Crystal Structure

The crystal structure can be described in terms of a space lattice (which is a regular periodic array of points in space), with a group of atoms attached to every lattice point. In other words, it is called a lattice with basis {where a basis is a set of atoms (or may be a single atom) that can be placed near (or on) each lattice point (or lattice site)}. Thus crystal structure is formed by placing a basis at each lattice site repeatedly, namely,

$\Rightarrow$ Crystal structure = Space Lattice + Basis

[Note: This arrangement of atoms in a crystal lattice is periodic, as shown in figure 1]

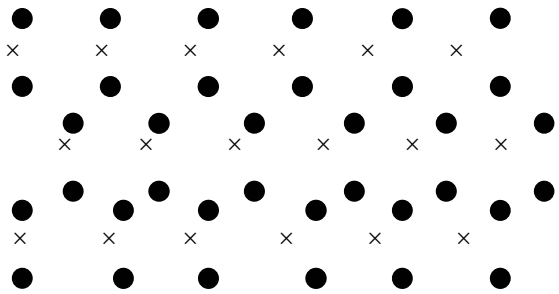

Figure 1: Periodic crystal structure is described as a lattice with basis

Crystal lattice can be classified to

1. Bravais crystal lattice
2. NonBravais crystal lattice

1. Bravais crystal lattice:

All lattice points (or lattice sites) look equivalent no matter from which orientation you look at them. Also all atoms at the lattice points are of the same kind.

[Note: There are 14 different lattice types in 3-D (see chap.7)]

Formation of Bravais lattice:

In 3-D, a Bravais lattice can be defined and generated by three fundamental vectors i.e. $\vec{a}_1$, $\vec{a}_2$ and $\vec{a}_3$ which are called the primitive vectors.

[Note: Primitive vectors are not necessarily perpendicular to each other and they are not all in the same plane].

The position vector of a lattice point:

Any lattice point of the 3-D Bravais lattice can be defined by the position vector $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$.

Here n_1, n_2 and n_3 are integers {each may have zero, negative or positive value}. Also $0 \le n_1 < N_1$, $0 \le n_2 < N_2$ and $0 \le n_3 < N_3$, where $N = N_1 N_2 N_3$ is the number of lattice sites of a finite 3-D lattice.

[Note: All crystal lattices have discrete translational symmetry. If displaced by a properly selected lattice vector $\vec{R}$, every atom moves to the position of an identical atom in the crystal].

A simple version of a Bravais lattice☹(2-D Bravais lattice):

For example, if $\vec{a}_1$ and $\vec{a}_2$ are drawn from a common origin, as shown in figure 2, for a 2-D Bravais lattice then the point , P, will have a position vector w.r.t this origin as: $\vec{R} = 2\vec{a}_1 + 2\vec{a}_2$ (where $n_1 = n_2 = 2$) , while another lattice point , Q, may have a different position vector, namely, $\vec{R} = -\vec{a}_1 - \vec{a}_2$ (where $n_1 = n_2 = -1$).

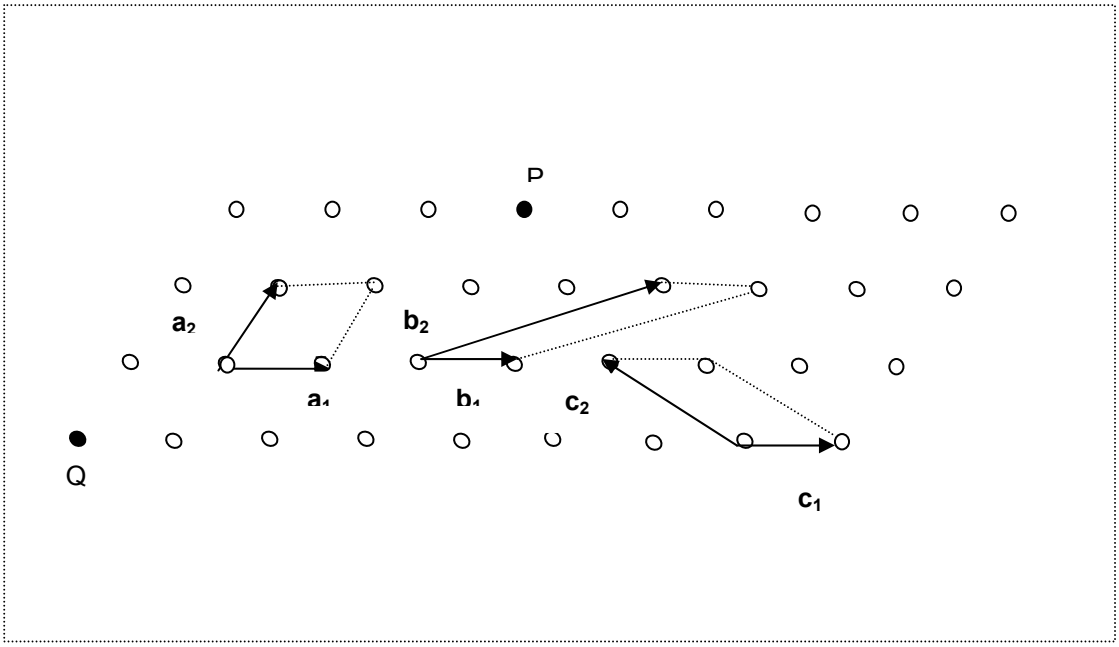

Figure 2: Three different choices of pairs of primitive vectors. Each set gives the smallest possible parallelogram area.

We need to justify the argument that a Bravais lattice is an infinite array of discrete points with an arrangement and orientation that appear the same no matter from which orientation you look at it. It is easy to prove that, in 2-D, by constructing different areas from the three set of vectors ($\vec{a}_1$ and $\vec{a}_2$), ($\vec{b}_1$ and $\vec{b}_2$), and ($\vec{c}_1$ and $\vec{c}_2$). Now if each constructed area gives the smallest parallelogram then the vectors constructing this area are primitive. When the area of all parallelograms turn to be the same it means that there is more than one choice for set of primitive vectors. [You should try to prove the above example analytically].

Example of a 3-D Bravais lattice:

The simple Cubic Bravais lattice is a primitive lattice. This is shown in figure 3.

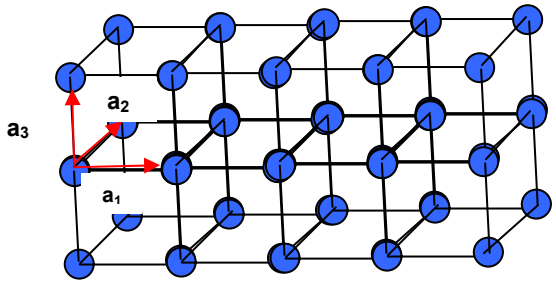

Figure 3: Three dimensional primitive cell is shown in a periodic crystal structure.

Exercise: Solve problem 8a in the text book.