the volume defined for the unit cell) and the origin of the unit cell, the origin and the three axes **a, b** and **c** which define the crystalline unit cell.

Draw Labels turn on/off the drawing of the chemical symbol on each of atom.

Draw Zone Axis turns on/off the drawing of the current zone axes when drawing a crystal unit cell.

Plane Control...

It is possible to draw a crystalline plane when drawing a crystal unit cell. The plane is specified by its indices [hkl] and the plane can be

drawn with a specified color and transparency. Selecting **Plane Control** brings up the following window
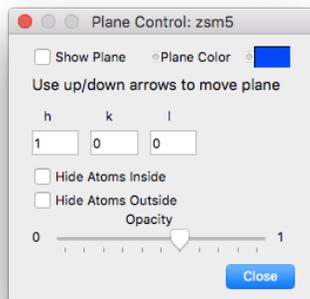
In addition to controlling the appearance of the plane it is possible to hide atoms above or below the plane.
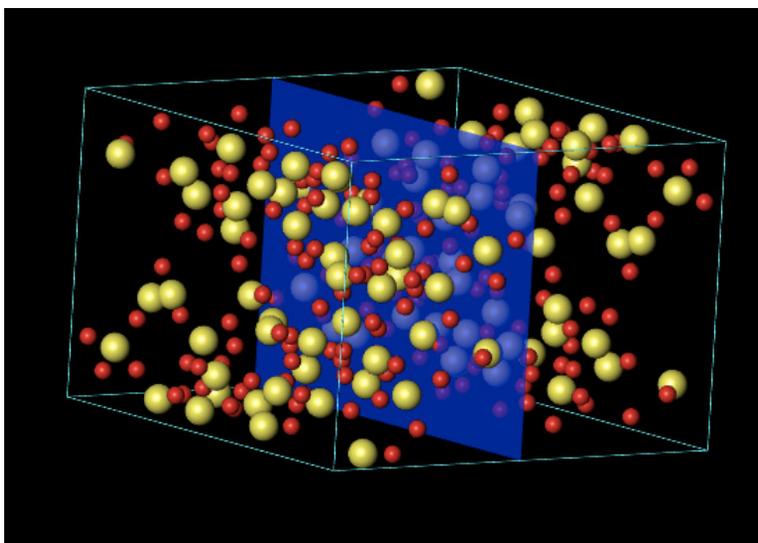
The plane itself can be moved up or down by using the up/down arrow keys..

The last two entries are only relevant when drawing cross-sections or interfaces and they will be described when covering cross sections and interfaces.

CrossSection/Interface Menu

New Cross Section

New Cross Section when activated with a Crystal Front Window will bring up the following Dialog for creating a cross section of the crystal perpendicular to a specified zone axis and of a specified extent.
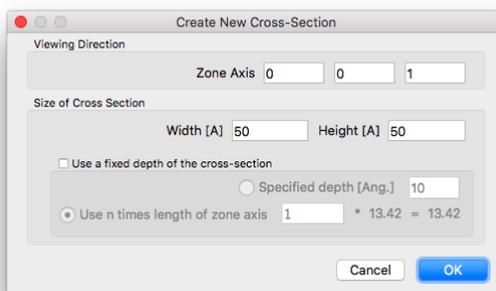
The depth of the cross-section will be the repeat distance in the viewing direction unless specified differently ("Use a fixed depth.." checkbox).

The following is a Cross-Section window (different from a Crystal Window) showing a section of Zeolite (Zsm5) in the [010] direction.
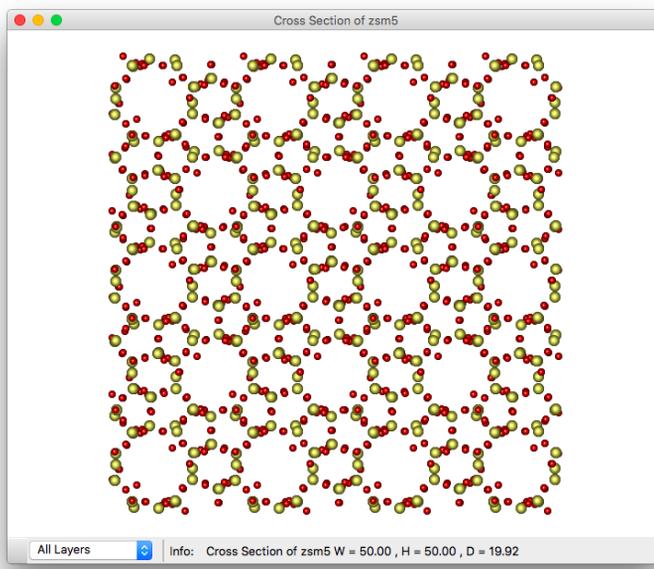
The CrossSection Window has a different appearance from the normal Crystal Window. It has a popup menu which lets you control which layer (depth-wise) that is being displayed. The appearance of the atoms not in the active layer depends on the setting "**Outline Atoms Not In Layer**" menu item in the **Display Options Menu.** OpenGL drawing is not available for Cross Sections and Interfaces.

Similarly, the drawing of bonds when displaying an active layer depends on the setting of the menu item "**Draw Bonds Not in Visible Layer**" in the **Display Options Menu.**
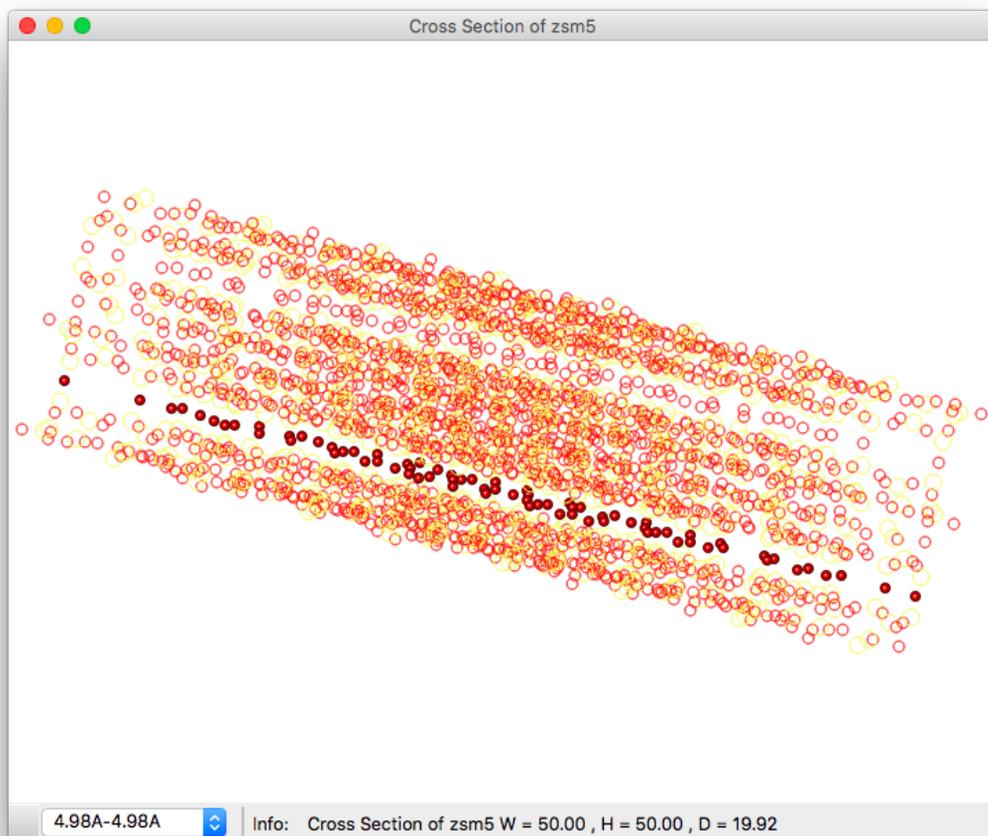
Apart from choosing which layer to display (unless all are shown) from the popup menu , one can move the active plane up/down by using the Up/Down Arrow Keys. The window has a contextual menu which is

accessible via Right-Clicking (Control+Click) in the active part of the window. The contextual menu is the following.

Edit.. allows modification of the cross section after its creation.
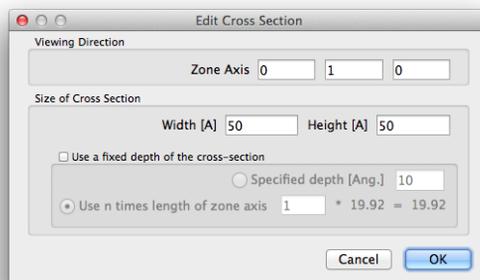
Model View brings up while **View Options** brings up

If the View is "**View Reciprocal Lattice**" the "**Edit...**" menu item changes to "**Edit Reciprocal Lattice Parameters...**"
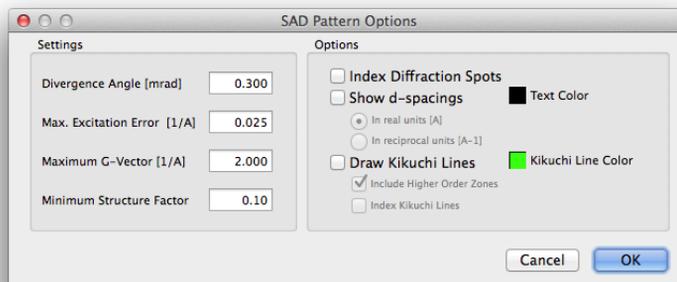
The Reciprocal Lattice Display corresponds to the zone axis orientation

of the Cross Section as defined at the time of creation. Hence the pattern will not change as the cross section is being rotated.
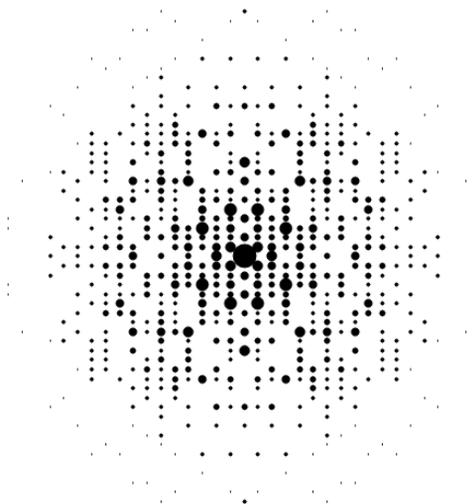
As with the two other windows that show atomic models (Crystal-Window and Interface-Window), the CrossSection-Window lets the use of Option+RightArrow/LeftArrow control the relative size of the atoms. Basically all atoms are drawn using a scaling factor times the atom radius and the key combination Option+RightArrow/LeftArrow changes the scaling factor.
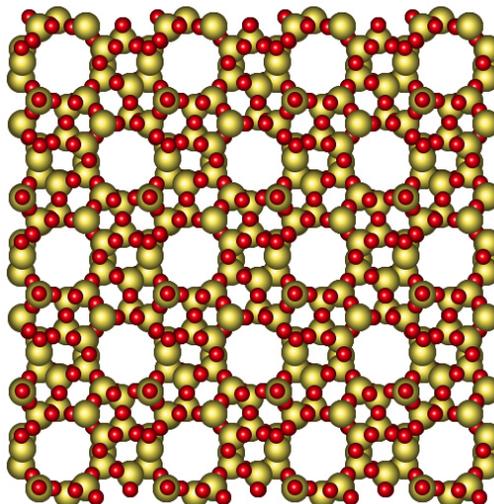
When rotation the Cross-Section the view can always be reset to the initial view by Double-Clicking in the window with the Rotate Tool being the active tool

New Interface...

With one Crystal Window being displayed the menu item "New Interface..." will be active.

An interface is defined by specifying the orientation relationship between two crystals. The two crystals can be the same crystal.

Selecting the "New Interface..." menu item brings up the following Dialog
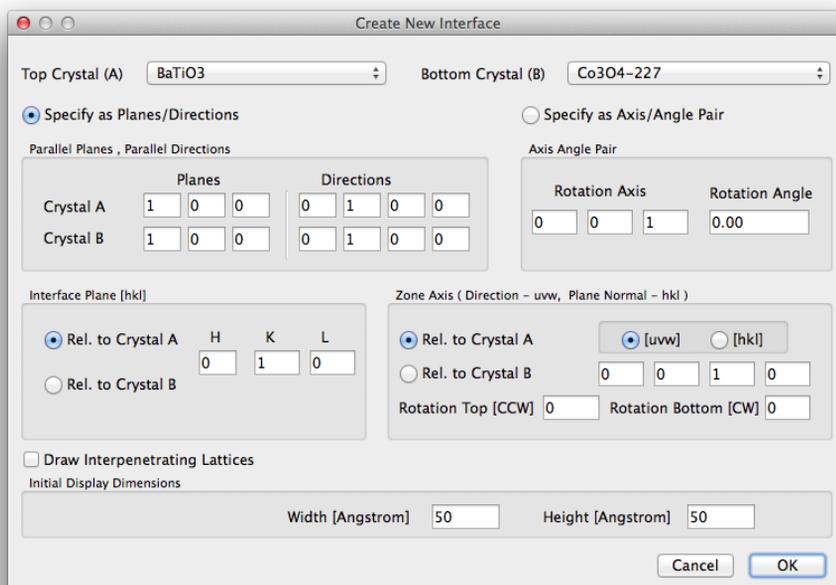
This Dialog contains all the required entries needed to specify a geometric interface between two crystals. In addition to defining the Orientation Relationship between the two crystals, it is necessary to define the interface plane and the zone axis (the electron beam direction). Either of these can be specified relative to either Crystal A or Crystal B. A and B just denote the two crystals.

Finally the extent of the interface must be set. It is important to note

that whichever extent is given, the unit cell containing the interface will represent a periodic structure in both X and Y if it is used in a simulation of a HRTEM image. It is likely that in most situation the real interface will not be periodic in X unless there is a commensurate repeat for both crystals in the X direction. Likewise the structure will "become" periodic in the Y-direction as well.
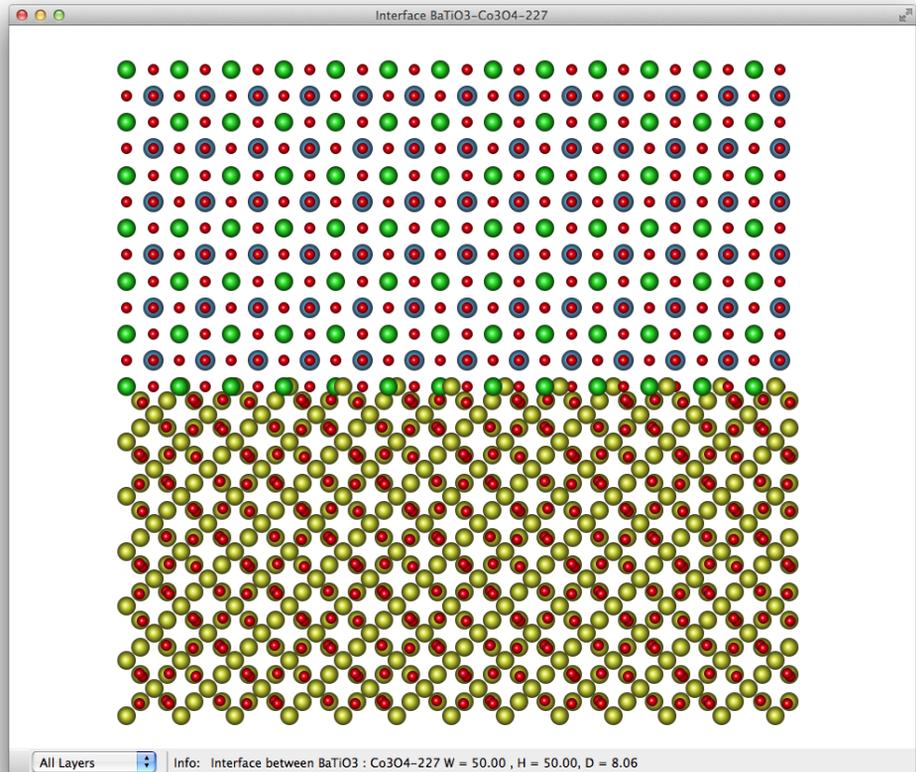

The Pointer Tool and the Rotate Tool serve a dual purpose. Used as is, the Pointer Tool will translate the interface in the window. Likewise, the Rotate Tool will rotate the view of the Interface so that it can be displayed from arbitrary directions.

IMPORTANT:

*Used with the Option Key down, the **Pointer Tool** will translate one of the grains relative to the other in any of the 3 directions. The mouse will need to be down in one of the grains and when dragged in any direction, the grain will shift relative to the other. Holding down the Shift Key will constrain the direction to the initial direction of the drag. In order to shift the grains in the Z-direction, the direction of the Zone Axis, it is necessary to rotate the whole interface such that it is viewed from the side. Dragging with the Option Key down will then move the grain in the Z-Direction.*

*Likewise with the Option Key down, the **Rotate Tool** will rotate either of the grain relative to the other grain. The rotation is around the Zone Axis. If the view is such that the Reciprocal Lattices are shown as well, the patterns will rotate together with the real lattices. The drag can be initiated by clicking down in either an atom belonging to a grain or one of the diffraction spots of the grain.*
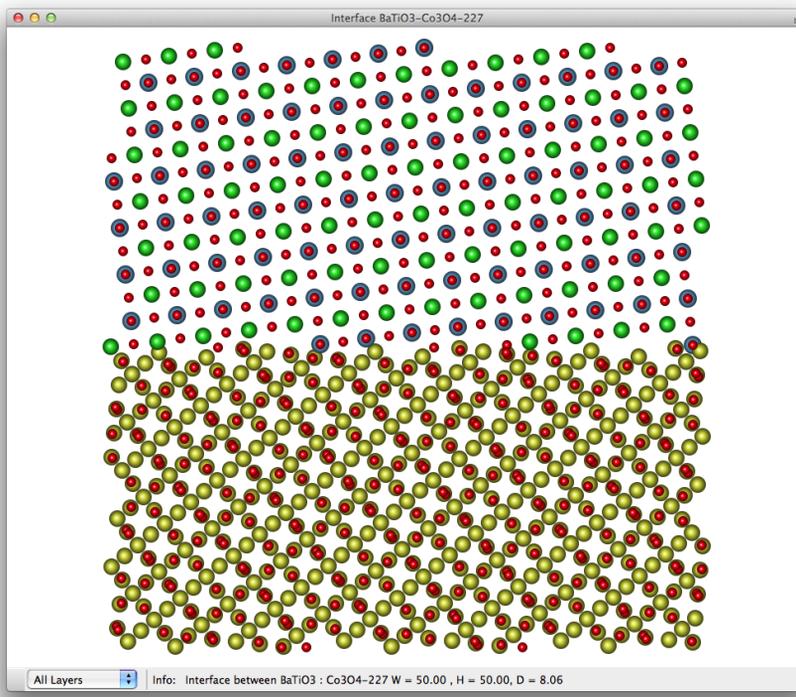
Using CrystalKit

Creating a new structure

Creating a new crystalline structure is normally done by invoking "New…" from the "File" menu. This opens a simple structure with lattice parameters a = b = c = 4.0 Å, alpha = beta = gamma = 90 Degrees, spacegroup = 1 and one Copper atom in the corner of the unit cell. At the same time the dialog box for changing the structure is shown.
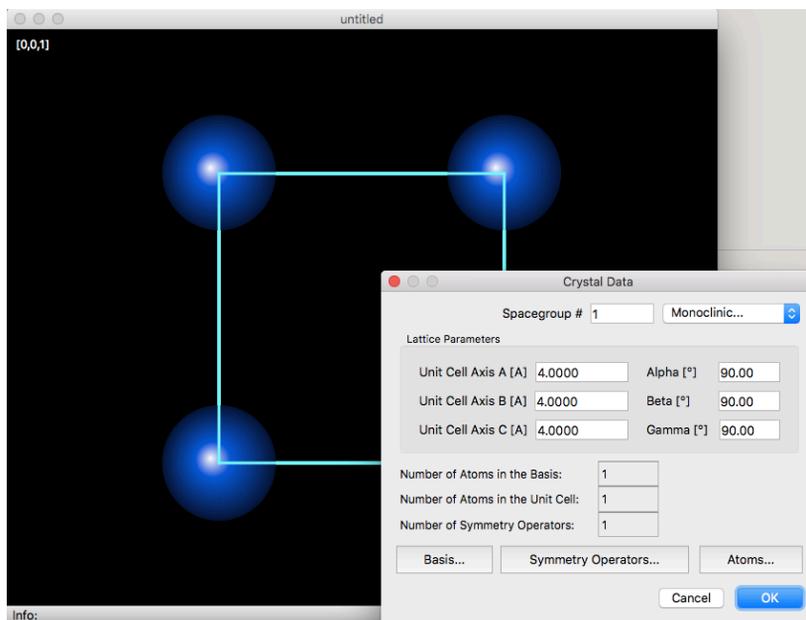
In order to understand how the structure is built up, one has to know the following:

The atoms start with a Motif. From here on the word Motif and Basis will be used interchangeably. The Motif can consist of anything from one atom to all the atoms in the structure.

The atoms in the Motif is entered through adding or modifying existing ones in the Basis Dialog. When creating a new structure, the motif

always has a single atom in the corner of the unit cell.

Basis Dialog...
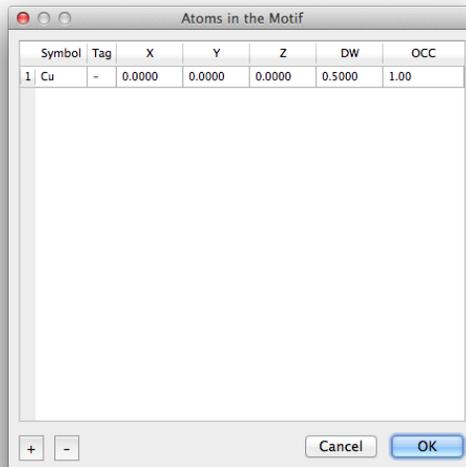
In addition to the atoms in the Motif, the crystal is associated with a set of symmetry operators. The atoms in the unit cell is created by having all the symmetry operators operate on the atoms in the Motif. By default the structure created by invoking "New..." has a single symmetry operator, the identity operator. The identity operator is "x,y,z", meaning that an atom in the Motif at the position (x1,y1,z1) will result in an atom in the unit cell at the same position (x1,y1,z1). Two symmetry operators x,y,z and x+1/2,y+1/2,z+1/2 together with an atom in the Motif at position (x1,y1,z1), will result in two atoms in the unit cell, one at (x1,y1,z1) and the other at (x1+1/2,y1+1/2,z1+1/2). The other thing to remember is that all the atom positions at this point are relative, meaning they are fractions of the unit cell vectors. The unit cell axes are the three vectors **a**, **b**, **c**. An atom at (0.5,0.5,0.5) is positioned at 0.5**a** + 0.5**b** + 0.5**c.**

If the symmetry operators consist of a single operator, then all the atoms in the unit cell will need to be specified in the Basis (Motif).

The atoms in a "perfect" crystalline structure is then defined by the

Basis and the symmetry operators. The symmetry operators are given by the Spacegroup, meaning the Symmetry of the atoms in the unit cell.

If one knows the Spacegroup of the structure, one chooses the correct one from the drop down menu in the Dialog Box.
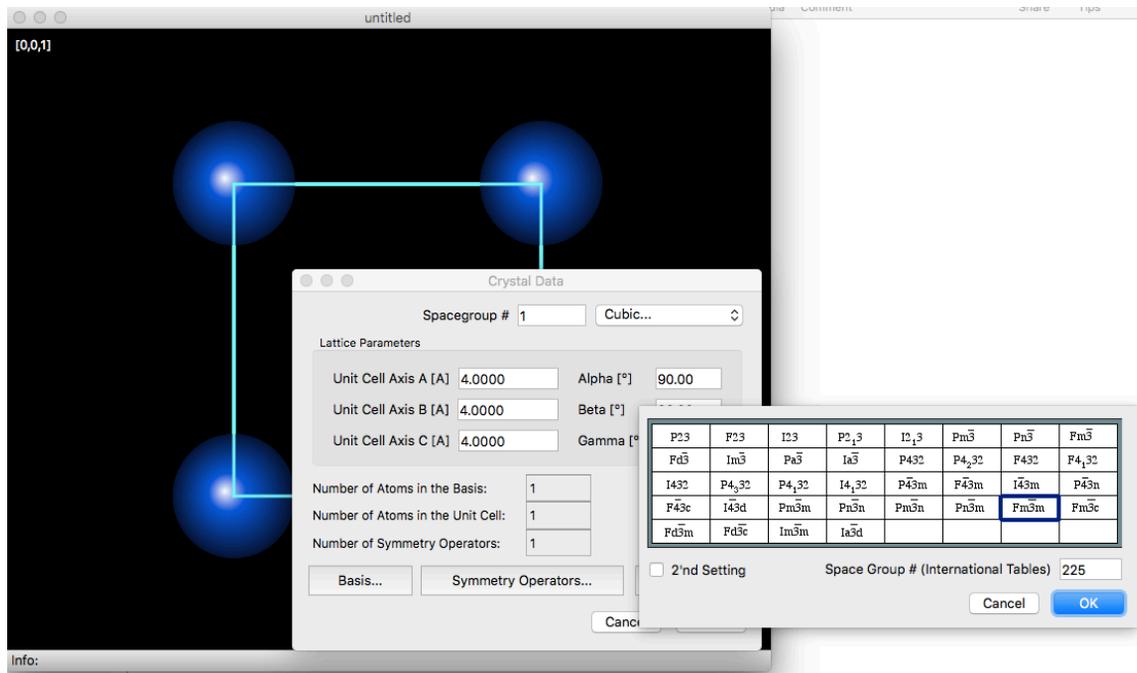
In this example the spacegroup corresponds to Face-Centered Cubic structure. The number of symmetry operators is 192.

While the number of symmetry operators is 192, many of the operators reproduce (transforms into) the same atom. Thus the total number of atoms in the unit cell is 4, total one of atom in the corner of the cell and total of one atom on each of the faces $x = 0$, $y = 0$ and $z = 0$. When one draws the unit cell one is tempted to conclude that there are 8 corner atoms, one for each of the 8 corners. However one can make the statement that the atom in the corner $(0,0,0)$ is the only corner atom, the others being equivalent atoms or that each corner atom has only 1/8th of the volume inside the unit cell. Likewise a face atom has 1/2 of the atom inside the unit cell, such that the 2 atoms at opposing faces make up a total of 1 atom, and not 2.

The final thing left to do to make the structure into FCC Copper is to change the lattice constant a to 3.6147Å.

The Symmetry Operators are shown in the "Symmetry Operators." Dialog under the "Crystal Data" Dialog which is also accessible through the "Show Crystal Data" menu item in the Commands Menu.

The Symmetry Operators for Spacegroup # 235 are shown here.
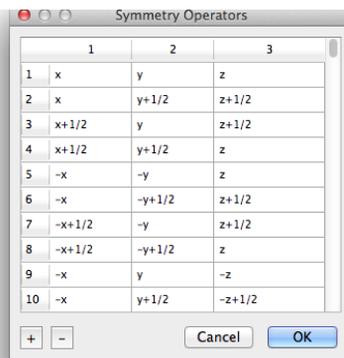
The total number of atoms in the unit cell which comes from applying the 192 symmetry operators on the single Copper atom in the corner of the unit cell is shown in the "Atoms" Dialog.
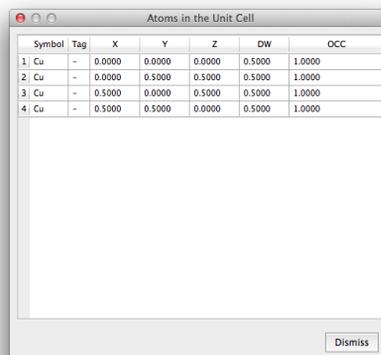
Creating other predefined structures

CrystalKit can also easily create the following structures
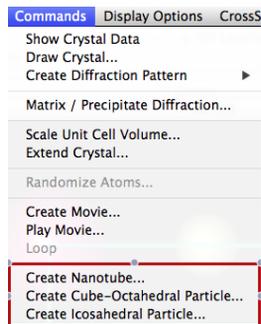
Carbon Nanotube

A Carbon nanotube is defined by its diameter and chirality, its Chiral Vector (n,m). As the tube needs to close properly and repeat without any discontinuity, the values are essentially quantized. Any set of (n,m) will determine the diameter of the tube and the Chiral Angle. Likewise the repeating length of the tube is given for a given set (n,m). In addition to creating a single walled carbon nanotube, CrystalKit can also create a many-walled tube, walls with the same chirality. When specifying additional walls, it is necessary to specify the wall separation, the translation between the "start" of the walls and a relative rotation between the walls.
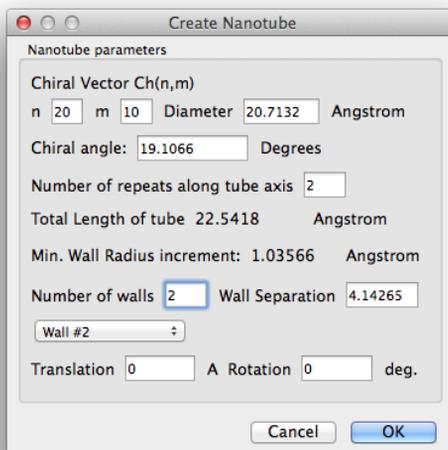
The parameters entered in the Carbon Nanotube creation Dialog gives the following structure.
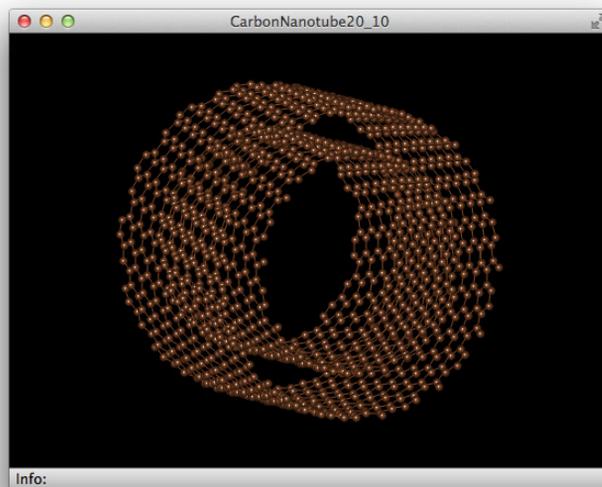
Cube-Octahedral Particle

The geometry of a Cube-Octahedral particle is specified entirely by the number of shells and the bond length between the atoms. Hence all the information needed is contained in the following dialog
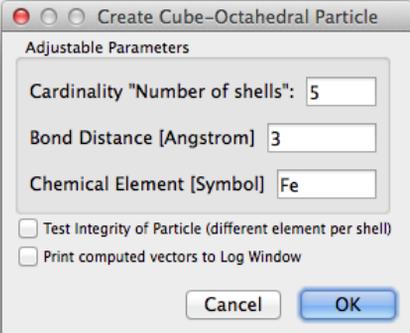
A Cube-Octahedral Particle with Cardinality (#Shells) of 5 would result in the following particle:
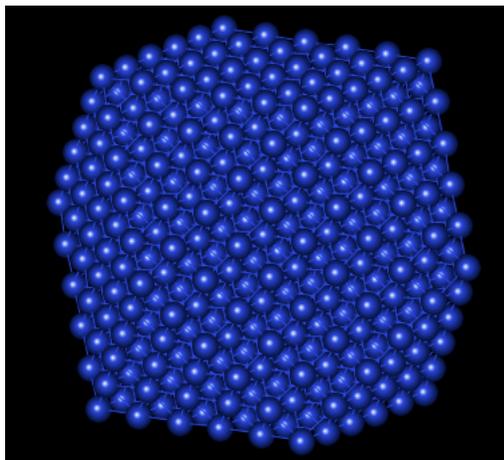
There are a few options available when displaying the particle. The particular keyboard sequence "**Option + UpArrow**" will result in the following display of the same particle.
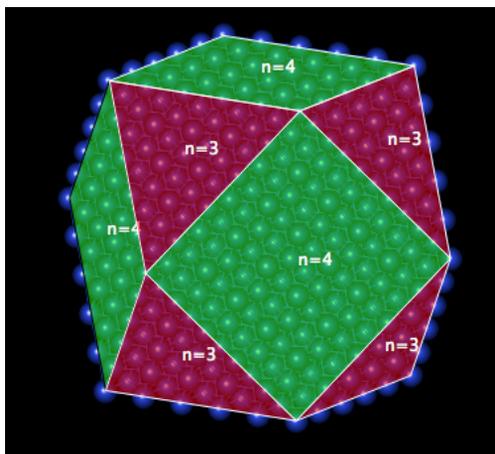
This view clearly shows the faces of the particle together with the symmetry of the faces.

"**Option + DownArrow**" will remove the particle faces.

Other key combinations:

"**Option + RightArrow**": Will show only the faces of the particle as in the view above, but without displaying any of the atomic structure.

"**Command + LeftArrow**": Will reset the view to showing the atomic structure.

"**Command + RightArrow**": Will cycle through displaying each shell at a time. Sequence from lower shell to higher.

"**Command + UpArrow**": Will "build up" the particle by adding one shell at a time.

"**Command + DownArrow**": Will "take apart" the particle by removing one shell at a time.

Icosahedral Particle

A similar particle to the CubeOctahedral particle but with different symmetry is the Icosahedral particle. Creating a Icosahedral particle is very similar to creating the CubeOctahedral particle through the equivalent Dialog
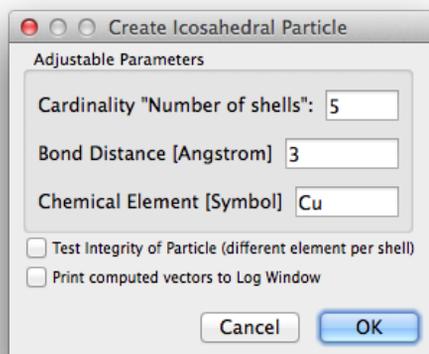
The resulting particle shown with bonds drawn and no cell outline is
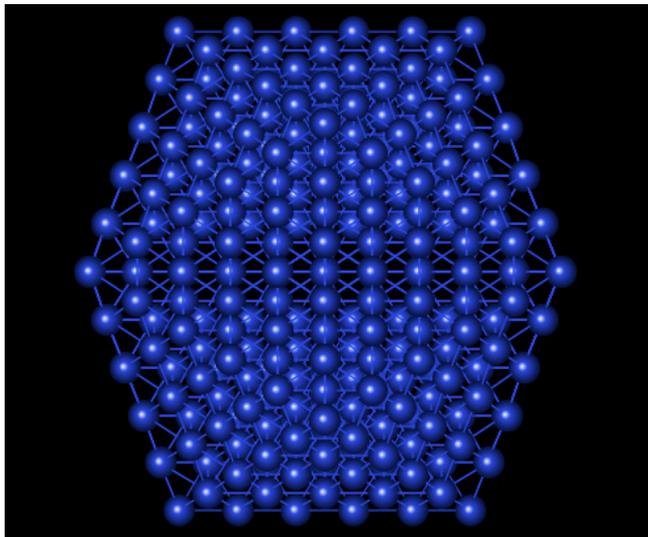
The keyboard combinations are the same as for the CubeOctahedral particle. Hence using the same key combination

"Option + RightArrow":

results in the hybrid view of atomic structure plus particle faces including showing the symmetry of each face.
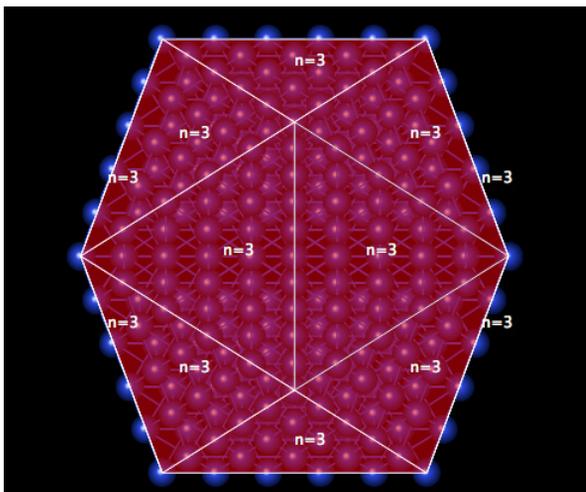
The option "Test Integrity of the particle..." is just a quick way to assign different elements to each of the shell for visualization.
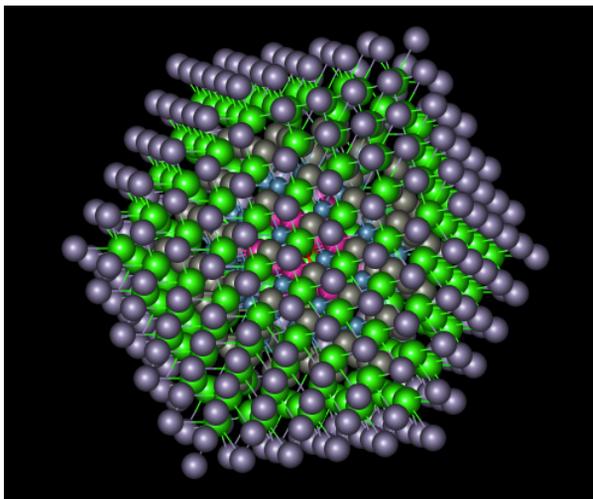
Creating Structures from Cross Sectional Views

Using the various selection tools it is possible to create a number of atom models starting from a cross section of a perfect crystal.

As an example we are starting with a perfect crystal Co3O4 to create a cross section as follows
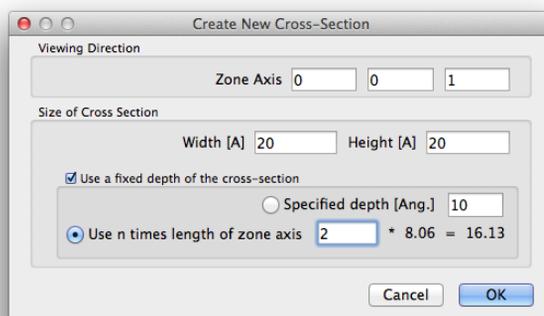
which gives a cross section as displayed here
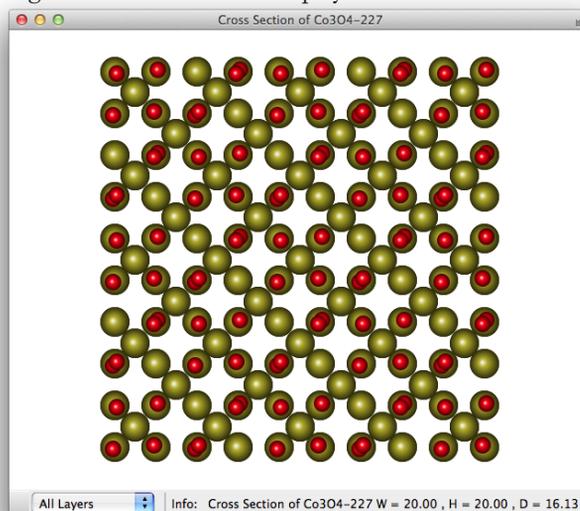
Using the Polygon Selection tool it is possible to outline various structures of "arbitrary" extent as shown here
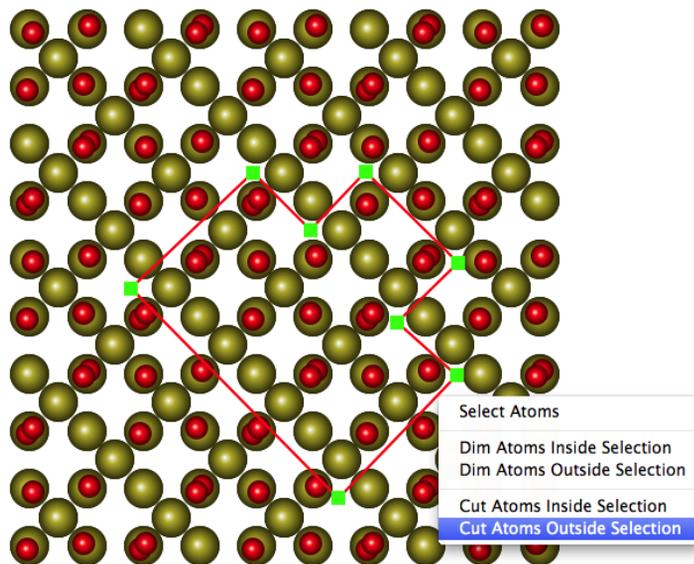
Right-Clicking (Control+Click) in the selection when it is active (green handles) brings up a contextual menu from which further choices are possible, giving the following "particle".
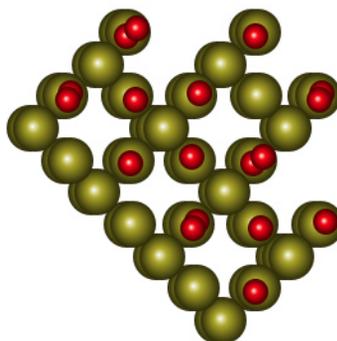
The Selection is "Live" meaning that if one dims the atoms inside the selection, one can move the selection around and the atoms will update accordingly to reflect the selected option for atoms inside/outside the selection. This will work for dimming, but not if one has already cut the

atoms inside/outside.

Cutting/Pasting Atoms

Atoms which are selected through one of the selection tools can be cut or copied.
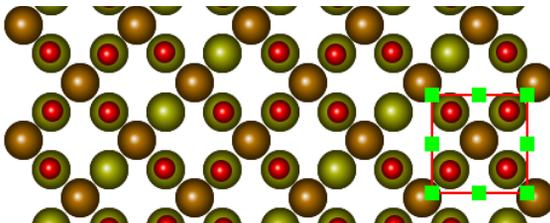
After they are cut, the atoms can be pasted back into the structure, upon which the atoms initially enter into their original positions and the atoms as a block can be moved in all three dimensions. In order to move the block of atoms, the pointer tool must be selected and the Option Key held down. If the Option Key is not held down when attempting to move the block of atoms, the entire structure is moved.

In order to become part of the structure, the selected block of atoms must be merged with the rest of the atoms making up the structure. In order to do this, Control+Click the selected block to bring up the contextual menu containing one entry, "Merge Atoms". After executing
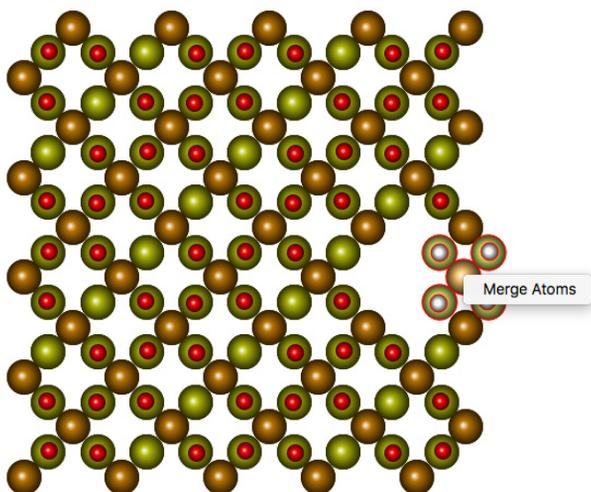
"Merge Atoms", the selected block of atoms becomes "fused" with the rest of the structure.
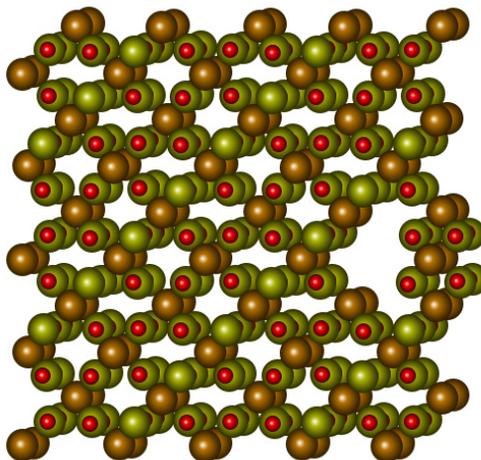
Adding / Moving / Removing Atoms

The "**Add Atom**" Tool is used to add a single atom into the structure. When selecting the "Add Atom" tool, a map of the chemical table is presented from which to choose the chemical symbol of the atom to be added.
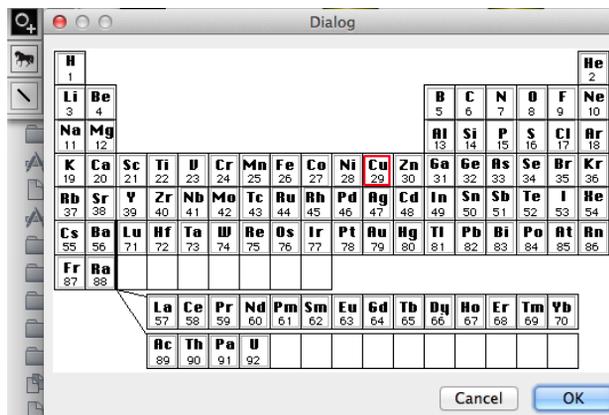
The atoms is added at a specific position by clicking at the selected position with the mouse. When adding an atom it will by default be added to the top layer (closest to the observer). If one is displaying layers one at a time, the atom will be added at the depth of the active layer.
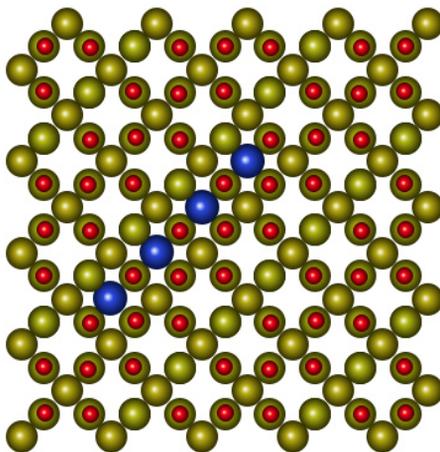
"**Remove Atom**" Tool are used to remove either a single atom or a column of atoms.

By itself, the "Remove Atom" tool deletes a single atom. By holding down the Option Key, all the atoms that lie in the same column as the atom being clicked are deleted.

"**Move Atom**" Tool will move individual atoms. The movement can be in 3 directions by rotating the structure in a way such that the 3rd dimension is "exposed". Clicking in an atom will select the atom and make it active for moving by dragging the atom to the desired position. If the atom is selected as a result of selecting it through the "Move Atom" tool, it is also active for being moved using the combination "Option Key" plus "Pointer" tool dragging. The atom can be deselected by clicking outside any atom with the "Move Atom" tool being active. Right-Clicking in the selected atom will also bring up a contextual menu with the option to deselect the atom.

Moving a Block of Atoms

There are several ways of doing this. One simple way is to create a

selection around the atoms that are to be moved. By Right-Clicking in the selected "selection", the contextual menu is shown as is illustrated below.
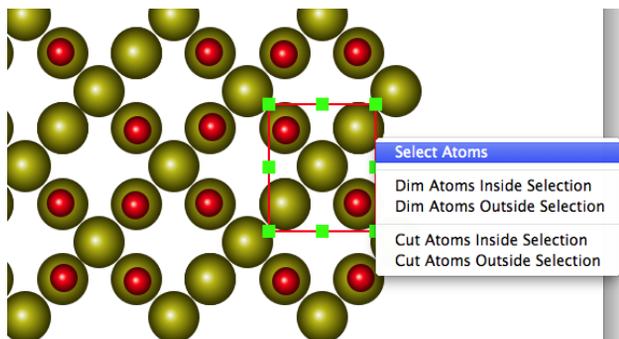
Then with the block of atoms being selected, they can be moved as a unit by dragging with the mouse (pointer tool active) and holding down the Option Key. If the Shift Key is held down as well, the movement is constrained to one of the x,y or z directions depending on the initial movement.. Once the block of atoms have been moved to the desired position, it is just a matter of right-clicking in the block to bring up the option to deselect the block and place the atoms at that position.
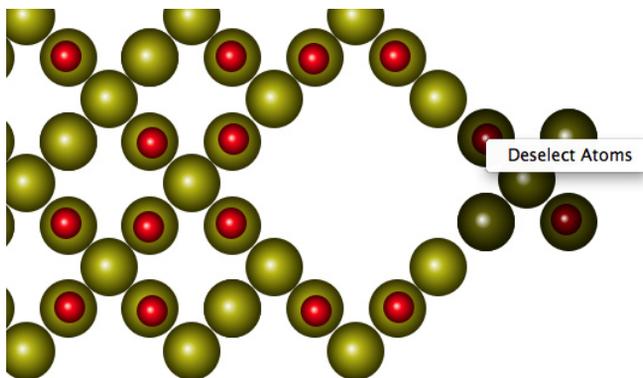
It's worth remembering that atoms can also be moved in the 3rd direction.

Rotating a crystal /cross-section / interface

The objects are rotated when the "Rotate" Tool is selected. When doing rotations in general, objects are rotated around the Z-axis (The viewing direction) by holding down the SHIFT Key. Holding down the Shift

Key constrains the rotation to be around the axis coming towards the viewer.

Horizontal movements of the mouse or fingers on the trackpad will cause the model to rotate around the vertical axis (y-axis).

**Up/Down movements** will cause a rotation around the horizontal axis (x-axis).

Resetting the View: By double clicking with the Rotate tool in the window, the structure is reset to its initial orientation.

Translating Objects: The entire objects are translated via the "Hand" Tool or the "Pointer" Tool. When using the Pointer Tool, holding down the Option Key will translate atoms. Using the Shift Key will constrain the movement to either being in the horizontal or the vertical direction.

Creating a Unit Cell from a Cross Sectional View

After displaying a cross section and thereafter creating a structure which can be used for further study, the structure of interest can be defined and extracted. This is done by using the "Unit Cell" Tool. The first step is to click at the position of the origin of the unit cell to be defined.

By default the click will be constrained to an atomic position. Holding down the Option Key will remove this constraint. Likewise unchecking the menu item "Constrain Clicks to Atoms" in the "CrossSection/Interface" Menu will allow the clicks to be at any position in the window.
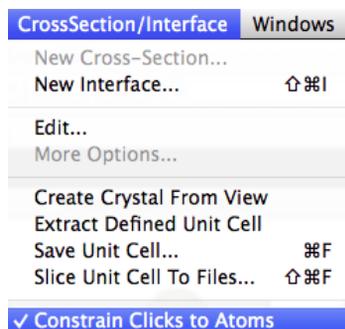

The Unit Cell is defined by first selecting the Origin of the unit cell followed by the point defining the Unit Cell A-Axis and ending by

defining the B-Axis. By default the Unit Cell will be the depth of the crystalline material being displayed.
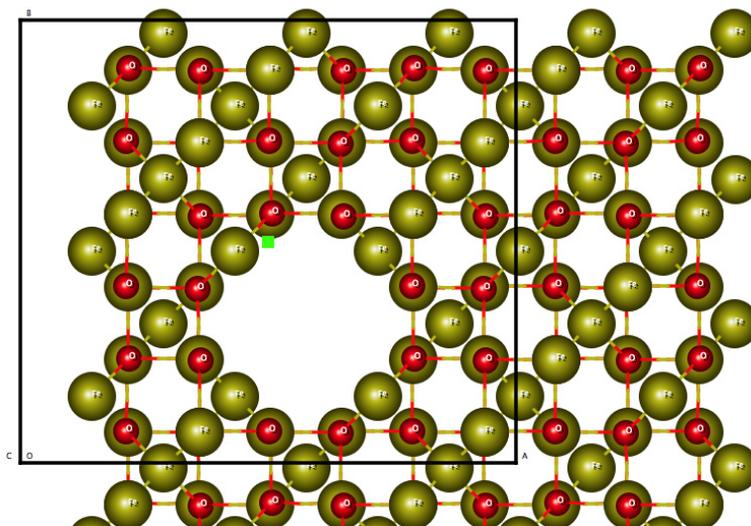

If the Shift Key is held down the Axes will be constrained to be in the horizontal and vertical direction. The final step in creating the unit cell is to using one of the commands in the "CrossSection/interface" menu. The menu item action "Extract Defined Unit Cell" extracts the unit cell and displays it in a new Crystal Window. All the atoms will be added to the Motif (Basis) atoms of the crystal and the spacegroup will be set to 1 with the single symmetry operator "x,y,z".
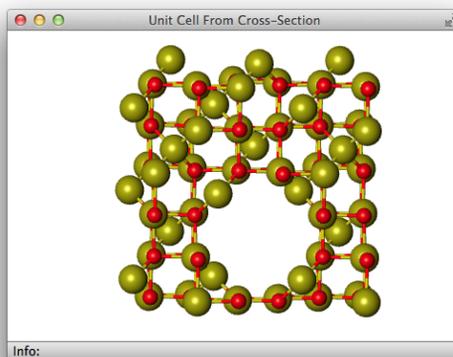
The actions "Save Unit Cell…" saves the unit cell directly without showing it in its own window and the "Slice Unit Cell To Files…" will divide the unit cell into a number of slices in the z-direction and save each slice as a crystalline unit using the base name supplied in the Save Dialog.

The "Edit…" command is used to adjust the cross section after its initial creation.
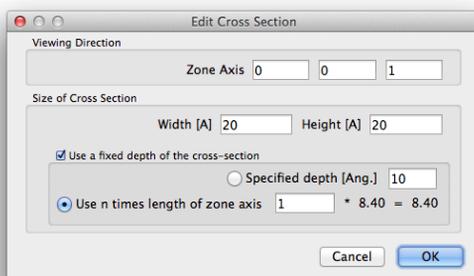
The Cross Section Window has its own contextual menu which is brought up by right-clicking in the window with the mouse (or Control-Click). The contextual menu is
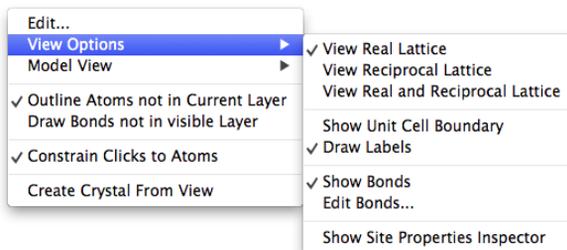
The "Create Crystal From View" will create a crystalline unit cell from the structure as it is shown by selecting a boundary slightly outside the extent of the atoms. This unit cell boundary can be adjusted easily later.

Creating Interfaces

An interface is easily created from two crystals making up the material on the two sides of the interface. The two crystals can be of the same material.

The interface is created by filling out the following dialog.

First the two crystals must be selected from crystals in open Crystal Windows.

Once the two structures are chosen, the orientation relationship between the two crystals must be defined. This is normally done by defining two orientations in the two crystals that are parallel together with two parallel planes. If the structures are aligned with all the axes initially being parallel (a || a', b || b' and c || c'), it might be possible to define the interface by a given rotation about an axis.

Once the orientation relationship is set, the plane of the interface must be given. Finally the Zone-Axis must be defined. Any of these planes

and/or directions can be defined with respect to either of the two crystals. The following is a fictional interface between Fe3O4 and zsm5.
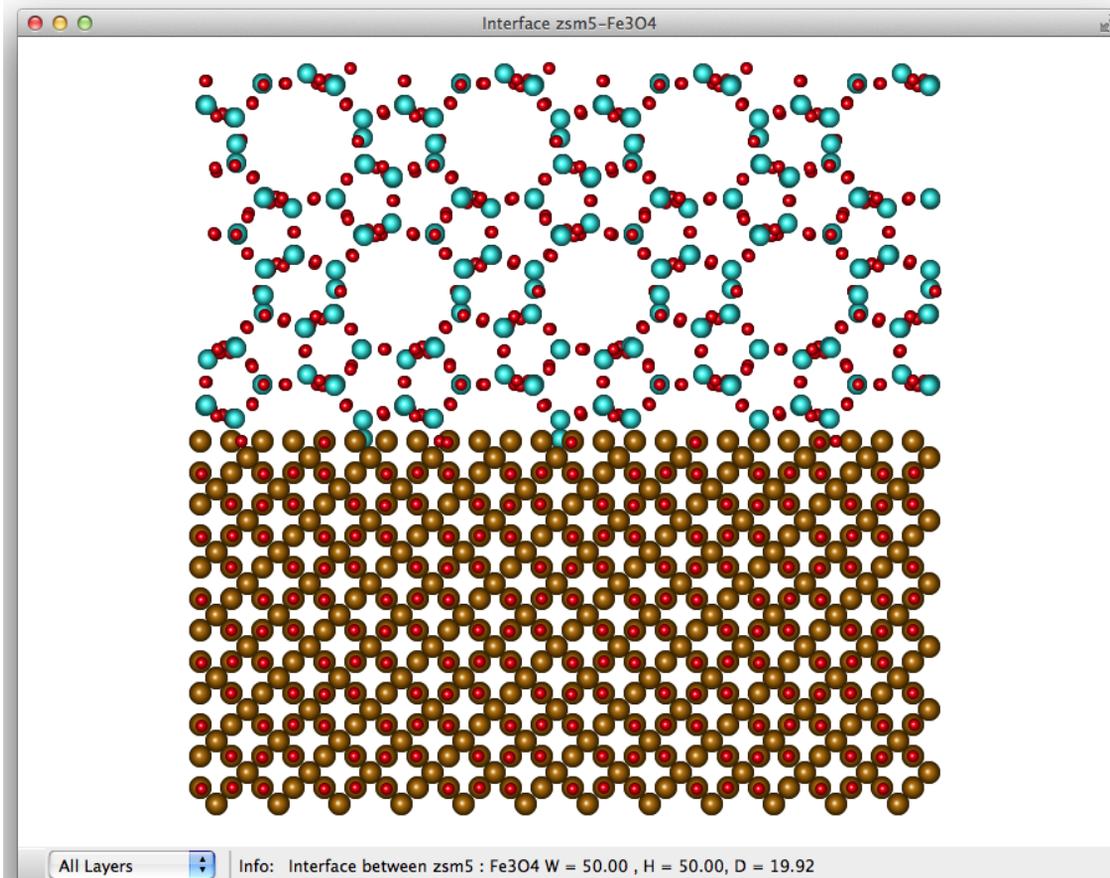
Rotating Grains:

From the initial geometric interface it is easy to add rotations by rotating any of the grains using the "Rotate" Tool while holding down the Option Key. If the Option Key is not used, the view of the structures is rotated.

Translating Grains:

The grains on either side of the interface can be translated with respect to each other. By using the Pointer Tool and holding down the Option Key, any grain can be moved in any of the tree directions.

Using Grids and Guides

Show Grid

Grid lines can be shown in Cross Section and Interface Windows by checking the option "Show Grid" in the View Menu.
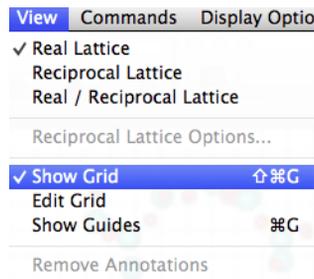
Edit Grid

The Grid can easily be adjusted by the "Edit Grid" command once the Grid is shown.
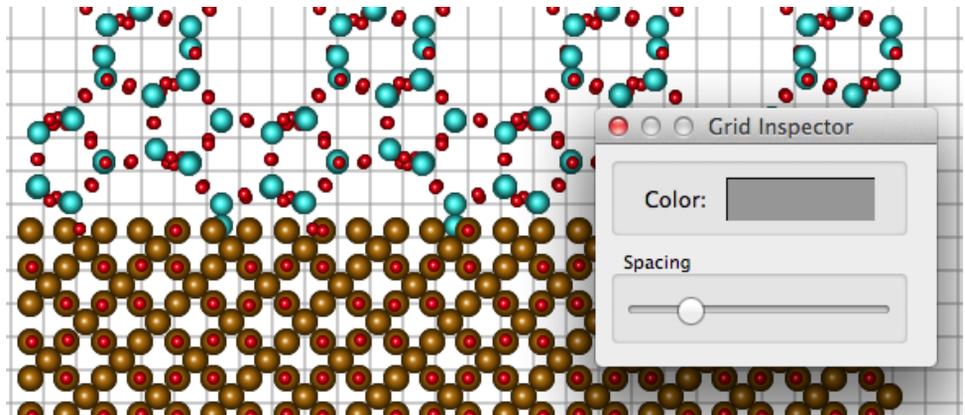
Show Guides

The command "Show Guides" will place 2 fixed guides in the window, one horizontal and one vertical position in the middle of the window.

Additionally there will be two strips, one at the left side of the window and one at the top of the window. These two strips (regions) serves as sources for movable guides to be added to the window.
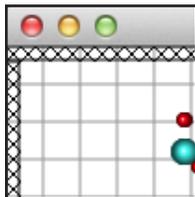
By dragging from the horizontal area (top) or the vertical area (left), horizontal and vertical guides are added to the window. As many guides as wanted can be placed in the window. These guides will remain fixed to the model such that they will move with the position and scale of the structure being viewed. A guide that is already placed in the window can freely be translated by dragging with the mouse. These guides are very handy for creating markers for selecting unit cells or otherwise marking the structure in some way.

Cross Section of zsm5
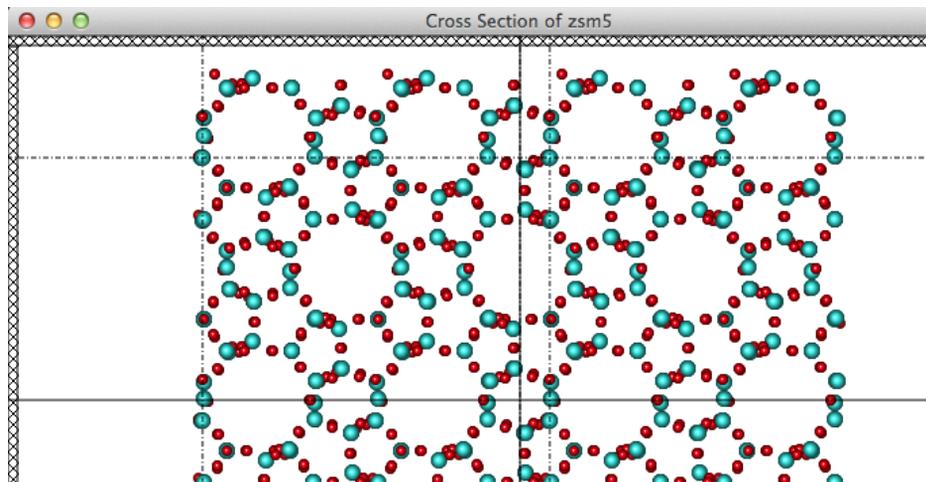
Creating a Precipitate

Creating a precipitate is normally done by defining the orientation relationships as previously shown and showing the structures as interpenetrating lattices.


This will show the structures as such. Here a Cylindrical Selection is defined and the Contextual Menu is shown (Right Clicking the selection).
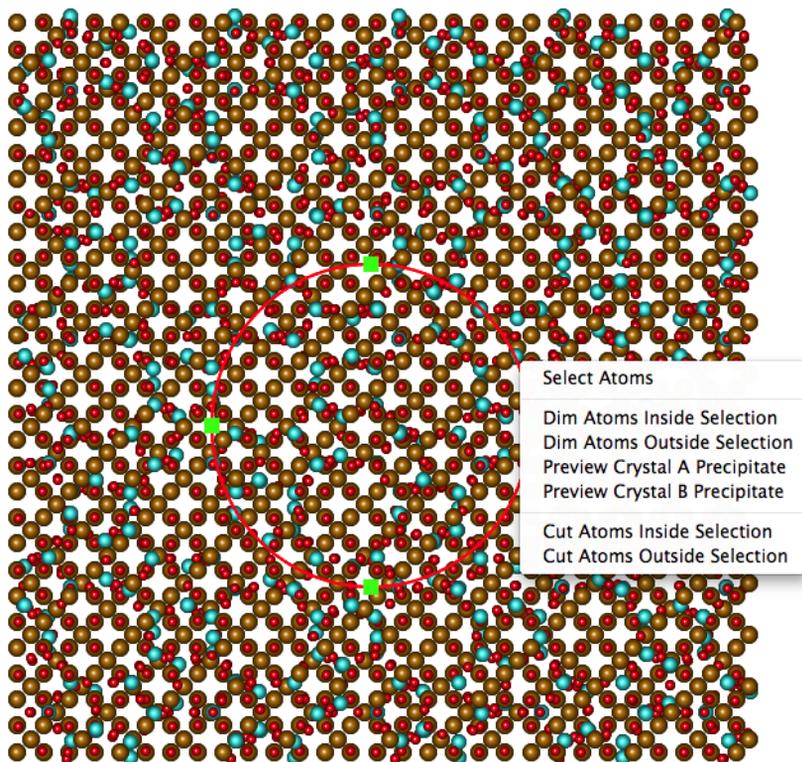

Selecting the menu item "Preview Crystal A Precipitate" will cause the

structure A to be shown inside the selection and Crystal B to be shown outside the selection. Moving the Selection around will give a "Live" view of the precipitate as the Selection is moved and also modified in size.
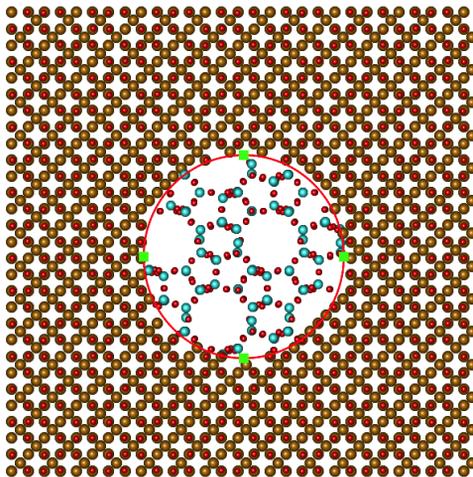
All the tools like Cutting Atoms, Pasting Atoms, Adding Atoms, Deleting Atoms etc. are available as expected. "Create zsm5 Precipitate" from the "Edit" Menu will create the Precipitate When everything has been adjusted as desired, the structure can be extracted as a unit cell.
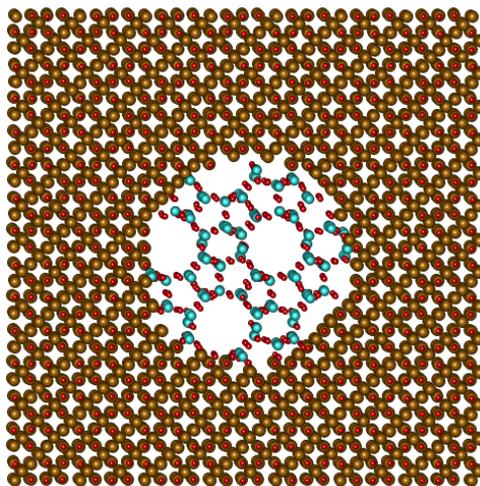
Creating an Irregular Interface

Creating an irregular interface can be done by starting with the two grains shown as overlapping lattices just as when creating precipitates.

Starting with the two grains of Zsm5 and Fe3O4 one can define the following interface starting point.
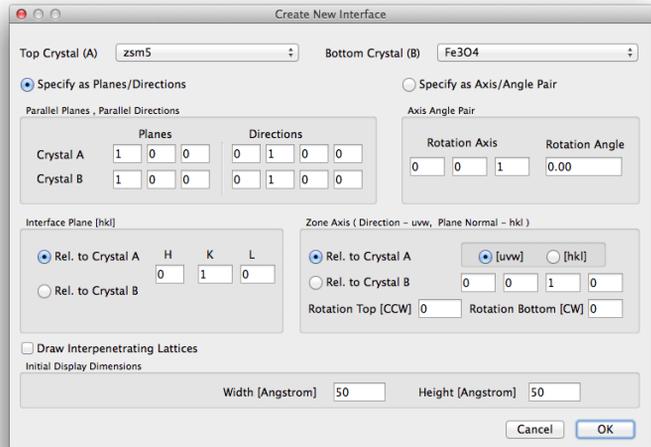
This creates the following geometric interface
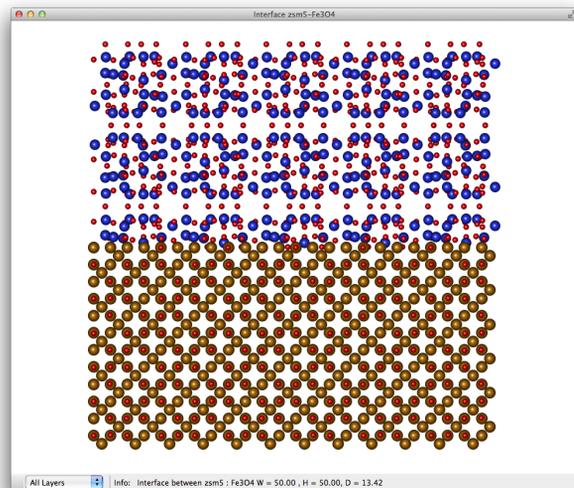
Again using the option of creating interpenetrating lattices
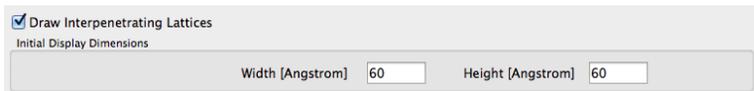
one gets
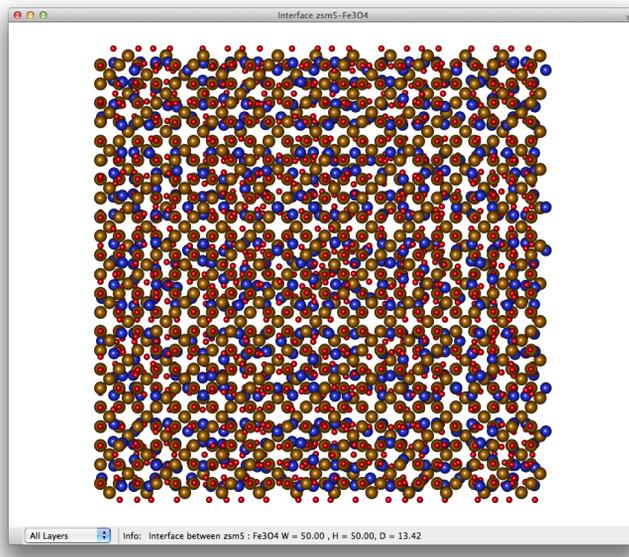
From here there are a couple of different ways of creating an "arbitrary" interface. One straight forward way is to use the "Interface" tool. With this tool one starts by clicking in a starting point to the left of the displayed structure. From there on, one defines the interface by clicking in successive points, from left to right without moving back in x, each point defining the boundary between the top and bottom crystal.
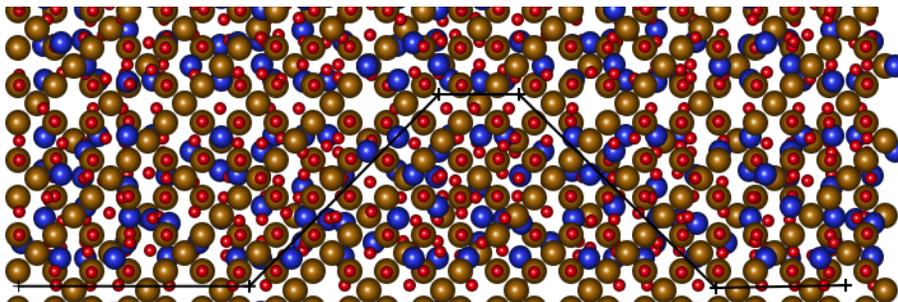
When one reaches to the right of the displayed structure, the interface is defined and is displayed.
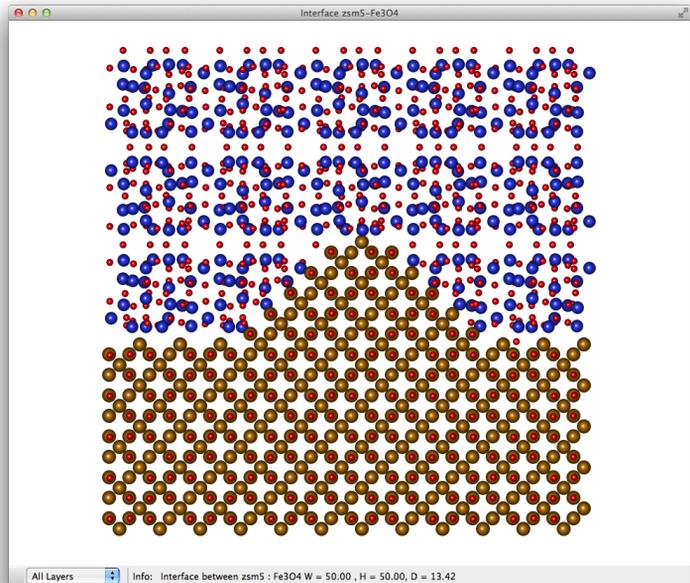
There are some additional options (constraints) that can be defined for the interface. These are set from "More Options..." from either the "CrossSection/Interface" Menu or the contextual menu shown when right-clicking (or Control+click) in the Interface Window.
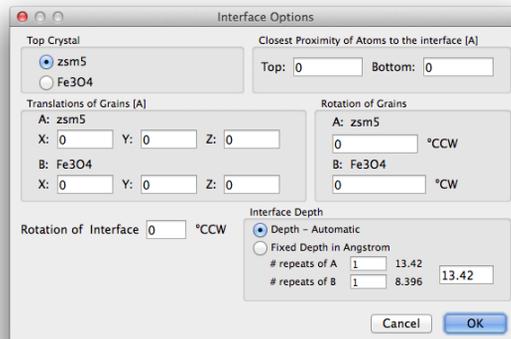

Using the "Interface Options" dialog, the minimum distance from the interface can be set. One can also specify any translation of the grains

and a rotation around the z-axis by entering the appropriate values in the dialog.

Again keep in mind that the two grains can be rotated with respect to each other (Rotate tool) as well be translated relative to each other in all 3 directions (Pointer tool).

In order to translate a grain it is necessary to hold down the "Option" key and move the grain with the "Pointer" tool. Holding down the "Shift" key will constrain the translation to the initial direction of the move. In order to translate the grain in the z-direction, rotate (without the Option key) the whole interface such that it is shown from the side of interest. This "exposes" the z-direction (the depth direction) such that the grain can be translated in that direction (use Option key).

Another way to define the boundary which removes the constraint of having to click in points of increasing x is to use the "Polygon" selection tool. Using the Polygon Selection tool makes it possible to preview the interface as well as tailoring the boundary to "perfection".
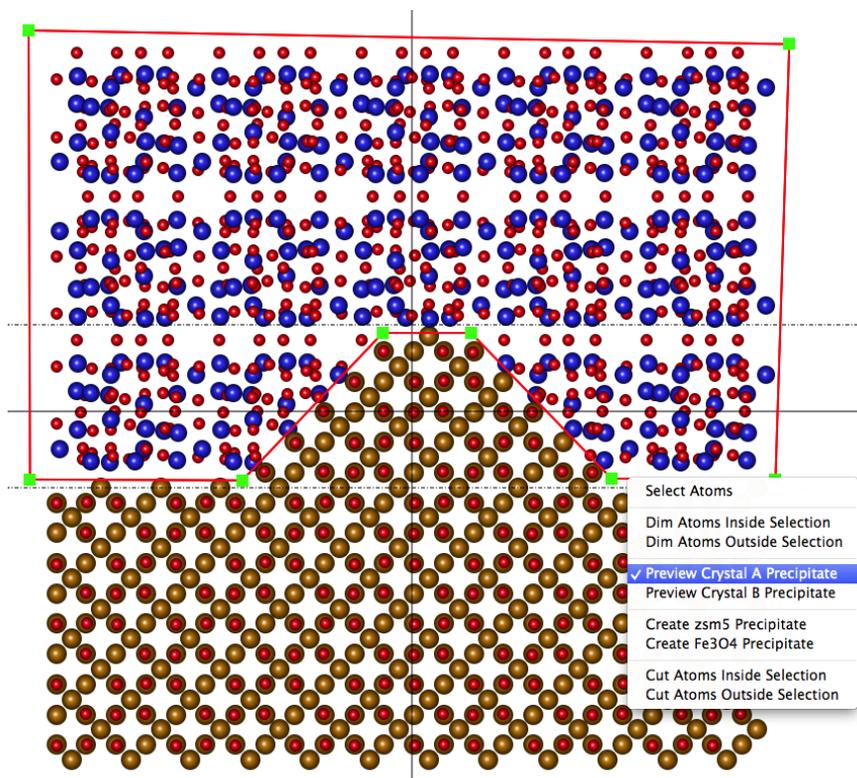
As mentioned already, using the Polygon selection tool removes the constraint of having to have increasing x for every interface point defining the boundary between the two crystals. This makes it possible to define such boundaries as this.
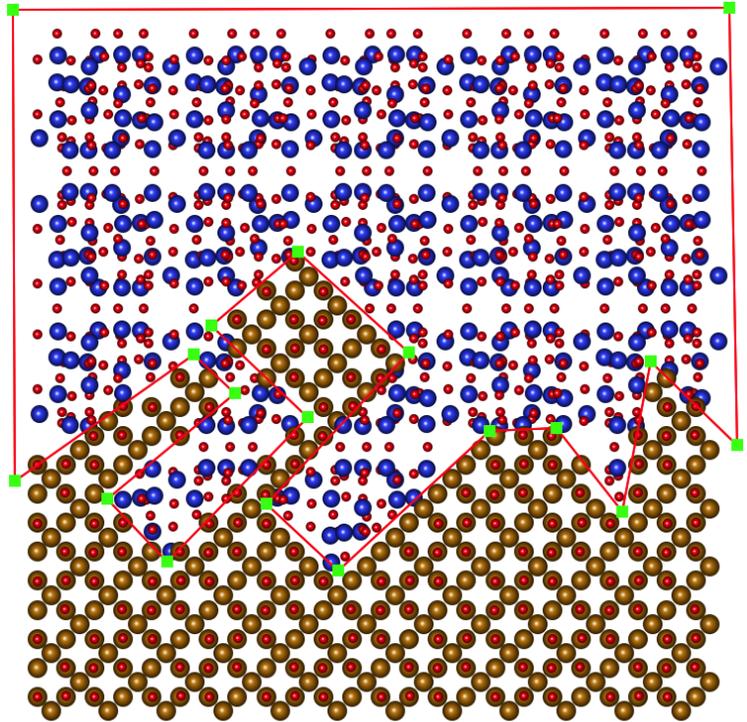
As a final step to create the boundary, one creates the precipitate rather than thinking of it as a boundary moving from left to right. This is done from the menu item "Create zsm5 Precipitate" in either the "Edit" Menu or the contextual menu shown when right-clicking in the selection when it is selected (active).
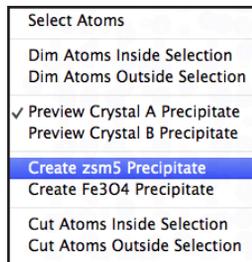
In order to continue to work with the structure as such defined, one extracts the structure as a new crystalline unit cell. This is done through "Create Crystal From View" in the "CrossSection/Interface" Menu. A crystal unit cell is defined by making an origin slightly to the bottom left of the structure and axes A and B extending slightly to the left and to the top of the structure. The C-axis is the depth of the interface. The unit cell volume can be modified later if desired.
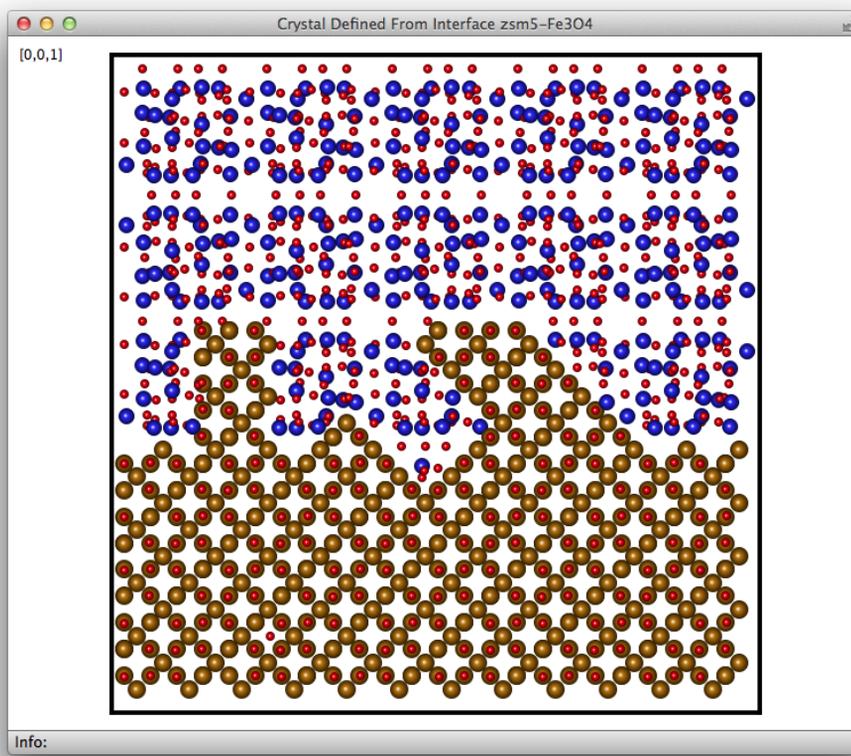
The use of 3d selection tools such as the box selection and the polygon selection allows for a lot of flexibility when it comes to creating interfaces. As shown above, the ability to create precipitates of one crystal in another, also leaves open the ability to create interfaces between two crystals.

Similarly, it become easy to create a layered structure with two interfaces, simulating epitaxial growth or vapor deposition of materials. The possibilities are many and since one can preview the boundaries between the materials as the boundaries are defined, the task is greatly facilitated.

As an example of a highly unlikely boundary, but just for the sake of showing how such a boundary is created, is the structure below. With the polygon selection tool it is trivial to add new vertices to the polygon by Option+Clicking with the Pointer tool wherever it is needed in the sides of the polygon. One can keep on adding new points to the polygon and drag them around while one is previewing the structure at all times. When one has finished defining all the boundaries between the structures, one can try to "clean up" the structure along the geometric boundaries. It is easy to remove atoms or columns of atoms at various sites if it is determined that these sites do not exist in the experimental structure. Likewise it is easy to add atoms at various sites as well.
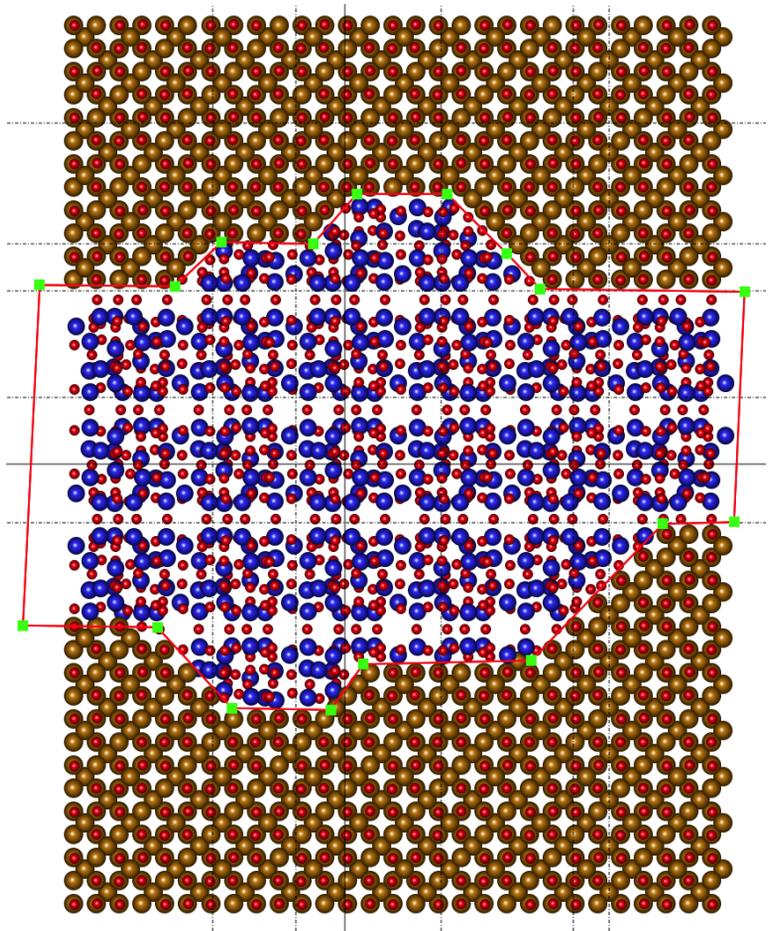
The one limitation to the creation of the structures is that it is defined by geometry.

If one does have an experimental image available, one can use the experimental image as a background image to the model.

Load Background Image
Loads an image and places it as an object behind the structural model

Remove Background Image
As the title says, removes the background image.

One can then calibrate the image (if it's not already) and scale the model to the image. Then using the "Move Atom" tool, one can attempt to shift atomic positions to further fit the experimental data.
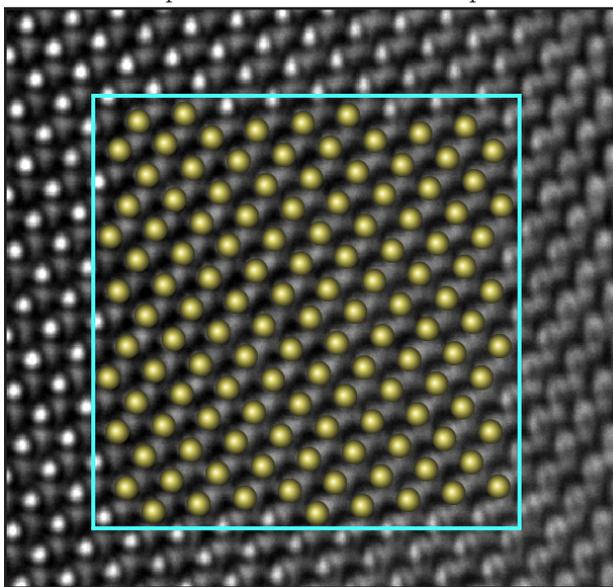
Currently any attempt to minimize the energy of the atomic configuration based on optimizing the position of atoms is outside the scope of CrystalKit. It is possible that some fairly simple energy minimization code will be added in the future, but it is not known if or when at this time.

Anyone wishing to try to refine the atomic positions based on the electrostatic atomic potentials will need to use the structure coming from CrystalKit as a starting point for applications that can perform energy minimization, using Molecular Dynamics Calculation on the structure.

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