

Crystals

The atoms in a crystal are arranged in a periodic pattern. A crystal is made up of unit cells that are repeated at a pattern of points, which is called the Bravais lattice (fig. (1)). The Bravais lattice is basically a three dimensional abstract lattice of points.

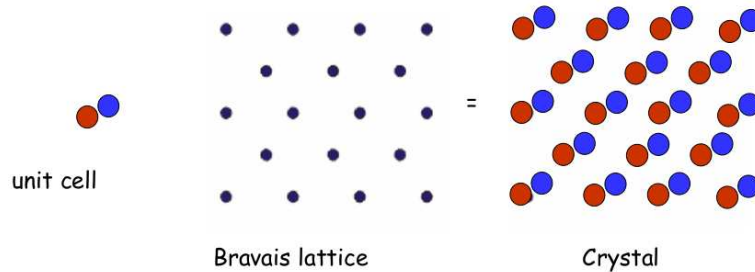


Figure 1: Unit cell - Bravais lattice - Crystal

Unit cell

The **unit cell** is the description of the arrangement of the atoms that get repeated, and is not unique - there are a various possibilities to choose it.

The **primitive unit cell** is the smallest possible pattern to reproduce the crystal and is also not unique. As shown in fig. (2) for 2 dimensions there is a number of options of choosing the primitive unit cell. Nevertheless all have the same area.

The same is true in three dimensions (various ways to choose primitive unit cell; same volume).

An example for a possible three dimensional primitive unit cell and the formula for calculating the volume can be seen in fig. (2).

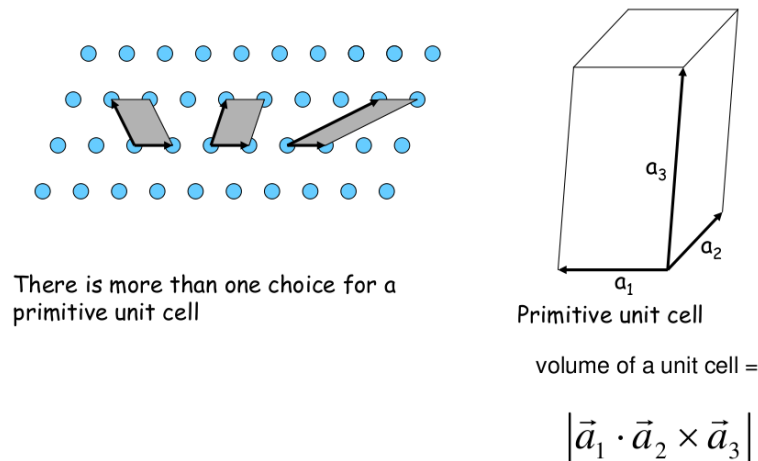


Figure 2: Illustration of primitive unit cells

The conventional unit cell is agreed upon. It is chosen in a way to display the crystal or the crystal symmetries as good as possible. Normally it is easier to imagine things when looking at the conventional unit cell.

A few conventional unit cells are displayed in fig. (3).

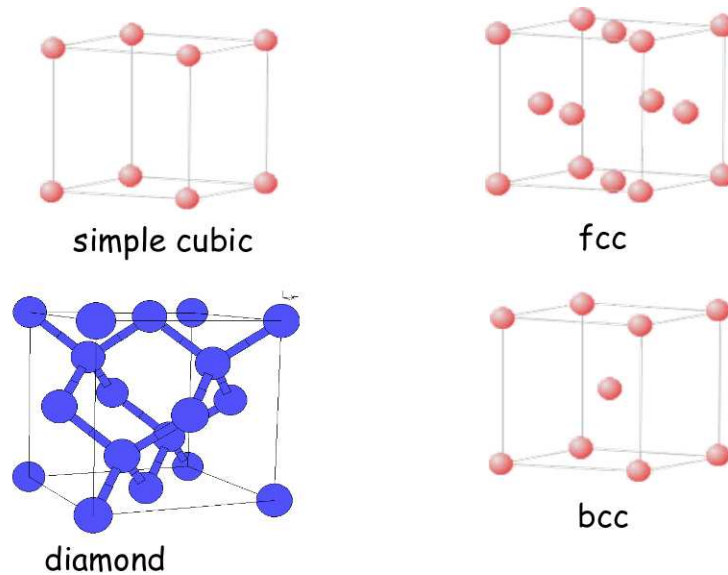


Figure 3: Illustration of conventional unit cells

- sc (simple cubic): Conventional and primitive unit cell are identical
- fcc (face centered cubic): The conventional unit cell consists of 4 atoms in comparison to the primitive unit cell which consists of only 1 atom. But the primitive unit cell doesn't describe fcc very well.
- bcc (body centered cubic): The conventional unit cell consists of 2 atoms in comparison to the primitive unit cell which consists of only 1 atom.
- diamond: The conventional unit cell consists of 8 atoms in comparison to the primitive unit cell which consists of 2 atoms. Examples for materials in diamond structure are carbon in form of diamond and silicon (which is used for semiconductors)

Details about the unit cell:

There can be two atoms of the same element but with different positions in the unit cell. This concept can be explained with the drawing fig. (4). It consists of orange and black crabs (two kinds of atoms). But some have the claws up and some have them down. So although they are the same atom they can't be put on top of another just by translations.

Which is what is done when taking the unit cell and mapping it on all the points of the Bravais lattice to create a crystal. But here also a rotation would be needed. So in this case the unit cell would consist of one orange crab with claws up, one with claws down, one black crab with claws down and one black one with claws up. But this would lead to a rather odd looking unit cell if taking all the legs and claws into concern.

So another and easier way to define the unit cell would be to start at an eye and go up to the equivalent point of an equivalent crab. Then do the same going to the right, down and back to the starting point. The resulting unit cell is rectangular and rather easy to handle. Also both primitive unit cells have the same area.



An element can have two distinct positions

Figure 4:

Diamond has a similar phenomena:

8 atoms in conventional unit cell

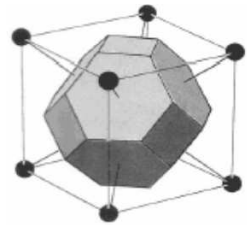
2 atoms in primitive unit cell

So more than one atom in unit cells are possible.

Wigner Seitz cell

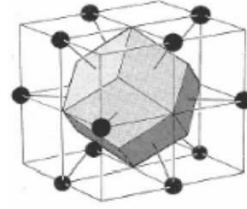
There are different ways of choosing a primitive unit cell. One of these ways is the Wigner-Seitz-cell. The Wigner-Seitz-cell has all the symmetries of the crystal (e.g. rotation by 90 degrees).

It is constructed by choosing one atom (e.g. bcc: central atom). Then draw lines to the nearest neighbours and cut all the lines in half with a plane. The Wigner-Seitz-cell consists of all points that can be reached from the central atom without crossing one of those planes. It also has the same volume as any other primitive unit cell and can also be stacked on the Bravais-lattice to construct the whole crystal. See fig. (5) for examples.



bcc

Truncated octahedron



fcc

Rhombic dodecahedron

Wigner-Seitz cells have the symmetry of the crystal

Figure 5: Wigner Seitz cell of bcc and fcc crystals

Crystall properties

Coordination Number:

Is the number of nearest neighbours an atom has in its crystall structure:

sc (simple cubic) = 6

bcc (body centered cubic) = 8

fcc (face centered cubic) = 12

hcp (hexagonal close pack) = 12

Diamond = 4

Graphite = 3

fcc and hcp have the highest possible coordination number. Diamond has a rather low number and its structure is therefore rather open.

Atomic Packing Density

Describes how much volume of the crystal is used and how much is 'filled' with empty space. hcp and fcc have the highest packing density.

The differences between the stacking of layers is displayed in fig. (6).

How to calculate the packing density:

Take a cube the size of the conventional unit cell and increase the radius of all atoms till their spheres are just touching. Then calculate how much volume is taken by the spheres and the total volume of the conventional unit cell. The ratio of those two equals the packing density.

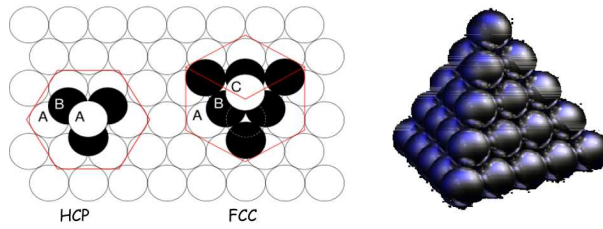


Figure 6: Illustration of hcp and fcc crystals

hcp, fcc = 0,74

bcc = 0,68

rcp (random close pack) = 0,64

sc = 0,52

Diamond is a very open structure with a lot of space inbetween. This for example is used in semiconductors where impurity atoms are purposely put into the silicon and then diffuse through it.

fcc

The shaded plain in fig. (7(a)) is the triangular lattice showing the close packed plane that is also displayed in fig. (6).

The primitive unit cell (7(b)) has only one atom but doesn't display very much. The Wigner-Seitz cell (7(c)) of fcc is a rhombicuboctahedron with only one atom inside.

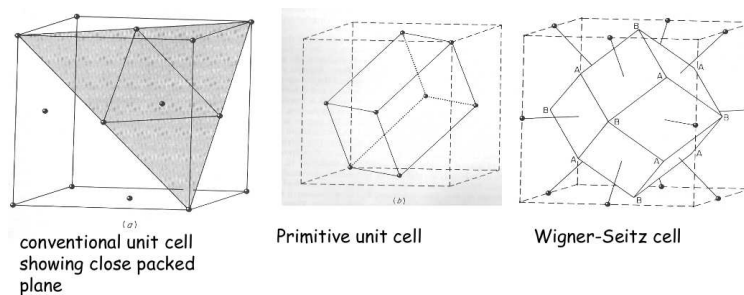


Figure 7: fcc crystal

Terminology - Miller Indices

Directions and planes are described with the Miller indices.

Directions

Are described with square brackets: $[\]$. There are three numbers in the brackets, each one indicating a direction. So the x,y,z directions are described as $[100],[010],[001]$ with Miller indices (the axes do not have to be orthogonal!).

Negative directions are described with a minus/bar over the number -> e.g.: $[\bar{1}00]$.
 45 degrees in the x,y-plane is the $[110]$ direction.

Families of directions:

Are written with $\langle \rangle$

Any set of equivalent directions belong to a family.

E.g. cubic crystal: $[100]$ is equivalent to $[001]$ is equivalent to $[010]$

Planes

Are also described with Miller indices, but with round brackets (e.g.: (100)).

If the crystal is cubic (equivalent to perpendicular axes) the planes are perpendicular to the corresponding directions. E.g.: (111) is perpendicular to $[111]$.

Families of planes:

Are written with $\{ \}$

Any set of equivalent planes belong to a family.

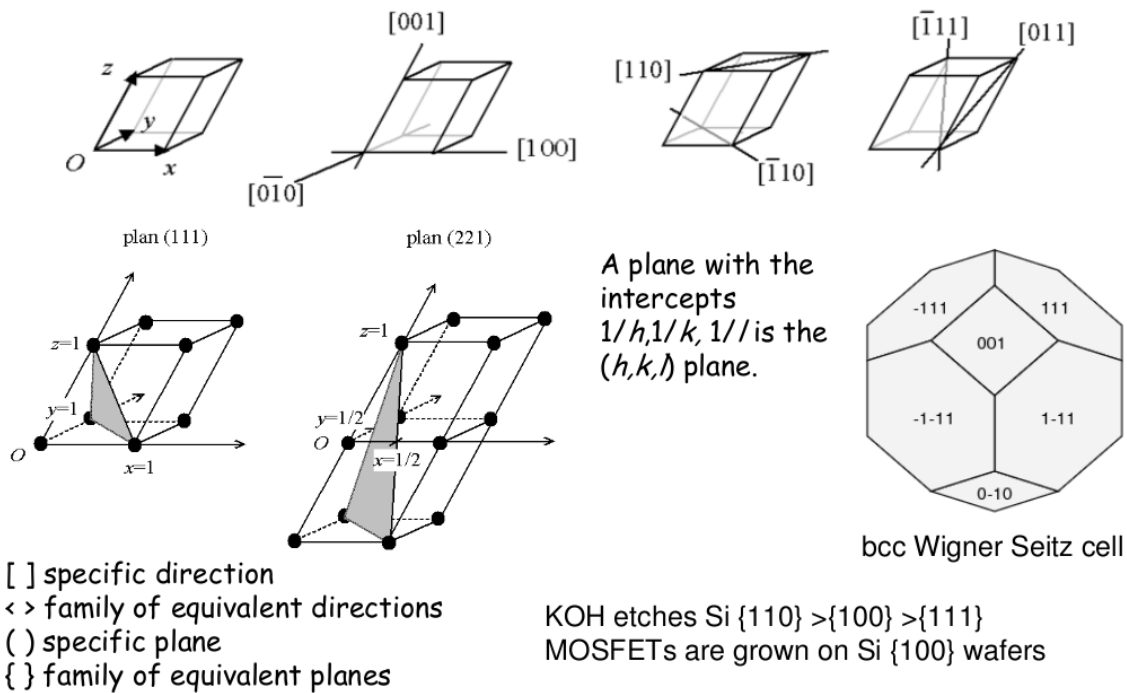


Figure 8: Miller indices

How to determine the Miller indices of a plane

1. Find the intercepts of the plane on the axes in terms of the lattice constants a_1, a_2, a_3 . (e.g.: intercepts at $3 * a_1, 2 * a_2, 2 * a_3$)

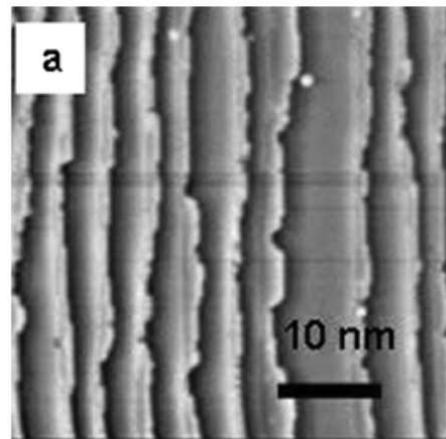
2. Take the reciprocal of those numbers. (e.g.: $\frac{1}{3}, \frac{1}{2}, \frac{1}{2}$)
3. Reduce the reciprocals to three integers having the same ratio, usually the smallest three integers. (e.g.: 2,3,3)
4. The result, enclosed in parantheses (hkl), is called the Miller index of the plane. (e.g. (233))

The Wigner-Seitz-cell displays the equivalent planes quite good.

KOH has different etch-rates in different directions on Si. So if you etch Si with it the (111)-plane will be exposed. This is used for microelectronics.

Example:

The picture in fig. 9 is an fcm-image of metal looking at the (15,15,13) pane. This is nearly (111). Steps can be seen in the picture because the picture is taken in that direction. If the picture would have been taken in (111) it would only show a smooth surface.



Rh(15,15,13) fcc

Figure 9: Rh (15,15,13)

Example:

The two pictures in fig. (10) are also fcm-images.

Si(100):

Atomic steps can be seen on the surface (and also that on some points atoms are missing on the surface). An interesting thing about it are the lines that come across. They come from the diamond structure: Every atom normally bonds to four other atoms. But the ones on the surface only bond with two atoms below and have the other two bonds hanging either to the one or the other side on the surface (they dimerize). So they bond with the atom next to them. The crystals on the surface then have bigger unit cells.

This is called the 2-by-1 reconstruction.

Si(111):

If the crystal is cut in (111) the result is a relatively complicated 7x7-reconstruction.

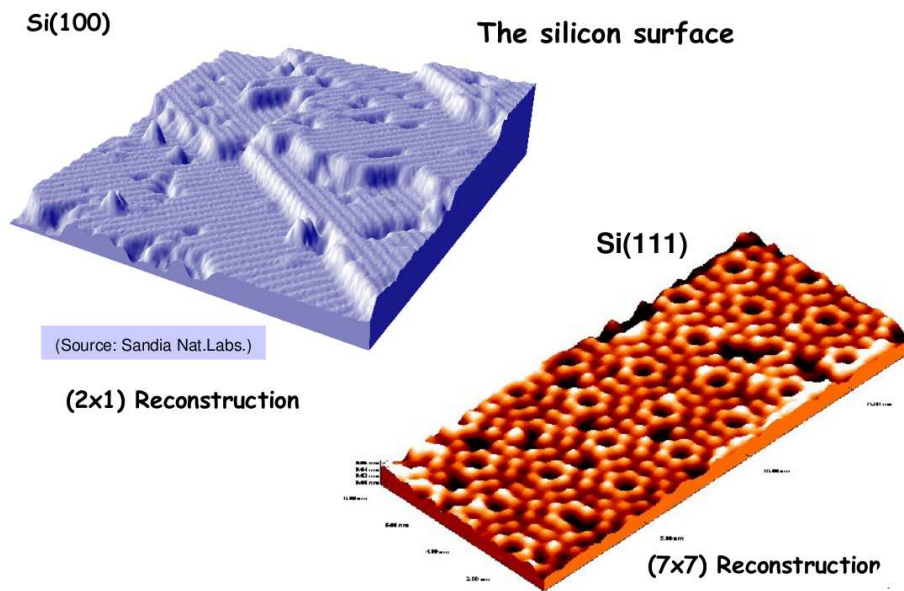


Figure 10: Si