nanoHUB Tool
Crystal Viewer 3.0
User Guide

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Part I : Introduction

A crystal or crystalline solid is a solid material whose constituent atoms, molecules or ions et cetera are arranged in an ordered pattern extending in all three spatial dimensions. In addition to their microscopic structure, large crystals are usually identifiable by their macroscopic geometrical shape, consisting of flat faces with specific, characteristic orientations.

Crystals actually have a huge number of uses in science. The biggest application of crystals in science is the basis for all microelectronics. Nowadays, every chip contains about one billion transistors which are all made from crystal materials. Besides, crystals are also very important in biological science, material science, optics and so on.

In order to explore various properties of crystal materials, it is essential to have a clear understanding of the crystal structure, and other basic concepts like unit cell, Bravais vector, miller plane et cetera. The Crystal Viewer tool is developed exactly for this purpose. The version 3.0 has a significant upgrade based on the 2.3.4 version and hopefully it can become a useful tool for your study and research.

Part II : Preparation

Unit cell

Simply stated, a unit cell is a small portion of any given crystal that can be used to reproduce the crystal. To help establish the unit cell concept, let us consider the two-dimensional lattice shown in Fig 1. In order to describe this lattice or to totally specify the physical characteristics of this lattice, one need only provide the unit cell shown in Fig 2. As indicated in Fig 3, the original lattice can be readily reproduced by merely duplicating the unit cell and stacking the duplicates next to each other in an orderly fashion.

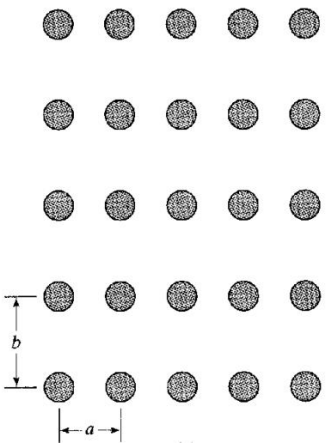


Figure 1

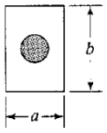


Figure 1

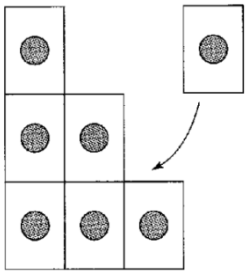


Figure 3

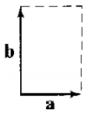


Figure 4

The relationship between a given unit cell and the lattice it characterizes can be more precisely described in terms of basis vectors. If $\vec{a}$ vector of length a parallel to the a-side of the unit cell, and $\vec{b}$ is a vector of length b parallel to the b-side of the unit cell (see Fig 4), then equivalent points of a two-dimensional lattice will be separated by $\vec{r} = h\vec{a} + k\vec{b}$ where h and k are integers. Hence, the lattice can be constructed by duplicating the unit cell and translating the duplicates $\vec{r} = \vec{a}$, $\vec{r} = \vec{b}$, $\vec{r} = \vec{a} + \vec{b}$ etc., relative to the original. Note that unit cells are not necessarily unique and a unit cell need not to be primitive (the smallest unit cell possible).

Semiconductor crystals are usually three-dimensional and are therefore described in terms of three-dimensional (3-D) unit cells. In Fig 5, we have pictured the simplest of all 3-D unit cells-namely, the simple cubic unit cell. It should be noted that only 1/8 of each corner atom is actually inside the cell, as pictured in Fig 6 (since the repetition of the unit cell cannot overlap). One could of course construct the lattice using the translation vectors $\vec{r} = h\vec{a} + k\vec{b} + l\vec{c}$, where $\vec{a}$, $\vec{b}$, and $\vec{c}$ are basis vectors and h, k, and I are integers.

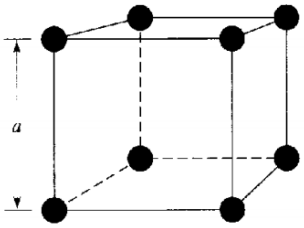


Figure 5

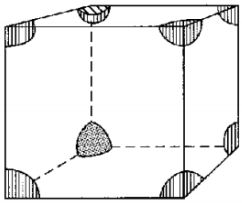


Figure 6

The Lattice and the basis

The crystal can be thought of as consisting of two separate parts: the lattice and the basis. The lattice is an ordered arrangement of points in space, while the basis consists of an arrangement of atoms which is repeated at every point in the lattice to build up the crystal structure. A good analogy is patterned wallpaper. The basis is like a motif on the wallpaper and the lattice would be periodic pattern of points on which of the motif is repeated. In Figure 7, the lattice points correspond with the center of the basis, but this does not have to be the case.

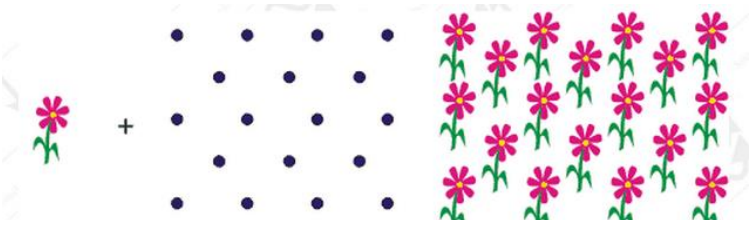


Figure 7

The Fourteen Bravais Lattices

The ways in which we can specify the lattice points in space and keep translational symmetry is limited. In 1848, Auguste Bravais demonstrated that there are in fact only fourteen possible point lattices and no more. For his efforts, the term Bravais lattice is often used in place of point lattice.

Table 1 lists all 14 Bravais lattices and their restrictions. Note that for 2-dimensional, there are 5 possible lattices. Note again that every blue dot here is not necessarily an atom; in fact it can also be any possible arrangement of multiple atoms.

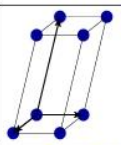
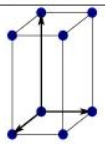
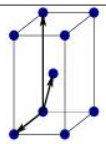
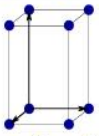
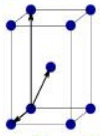
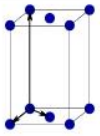
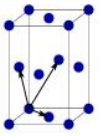
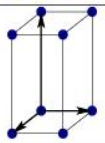
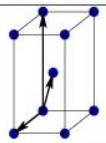
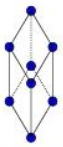
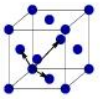
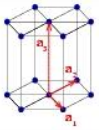
Bravais lattice	Parameters	Simple (P)	Volume centered (I)	Base centered (C)	Face centered (F)
Triclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} \neq \alpha_{23} \neq \alpha_{31}$				
Monoclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{23} = \alpha_{31} = 90°$ $\alpha_{12} \neq 90°$				
Orthorhombic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Tetragonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Trigonal	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} < 120°$				
Cubic	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Hexagonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = 120°$ $\alpha_{23} = \alpha_{31} = 90°$				

Table 1

Miller Indices and Notation

Miller Indices are used to identify planes of atoms within a crystal structure. Miller indices are written as three digits between brackets, (100) for example. Given the intercepts of the plane with the crystallographic axes, (directions of the lattice vectors), joining the intercepts with lines defines a plane which cuts through the crystal. The Miller indices are then calculated by taking the reciprocal of the intercepts and multiplying them by their highest common factor. Negative numbers are represented by placing a bar over the top of the digit. If this sounds at all complicated, it is easily illustrated with a few examples. If the intercept is at infinity, then the plane is parallel to that axis and the Miller index is zero, since, $1/\infty = 0$.

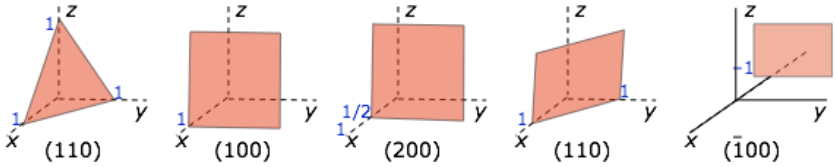


Figure 8

The diligent reader may have noticed that due to the symmetry of the unit-cell of the lattice, certain planes are equivalent. In the cubic lattice, for example, (100) is equivalent to five other planes, (010), (001), (100), (010), (001) and to acknowledge this, the set of Miller indices is written {100} which means the set of (100) planes equivalent by virtue of symmetry. The beauty of this system is that similar planes can be identified in any of the Bravais lattice point groups. The Miller indices are also similar in the way in which planes are described in mathematical terms.

A common shorthand notation to show the lattice vector directions is to write the three vector components coefficients in square brackets [uvw] where u, v, and w are integers. It is important not to confuse these with Miller indices. The direction is then

$$\vec{T} = u\vec{a} + v\vec{b} + w\vec{c}$$

Equivalent directions are designated using angled brackets <uvw>.

Part III : Tool usage

View a material

To view an available material, first select “view a material” and then select one of the available crystal structures in the Crystal structure section (as in Fig 9). When the crystal structure is selected, go down to the Material section and select a material in the list (as in Fig 10).

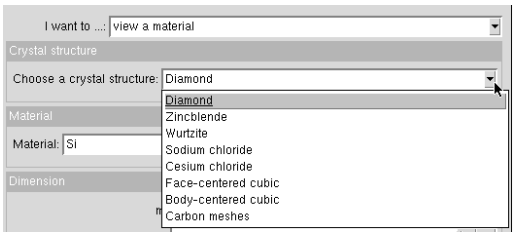


Figure 9

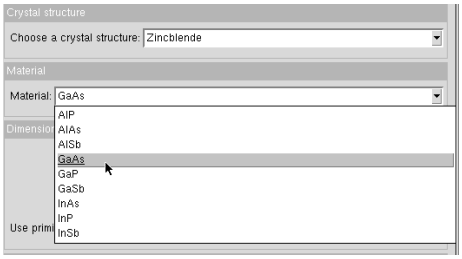


Figure 10

Specify the dimension of the crystal lattice and the Bravais vector (as in Fig 11).

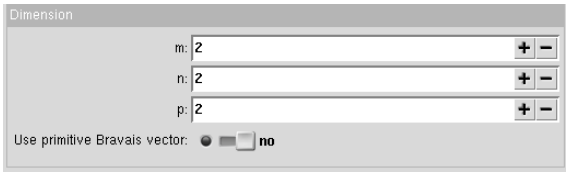


Figure 11

The option “Use primitive Bravais vector ” remains off in default which means the conventional Bravais vector is used. Toggle it on to use the primitive Bravais lattice. Both conventional and primitive Bravais vectors are shown for every material in the picture in the Bravais vector section. Figure 12 gives an example for GaAs.

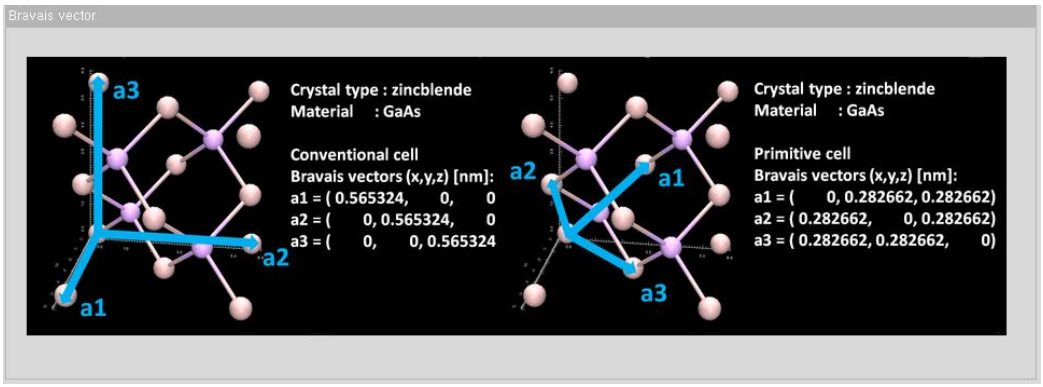


Figure 12

For Graphene/Graphite and carbon nano tube, the dimension setting is different from other materials.

Graphene/Graphite

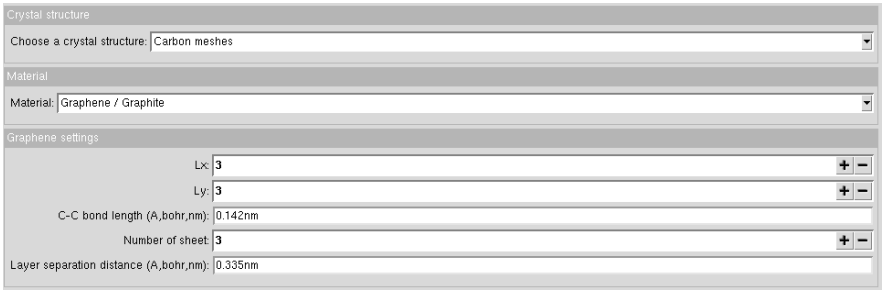


Figure 13

Here Lx and Ly are the translation along X and Y axis.

CNT

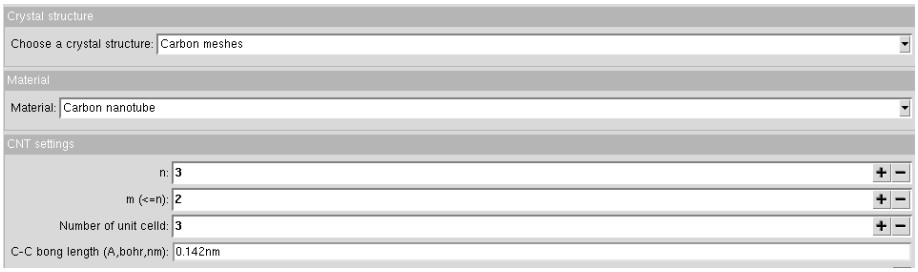


Figure 14

Here one needs to set the chiral vector. We provide a detailed explanation right below for people who don't know what the chiral vector is.

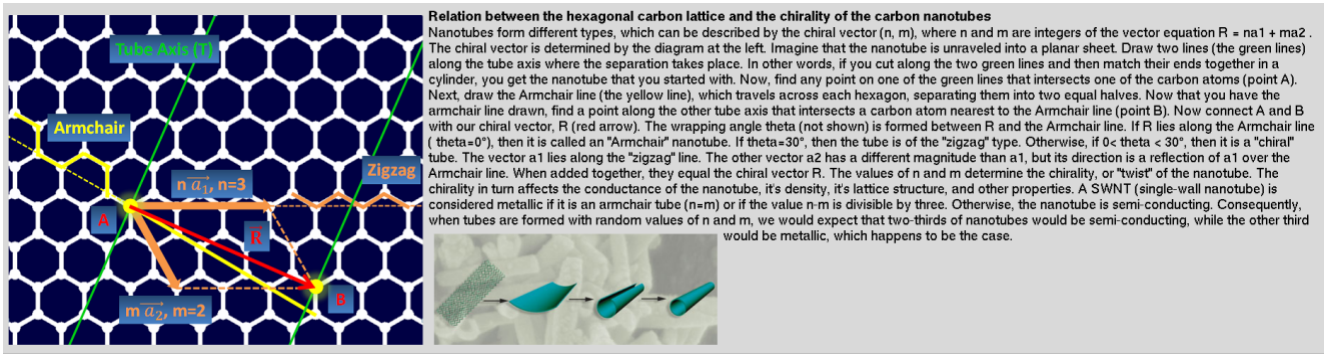


Figure 15

Example

Let's view a 3 by 3 by 3 AlP using conventional Bravais vector. After the simulation is finished, the tool will show the basis and the lattice grid. You can view each of them by selecting in the Result list.

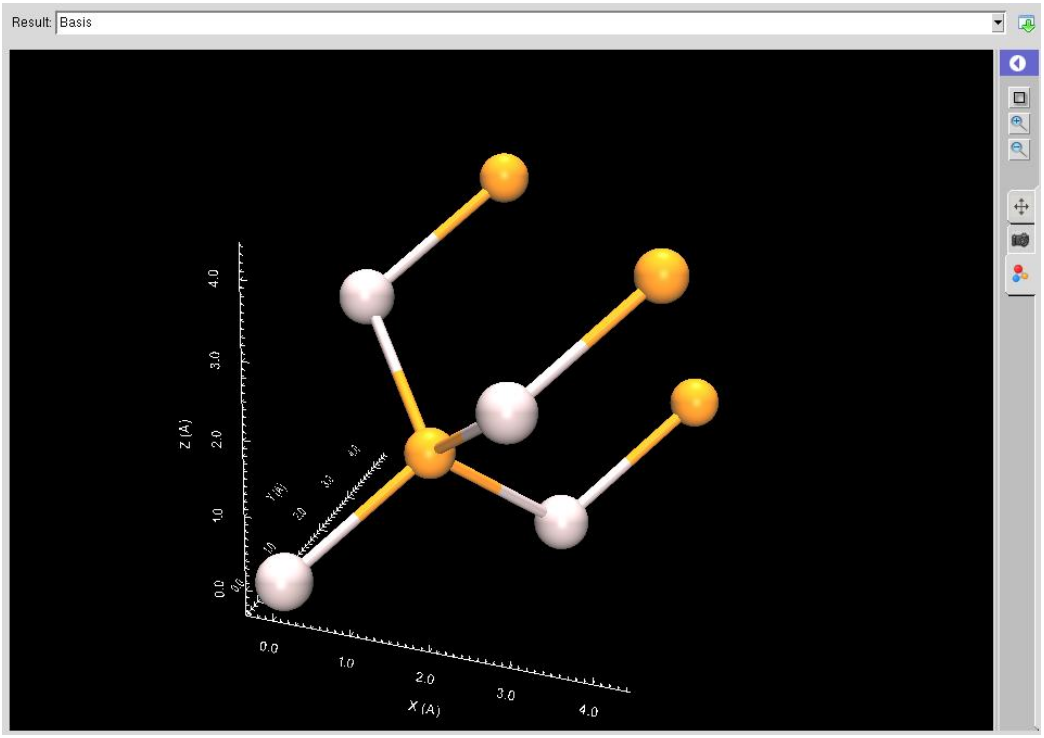


Figure 16

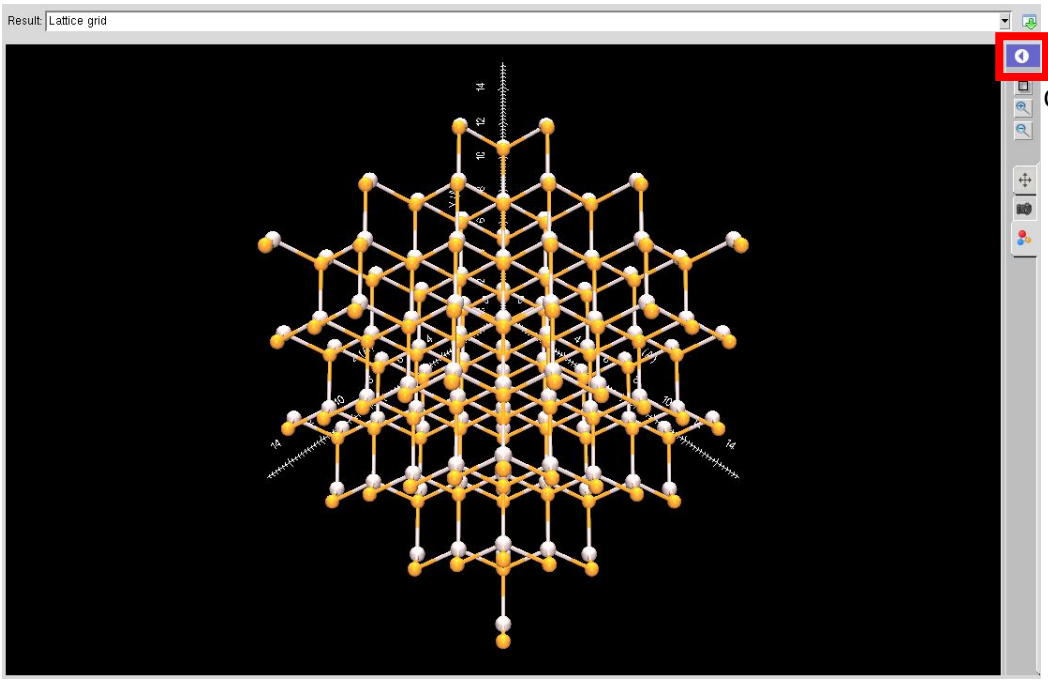


Figure 17

By opening the menu on the right, you can zoom in and out, show atom labels. You can also change the atom scale and the bond scale and the opacity.

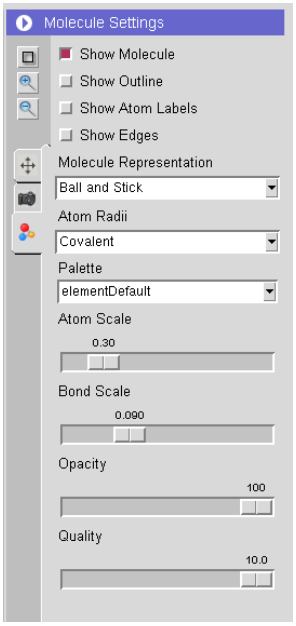


Figure 18

Moreover, you can choose different representation.

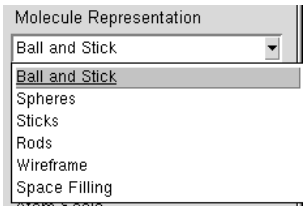


Figure 19

For example, the space filling model

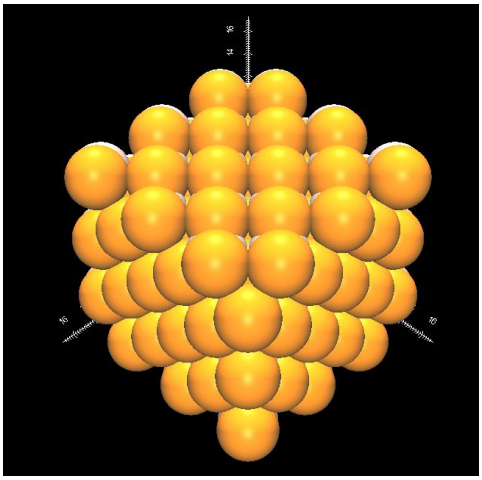


Figure 20

Besides, you can also choose different atom radii model.

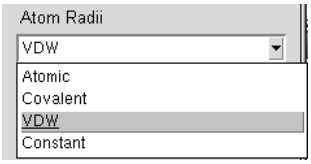


Figure 21

Figure 22 is atomic model and Figure 23 is VDW model

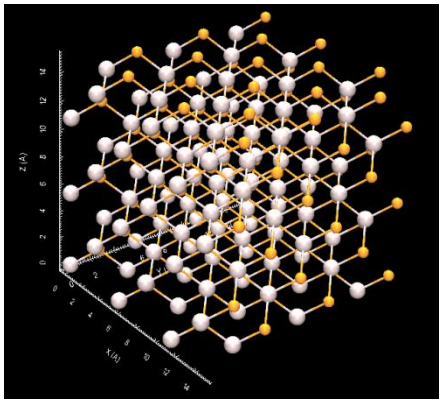


Figure 22

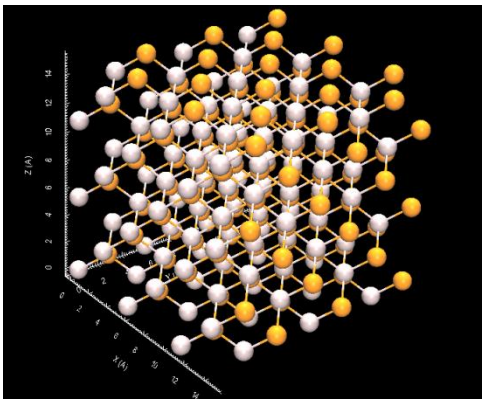


Figure 23

View a Bravais lattice

To view one of the 14 3-dimensional Bravais lattice, first select “view Bravais lattice” and then choose one of the 7 crystal systems in the Crystal system section and then select the available Bravais lattice.

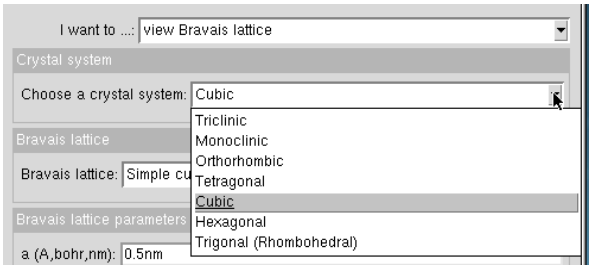


Figure 24

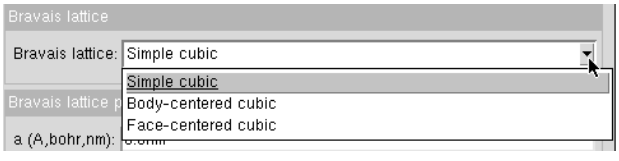


Figure 25

Then you need to set the parameters for this type of Bravais lattice and the dimension of the lattice grid.

Example

Let's view a 3 by 3 by 3 hexagonal Bravais lattice. For hexagonal Bravais lattice, we need to set the length of a and c.

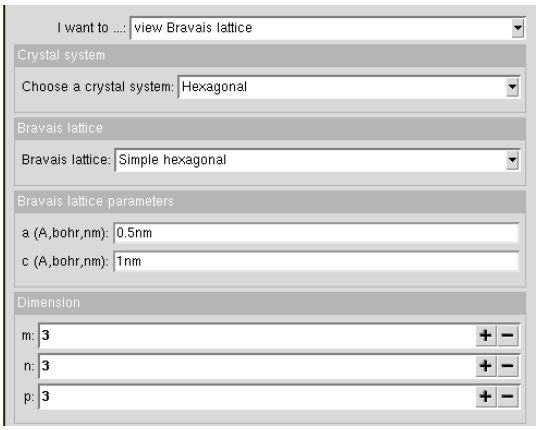


Figure 25

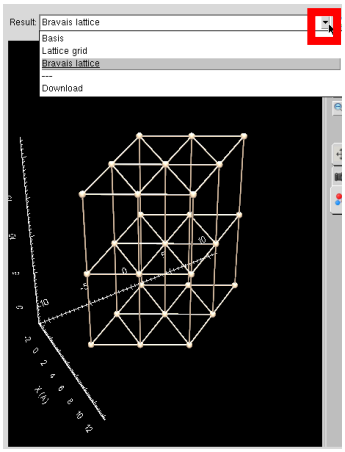


Figure 26

If your previous simulation was for viewing a material, you had two results which are the basis and the lattice grid. Then now you must choose Bravais lattice in the result list to view the bravais lattice because for a Bravais lattice simulation the basis and the lattice grid is empty.

Creat your own material

In "view a material", there contains finite number of crystal materials. The idea of "user-defined crystal" aims to allow

1. viewing all materials which have periodical structure
2. building crystal structure even not exists in nature

For doing that, you need to define:

1. The number of atom in the basis
2. Coordinate (x, y, z) for every atom in the basis
3. Material for every atom in the basis
4. Bravais vector a1, a2 and a3
5. Dimension of the lattice grid
6. Bond radius (the bond radius means the distance under which a covalent bond will be created between two atoms)

Example

Let's view Polonium which is not contained in our material database.

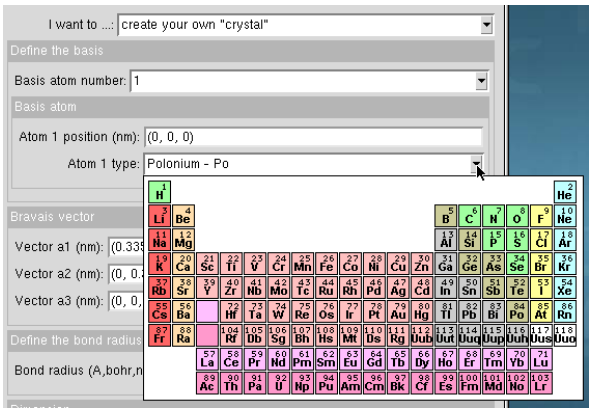


Figure 27

Polonium has a simple cubic crystal structure. Thus we set 1 basis atom number and set the position at (0, 0, 0). For atom type we choose Po in the periodic table.

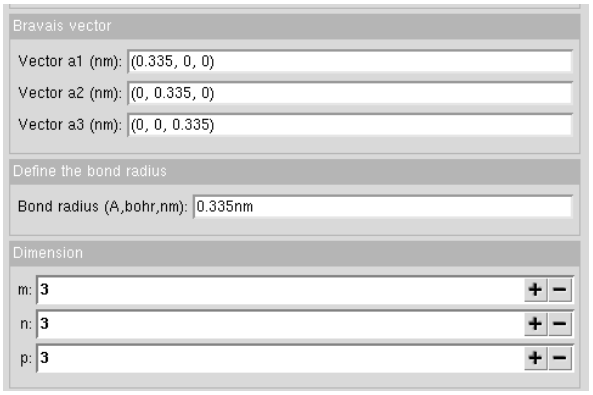


Figure 28

Then we set the Brvais lattice, the bond radius and the dimension.

Thus we created the Polonium lattice grid as in Fig 29.

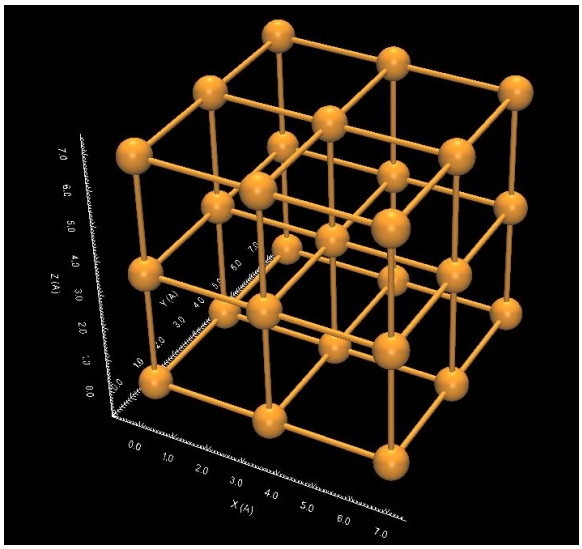


Figure 29

You can use this option to create other materials that are not in our database. Besides, you are also allowed to create your own “crazy” crystal as long as you set the data properly. Fig. 30 shows a user-defined crystal that does not exist in nature.

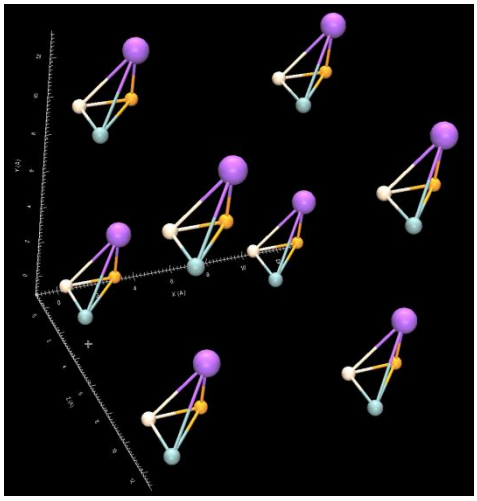


Figure 30

Miller plane

To draw miller planes, toggle on the option “Draw miller plane”. Note that miller plane is not allowed for Bravais lattice.

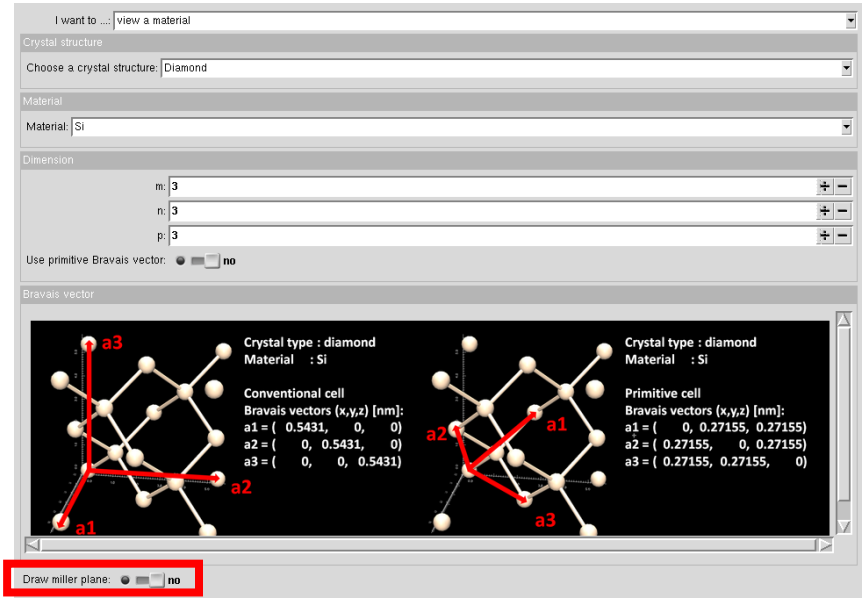


Figure 31

When toggled on, the miller plane setting menu will automatically show up.

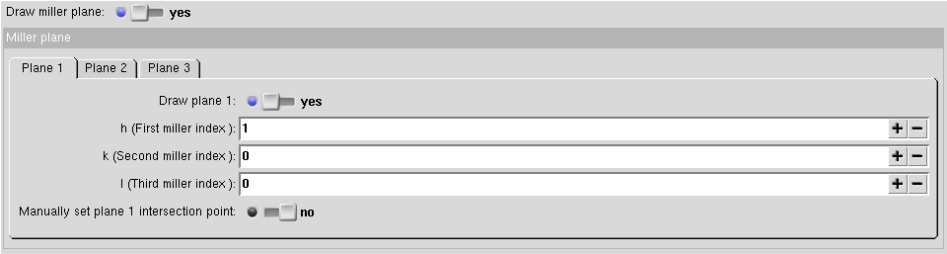


Figure 32

You can set the miller indices (h, l, k) from 0 to 7.
The size and the shape of the plane will change according to the size and the shape of the lattice grid.

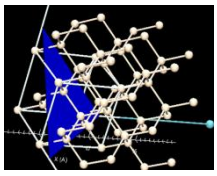


Figure 33

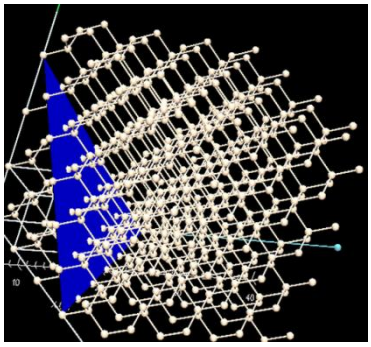


Figure 34

Plane size changed for different lattice grid size

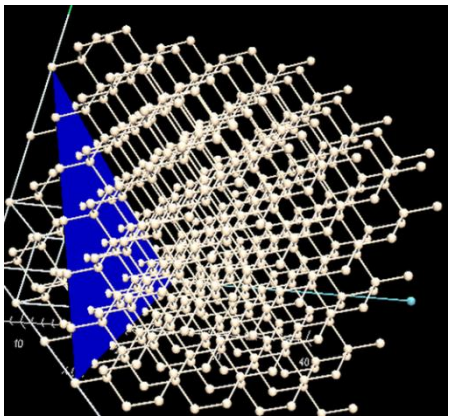


Figure 35

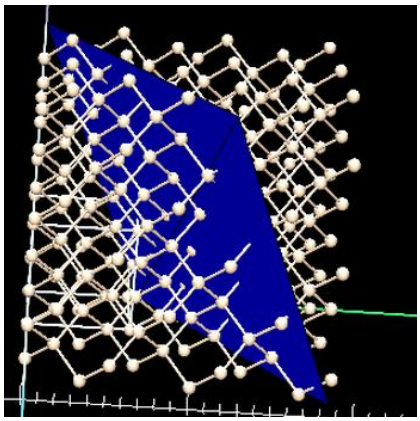


Figure 36

Plane shape changed for different miller indices

To shift the plane, toggle on the option “Manually set plane 1 intersection point”. The menu for setting the intercept points will pop up automatically

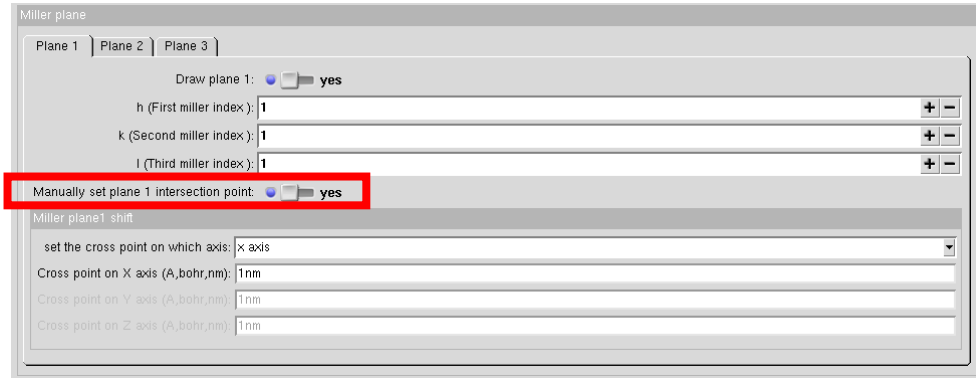


Figure 37

Select one of the 3 axes and then set the intercept point. The miller plane will cross the intercept point you set.

If you want to draw more than one plane, simply go to menu Plane 2 and Plane 3. The Miller planes will be plotted in different colors. Fig 38 shows a (1, 1, 1) plane and a (1, 1, -1) plane in a silicon lattice grid.

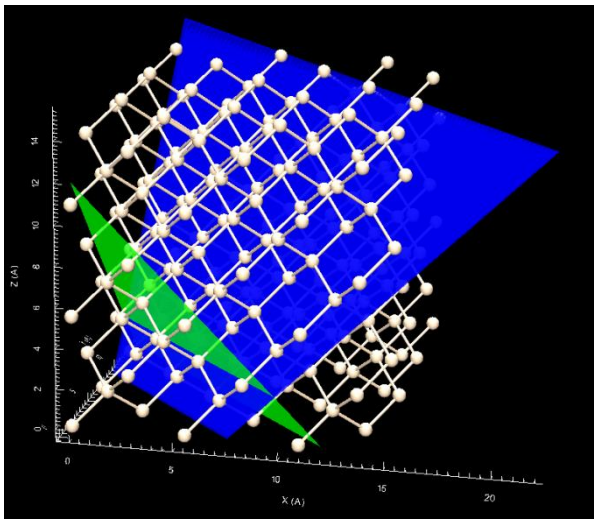


Figure 38

Together with a miller plane, we also provide views for the crystal on only one side of the plane. To view it, select “Crystal on one (the other) side of plane 1” in the result list.

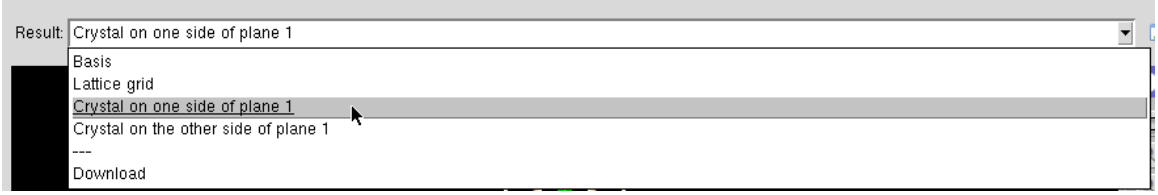


Figure 39

Figure 40 shows an example for the (1, 1, 1) plane in silicon lattice grid.

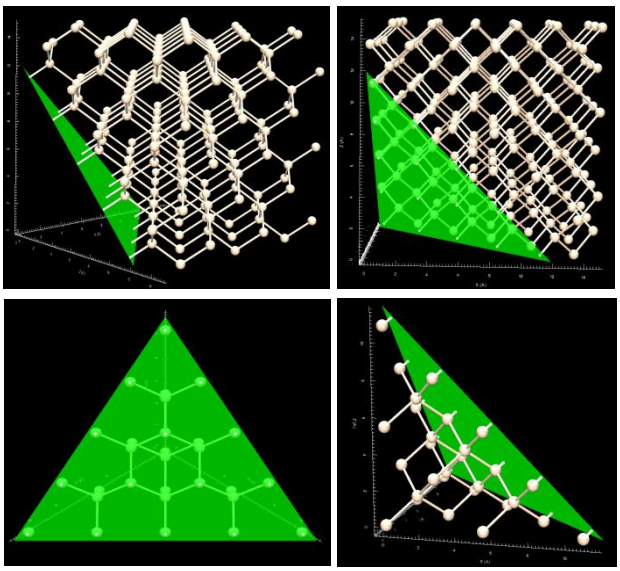
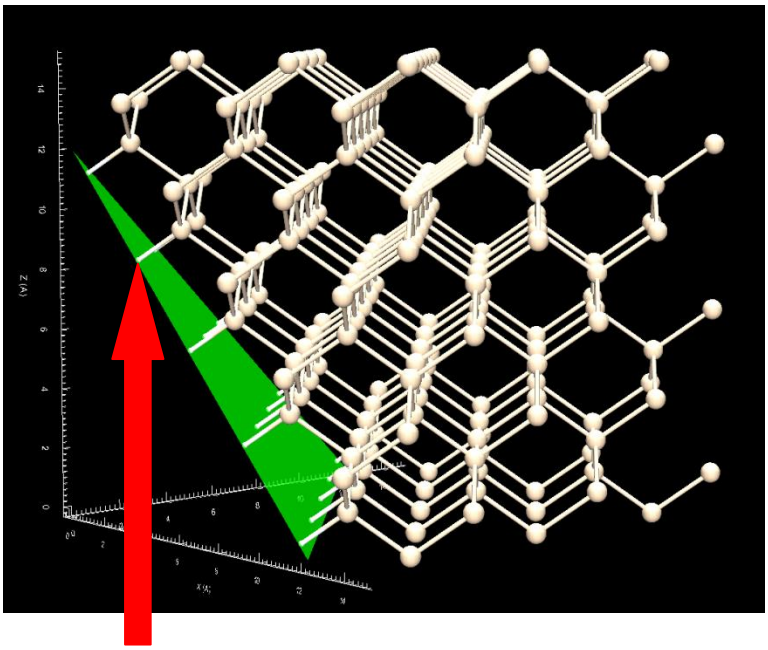


Figure 40

For every dangling bond cut by the plane, we use a hydrogen atom to terminate the bond.



Hydrogen atom

Figure 41

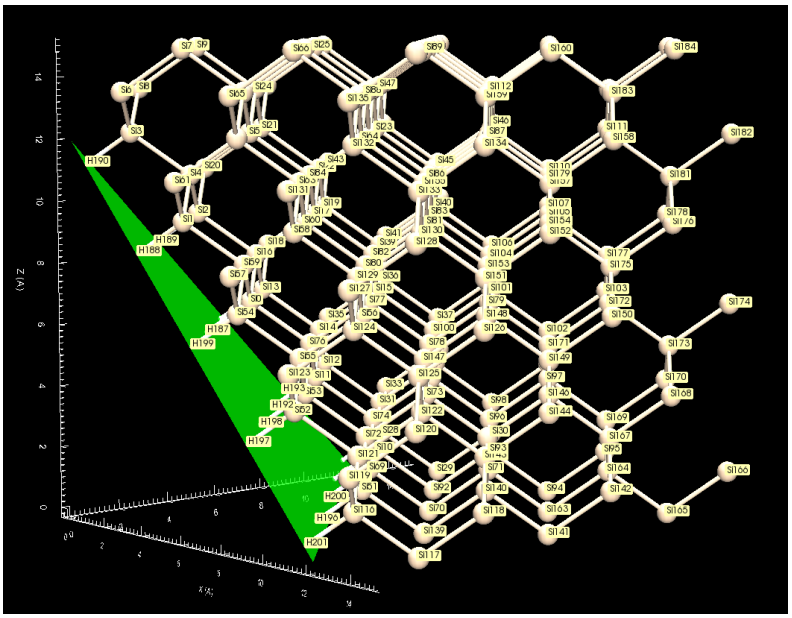


Figure 42