UNIT -IV CRYSTAL PHYSICS

TOPIC – IV CN AND PF FOR SC AND BCC

1.11 CHARACTERISTIC OF A UNIT CELL

A unit cell is characterized by the following properties

i) Number of atoms per unit cell

ii) Co-ordination number

iii) Nearest neighboring distance

iv) Atomic radius and

v) Packing factor or density factor

(i) Number of atoms per unit cell:

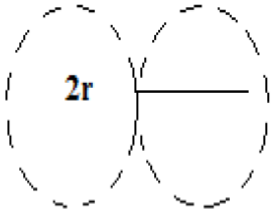
It is the number of atoms possessed by a unit cell. This can be determined if the arrangement of atoms inside the unit cell is known.

(ii) Co-ordination number:

It is the number of nearest atoms directly surrounding a particular atom in a crystal. The co-ordination number gives the information about the packing of atoms in the structure. i.e., whether the crystal structure is closely packed structure or loosely packed structure. If the co-ordination number is high, then the structure is more closely packed. If it is low, then the structure is loosely packed.

(iii) Nearest neighboring distance (2r):

The distance between the centers of two nearest atoms is called nearest neighboring distance. It is expressed in terms of the length of edge of the unit cell 'a' and it is 2r.



(iv) Atomic radius (r):

It is half of the nearest neighbouring distance in a crystal. It is denoted by 'r'. It is usually expressed in terms of cube edge 'a'(lattice parameter).(Fig 1.12).

$$r = \frac{a}{2}$$

(v) Packing factor (PF):

It is defined as the ratio of total volume occupied by the atoms in a unit cell to the total volume of a unit cell.

$$packing\ factor = \frac{Total\ volume\ occupied\ by\ the\ atoms\ in\ a\ unit\ cell\ (v)}{Total\ volume\ of\ the\ unit\ cell\ (V)}$$

$$PF = \frac{Number\ of\ atoms\ present\ in\ a\ unit\ cell\ \times\ Volume\ of\ one\ atom}{Total\ volume\ of\ the\ unit\ cell}$$

A high packing factor indicates that the atoms are very closely packed and therefore there is very little unoccupied space. On the other hand, a low packing factor indicates loose packing of atoms and hence there is relatively more unoccupied space. It also called as **density of packing.**

1.12 CRYSTAL STRUCTURES - SIMPLE CUBIC (SC) STRUCTURE

This is one of the most common and simplest shapes found in crystals. The simple cubic unit cell is a cube (all sides of the same length and all face perpendicular to each other) with an atom at each corner of the unit cell. These corner atoms touch each other along cube edges. The figure 1.13 represents the arrangement of atoms in simple cubic crystal.

Fig 1.13 simple cubic system

Number atoms per unit cell:

The unit of a simple cubic structure is shown in fig 1.14. There are 8 atoms, one atom at each corner of the unit cell. Each corner atom is shared by 8 surrounding unit cell.

Therefore, Share of each unit cell $= \frac{1}{8}$ of corner atom

Total number of atom in unit cell $= \frac{1}{8} \times 8$

$= 1$ atom

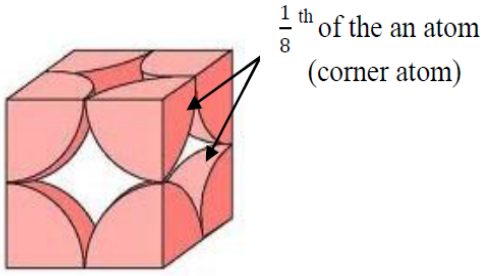


Fig 1.14

Co-ordination number:

Simple cubic unit cell has 8 corner atoms. Let us consider one of the corner atoms (say X). It is shared by 8 adjacent unit cells as shown in fig 1.15.

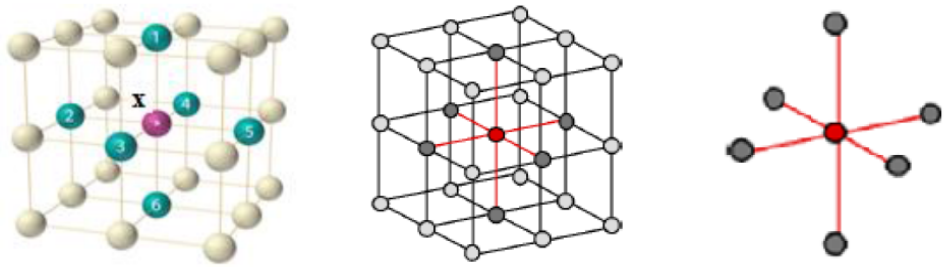


Fig 1.15

There are 4nearest neighbouring atoms to this particular atom 'X' which are shown by 2, 3, 4 and 5 in a plane (horizontal plane). Further, there are 2 more nearest atoms, one directly above (atom 1) and the other one directly below (atom 6) to the atom X. Thus, there are only six (4+2) nearest neighbours to the atom X.

Hence, the co-ordination number for simple cubic is 6.

Atomic radius:

Consider a face of the unit cell of a simple cubic structure (fig 1.16). The atoms touch each other along the edges of the cube. It is clear that the distance between the centers of two nearest atoms is just equal to the cube edge 'a'.

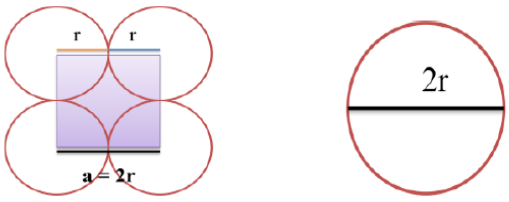


Fig 1.16

If 'a' is the side of the unit cell and 'r' its radius, then, from 1.16,

$$2r = a$$

$$\boxed{r = \frac{a}{2}}$$

Atomic Packing factor:

Number of atoms per unit cell = 1

Volume of one unit cell, $v = \frac{4}{3}\pi r^3$

Where r is the atomic radius

Atomic radius, $r = \frac{a}{2}$ and a = 2r

Total volume of the unit cell, $V = a^3$

We know that, Packing factor $= \frac{v}{V}$

Substituting the values of v and V in above equation we get,

$$PF = \frac{\frac{4}{3}\pi r^3}{a^3}$$

Substituting the value of 'a' in above equation we get,

$$PF = \frac{\frac{4}{3}\pi r^3}{(2r)^3} = \frac{\frac{4}{3}\pi r^3}{2^3 r^3}$$

$$= \frac{\frac{4}{3}\pi}{8} = \frac{4\pi}{24}$$

$$= \frac{\pi}{6} = 0.5236$$

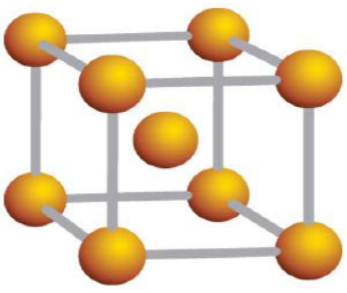
PF = 52 %

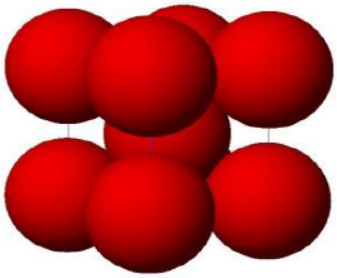
Thus, 52% of the volume is occupied by the atoms and remaining 48% volume is vacant.

Example: Only one element Polonium (Po) at a certain temperature range exhibits this crystal structure.

1.13 BODY CENTERED CUBIC (BCC) CRYSTAL SYSTEM

The body-centered cubic unit cell is a cube (all sides of the same length and all face perpendicular to each other) with an atom at each corner of the unit cell and an atom in the center of the unit cell. These corner atoms do not touch each other but all these corner atoms touch the body center atom. The figure 1.17 represents the arrangement of atoms in BCC crystal.





Number atoms per unit cell:

The unit of a Body-centered cubic structure is shown in fig 1.18.

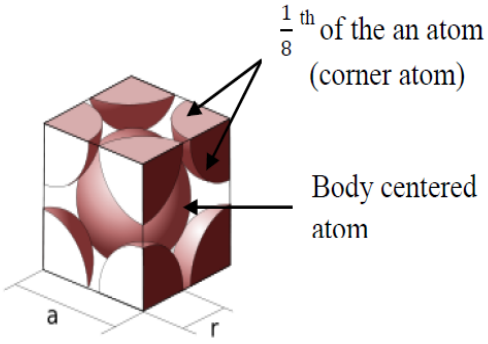


Fig 1.18 Body-centered cubic unit cell

There are 8 atoms, one atom at each corner of the unit cell. Each corner atom is shared by 8 surrounding unit cell. Therefore,

$$\text{Share of each unit cell} = \frac{1}{8} \text{ of corner atom}$$

$$\text{Total number of corner atom in unit cell} = \frac{1}{8} \times 8 = 1 \text{ atom}$$

There is one atom at the body center of every unit cell.

Therefore,

Total number of atoms per unit cell in BCC = Total number of corner atom in unit cell + Total number of body centered atom

= 1+1

= 2 atoms

Co-ordination number:

In the unit cell of BCC structure, there is one atom (say atom X) at the body center of the unit cell. Further there are '8' atoms at the 8 corners of the unit cell as shown in fig 1.19.

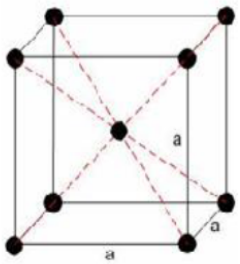


Fig 1.19

The corner atoms do not touch each other but all the '8' corner atoms touch the body center atom along the body diagonal. Thus, for body center atom 'X', there are 8 nearest neighbours (ie., 8 corner atoms). Hence, the co-ordination number of body centered cubic structure is 8.

Atomic radius:

The corner atoms do not touch each other. However, each corner atoms touches the body centered atom along the body diagonal of the cube. The unit cell for BCC is shown in fig 1.20.

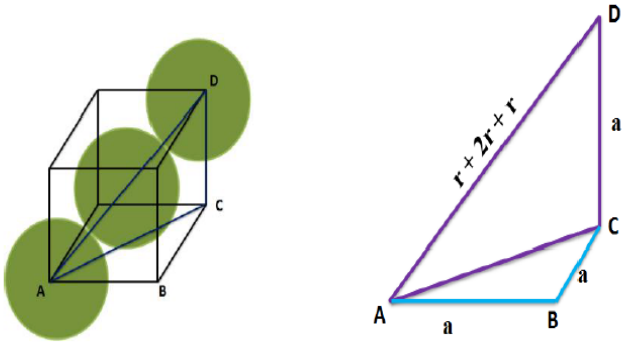


Fig 1.20

It is clear from fig 1.17 that the nearest neighbouring atoms are corner atoms A and D and the body center atom. Consider the atoms at A, D and the body center atom. These atoms lie in one straight line along the body diagonal AD of the cube.

From the right angled △ ABC,

$$AC^2 = AB^2 + BC^2$$

Substituting the values for AB and BC from the fig 1.17, we have

$$AC^2 = a^2 + a^2$$

$$AC^2 = 2a^2$$

From the geometry of figure 1.17,

$$AD = r + 2r + r = 4r$$

On squaring on both sides, we get

$$AD^2 = (4r)^2$$

From the right angled triangle ACD,

$$AD^2 = AC^2 + CD^2$$

$$= AB^2 + BC^2 + CD^2$$

Substituting the values for AD^2, AB^2, BC^2 and CD^2, we get

$$(4r)^2 = a^2 + a^2 + a^2$$

$$16r^2 = 3a^2$$

$$r^2 = 3a^2/16$$

Taking square root on both sides, we get

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

Atomic packing factor:

Number of atoms per unit cell = 2

$$\text{Volume of 2 atoms, } v = 2 \times \frac{4}{3}\pi r^3 = \frac{8}{3}\pi r^3$$

Where r is the atomic radius

$$\text{Atomic radius, } r = \frac{a\sqrt{3}}{4} \text{ and } a = \frac{4r}{\sqrt{3}}$$

Total volume of the unit cell, $V = a^3$

We know that, $\text{Packing factor} = \frac{v}{V}$

Substituting the values of v and V in above equation we get,

$$PF = \frac{\frac{8}{3}\pi r^3}{a^3}$$

Substituting the value of 'a' in above equation we get,

$$PF = \frac{\frac{8}{3}\pi r^3}{\left(\frac{4r}{\sqrt{3}}\right)^3} = \frac{\frac{8}{3}\pi r^3}{4^3 r^3/\sqrt{3}^3} \qquad (\sqrt{3} \times \sqrt{3} \times \sqrt{3} = 3\sqrt{3})$$

$$= \frac{\frac{8}{3}\pi r^3}{\frac{64r^3}{3\sqrt{3}}} = \frac{8}{3}\pi r^3 \times \frac{3\sqrt{3}}{64r^3}$$

$$= \frac{\sqrt{3}\pi}{8} = 0.6798$$

$$PF = 68\ \%$$

Thus, 68% of the volume is occupied by the atoms and remaining 32% volume is vacant.

Example: Tungsten, Chromium and Molybdenum.