

## Simple Crystal Structure

tion, reflection, and inversion are the point operations and their combination give certain symmetry elements which collectively determine the symmetry of space around a point. The group of such symmetry operation at a point is called a **point group**.

In two-dimension space, rotation and reflection are the only point operations. Their combinations yield 10 different point groups designated as 1,  $1m$ , 2,  $2mm$ , 3,  $3m$ , 4,  $4mm$ , 6, and  $6mm$ . In three-dimensional space, however, the situation is complicated due to the presence of additional point operations such as inversion. There are total of 32 point group in a three-dimensional lattice.

The crystals are classified on the basis of their symmetry which is compared with the symmetry of different point groups. Also, the lattices consistent with the point group operations are limited. Such lattices are known as *Bravais lattices*. These lattices may further be grouped into distinct crystal systems.

The point symmetry of crystal structures as a whole is determined by the point symmetry of the lattice as well as of the basis. Thus in order to determine the point symmetry of a crystal structure, it should be noted that

1. a unit cell might show point symmetry at more than one locations inside it, and
2. the symmetry element comprising combined point and translation operations might be existing at these locations.

The group of all the symmetry elements of a crystal structure is called *space group*. It determined the symmetry of a crystal structure as a whole. There are 17 and 230 distinct space group possible in two and three dimensions respectively.

### Types of Lattices

The number of point groups in three dimensions is 32. These point groups form the basis for construction of different types of lattices. Only those lattices are permissible which are consistent with the point group operations. Such lattices are called *Bravais lattices*. 32 point groups in three dimensions produce only 14 distinct Bravais lattices. These Bravais lattices further become parts of 7 distinct crystal systems.

All the seven crystal systems of three-dimensional space and corresponding Bravais lattice are listed in Figure.

A lattice point lying at the corner of a cell is shared by eight such cells and the one lying at the face center position is shared by two cells. Therefore, the contribution of the lattice point lying at the corner towards a particular cell is  $1/8$  and that of a point lying at the face center is  $1/2$ . The effective number of lattice points belonging to a particular cell is given by

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{8}$$

### Close-Packed Structure

Close-packed structures are mostly found in monoatomic crystals having non-directional bonding, such as metallic bonding. In these structures, the coordination number of each atom is 12, i.e., each atom is surrounded by twelve similar and equal sized neighbours. Out of these twelve neighbours, six lie in one plane, three in an adjacent parallel plane above this plane and three in a similar plane below it. There are two types of close-packed structures:

1. Hexagonal close-packed (*hcp*) structure
2. Face-centered cubic (*fcc*) structure

## Hexagonal close-packed structure

Consider a layer of similar atoms with each atom surrounded by six atoms in one plane as shown in fig(3). Another similar layer B can be placed on top of layer A such that the atoms of layer B occupy the alternate valleys formed by the atoms of layer A. If a third similar layer is placed on top of the B-layer in such a way that the atoms of B-layer exactly overlap the atoms of A-layer and this type of stacking is repeated successively, the following layered arrangement is obtained:  $\cdots ABABAB \cdots$ . This type of stacking is called *hcp stacking* and the structure is known as *hexagonal close-packed structure*. The name corresponds to the shape of the conventional unit cell which is hexagonal and is shown in figure (1). There are twelve atoms located at the corners, two at the centers of the basal planes, and three completely inside the hexagon forming a part of the B-layer. The effective number of atoms in a unit cell is

$$12(1/6) + 2(1/2) + 3 = 6$$

The interatomic distance for the atoms within a layer is  $a$ . The distance between the two adjacent layers is  $c/2$ ,  $c$  being the height of the unit cell. For an ideal *hcp* structure,  $c = 1.633a$ .

It may be noted that although the structure is *hcp*, the space lattice is simple hexagonal with basis consisting of two atoms placed in such a way that if one atom lies at the origin, the other atom lies at the point  $(2/3, 1/3, 1/2)$ . The shaded portion in figure (1) represents the primitive cell of this structure. It contains 2 atoms instead of one which is due to the presence of the basis. Also, the volume of the primitive cell is exactly one-third of the volume of the hexagonal cell.

The *packing fraction*,  $f$ , is defined as the ratio of the volume occupied by the atoms present in a unit cell to the total volume of the unit cell. It is also referred to as the *packing factor* or *packing efficiency* of the unit cell. From the primitive cell, we find

$$f = \frac{2(4/3)\pi r^3}{a(a \sin 60^\circ)c}$$

where  $r$  is the atomic radius. Using  $c = 1.633a$  and  $a = 2r$ , we get  $f = 0.74$ . Thus, in an ideal *hcp* structure, 74% of the total volume is occupied by atoms. Metals like Mg, Zn, Cd, Ti, etc. exhibit this type of structure.

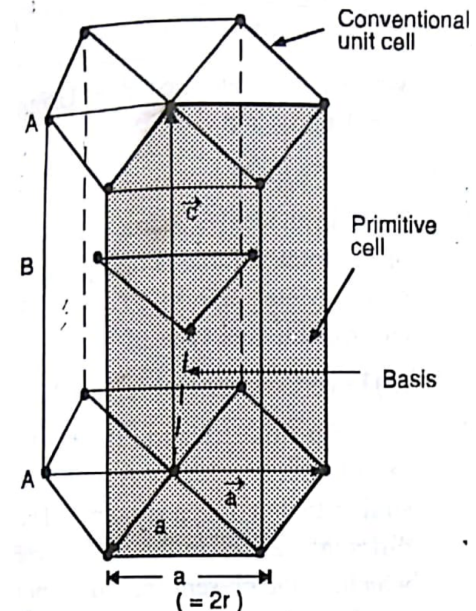


Figure 1: Conventional and primitive cells of hexagonal close-packed structure.

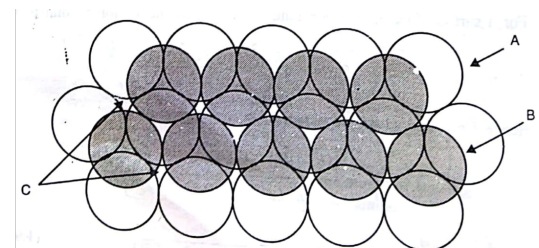


Figure 2: Layered arrangement of close-packed structure.

## Face-Centered Cubic Structure

In this structure, the stacking of first two layers A and B is similar to that of *hcp* structure. The difference arises in the third layer which, in the present case, does not overlap the first layer. The atoms of the third layer occupy the positions of those valleys of the A-layer which are not occupied by the B-layer atoms. The third layer is designated by the letter C. The fourth layer exactly overlaps the first layer and the sequence is repeated. Thus *fcc* structure is represented by the following stacking sequence:  $\dots ABCABCABC\dots$ . Unit cell of *fcc* has effective number of atoms equal to 4. The atoms touch one another along the face diagonals. The length of the cube edge,  $a$ , and the atomic radius,  $r$ , are related to each other as

$$4r = \sqrt{2}a$$

The packing fraction,  $f$ , is given by

$$f = \frac{4(4/3)\pi r^3}{a^3} = 0.74$$

Thus the packing fraction of *fcc* structure is exactly the same as that of the *hcp* structure which is expected because of the close-packed nature of both the structures. Also, the coordination number of each atom is 12. Examples of materials having this type of structure are Cu, Ag, Au, Al, etc.

## Loose-packed structures

A loose-packed structure is that in which the coordination number of an atom is less than 12 or the packing fraction is less than 0.74. Among the various possible loose-packed structures, the most common and the simplest are the *body-centered cubic (bcc)* and the *simple cubic (sc)* structures.

### Body-centered Cubic Structure (bcc)

The conventional unit cell of *bcc* structure has cubical shape with atoms located at the corners and body center. Thus the effective number of atoms per unit cell is 2. The coordination number of each atom is 8. The atoms touch one another along the body diagonal. Thus  $a$  is related to  $r$  as

$$4r = \sqrt{3}a$$

The packing fraction is given by

$$f = \frac{2(4/3)\pi r^3}{a^3} = 0.68$$

The example of materials exhibiting *bcc* structures are Na, K, Mo, W, etc.

### Simple Cubic Structure (sc)

The conventional unit cell of *sc* structure has atoms located at the corners only and touch one another along the cube edges. Thus in *sc* structures, we have,

$$a = 2r$$

The coordination number of each atom is 6. The packing fraction is given by

$$f = \frac{1(4/3)\pi r^3}{a^3} = 0.52$$

Only polonium exhibits this type of structure at room temperature.

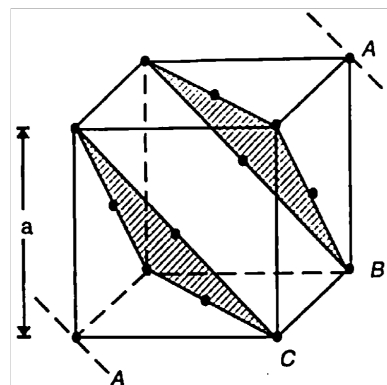


Figure 3: Layered arrangement of close-packed structure.