UNIT -IV CRYSTAL PHYSICS

TOPIC – V CN AND PF FOR FCC AND DIAMOND

1.14 FACE CENTERED CUBIC (FCC) CRYSTAL STRUCTURE

Face Center Cubic Structure consists of an atom at each cube corner and an atom in the center of each cube face. The FCC structure is shown in fig.l.21. These corner atoms do not touch each other but all these corner atoms touch the face center atom.

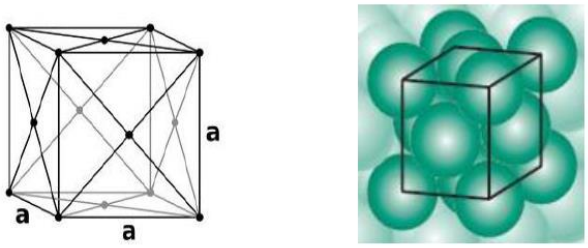


Fig 1.21

Number atoms per unit cell:

The unit of a Face-centered cubic structure is shown in fig 1.22. It consists of two types of atoms such as corner atoms and face centered atoms.

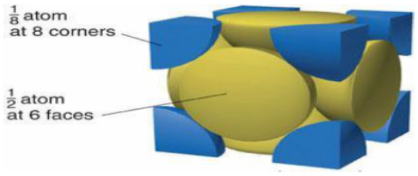


Fig 1.22 Face-centered cubic unit cell

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

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

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

Each face centered atom is shared by only two unit cell, which lie on either side of the atom. Similarly we have six face centered atoms in a unit cell.

Therefore,

$$\text{Total number of face centered atom in unit cell} = \frac{1}{2} \times 6 = 3 \text{ atoms}$$

Therefore,

$$\begin{aligned} \text{Total number of atoms per unit cell in FCC} &= \text{Total number of corner atom in unit cell} + \text{Total number of face centered atom} \\ &= 1 + 3 \\ &= 4 \text{ atoms} \end{aligned}$$

Co-ordination number:

To calculate the co-ordination number, for FCC, let us consider a corner atom (X) as shown in fig 1.23. In its own plane it has 4 face centered atoms (5, 6, 7, 8) as nearest neighbours. In a plane which is lie just above this corner atom, it has 4 more face centered atoms (1, 2, 3, 4) as nearest neighbours. In a plane which is lie just below this corner atom, it has 4 more face centered atoms (9, 10, 11, 12) as nearest neighbours. Therefore, the total number of nearest atoms to any corner atom is 4+4+4=12.Hence, the co-ordination number for FCC is 12.

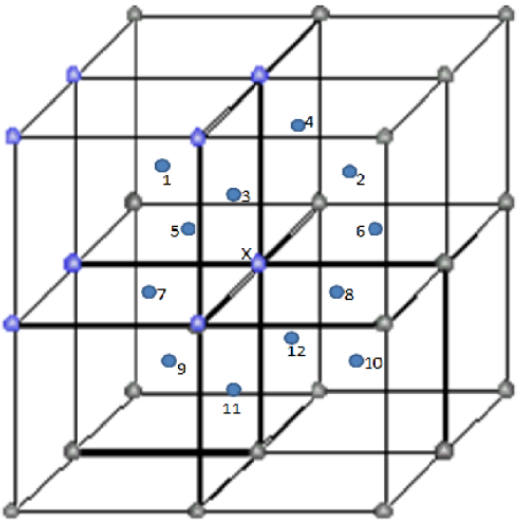


Fig 1.23

Atomic radius:

The corner atoms do not touch each other. However, each corner atoms touches the face centered atoms along the diagonal of the face of the cube as shown in fig 1.24 (a).

It is clear from fig 1.23 that the nearest neighbouring atoms are corner atoms A and C and the face center atom. Consider the atoms at A, C and the face center atom. These atoms lie in one straight line along the face diagonal AC of the cube.

From the right angled △ ABC,

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

Substituting the values for AB and BC from the fig 1.20 (b), we have

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

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

Taking square root on both sides, we get

$$AC = \sqrt{2}a$$

From the geometry of figure 1.20,

$$AC = r + 2r + r = 4r$$

Substituting the values for AC, we get

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

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

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

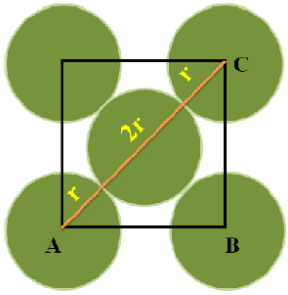


Fig 1.24 (a)

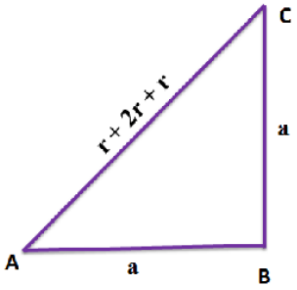


Fig 1.24 (b)

Atomic packing factor:

Number of atoms per unit cell = 4

Volume of 2 atoms, $v = 4 \times \frac{4}{3}\pi r^3 = \frac{16}{3}\pi r^3$

Where r is the atomic radius

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

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,

$$PF = \frac{\frac{16}{3}\pi r^3}{a^3}$$

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

$$PF = \frac{\frac{16}{3}\pi r^3}{(2\sqrt{2}r)^3} = \frac{\frac{16}{3}\pi r^3}{2^3 r^3 \sqrt{2^3}} \qquad (\sqrt{2} \times \sqrt{2} \times \sqrt{2} = 2\sqrt{2})$$

$$= \frac{\frac{16}{3}\pi r^3}{16\sqrt{2}r^3} = \frac{1}{3\sqrt{2}}\pi$$

$$= 0.7402$$

$$PF = 74\ \%$$

Thus, 74% of the volume is occupied by the atoms and remaining 26% volume is vacant.

1.16.1 DIAMOND CUBIC STRUCTURE

The diamond structure is an FCC with the basis of two carbon atoms, viz., 'X' and 'Y'. The 'X' atom is located with origin of (0, 0, 0) and the 'Y' atom is located with origin of $\left(\frac{a}{4}, \frac{a}{4}, \frac{a}{4}\right)$ where 'a' is the lattice constant of the FCC lattice. The figure 1.30 illustrates the diamond structure.

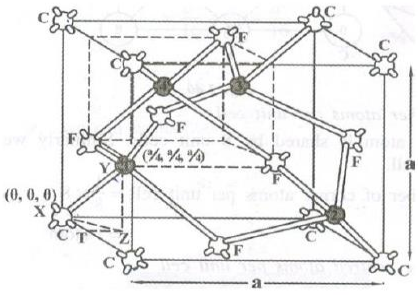


Fig 1.30: The diamond structure

Thus, from fig 1.30, we can say that the diamond structure is formed due to the combination of two interpenetrating FCC sub lattices, having the origin (0, 0, 0) and $\left(\frac{1}{4},\frac{1}{4},\frac{1}{4}\right)$, along the body diagonal.

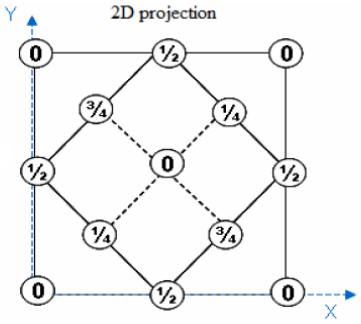


Fig 1.31 The diamond unit cell

The figure 1.31 shows a the unit cell of the diamond structure with co-ordinates of each point and the tetrahedral bonds of the nearest neighbours. The diamond unit cell has 4 tetrahedral bonds as shown in figure 1.27.

Number of atoms per unit cell:

The unit cell has 8 corner atoms, 6 face-centered atoms and 4 atoms inside the cube. Since each corner atom is shared by 8 adjacent unit cells and each face-centered atom is shared by 2 unit cells. Therefore,

The number of atoms /unit cell = (⅛) x 8 + (½) x 6 + 4 = 8

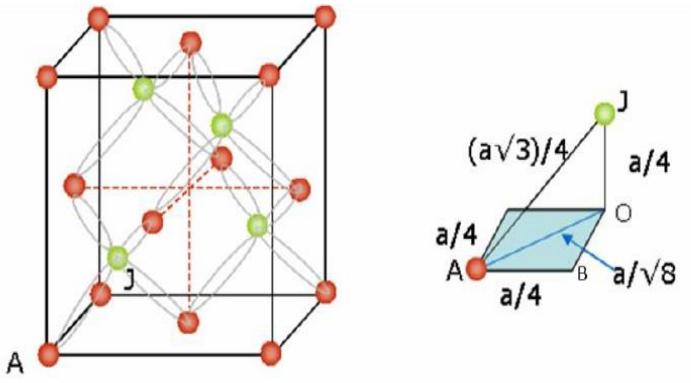
(Corner atoms) (FC atoms)

Co-ordination number:

The co-ordination number of an atom in diamond structure is obviously 4 as can be seen from the unit cell of diamond and is loosely packed.

Atomic radius:

To determine the distance between nearest neighbours one needs to estimate the distance AJ as shown in the figure 1.32.



The atom at J is displaced from that at A by a/4 along x-axis and a/4 along Y axis, therefore

$$AO^2 = AB^2 + BO^2 = (\frac{a}{4})^2 + (\frac{a}{4})^2 = 2a^2/16 = a^2/8$$

Then,

$$AJ^2 = AO^2 + OJ^2 = \frac{a^2}{8} + \frac{a^2}{16} = \frac{3a^2}{16}$$

Therefore,

$$AJ = \frac{a\sqrt{3}}{4}$$

Substituting the values for AJ from the fig 1.28, we get

$$2r = \frac{a\sqrt{3}}{4}$$

Therefore, $$r = \frac{a\sqrt{3}}{8}$$

From the atomic radius, the lattice constant becomes,

$$a = \frac{8r}{\sqrt{3}}$$

Packing factor:

Number of atoms per unit cell = 8

Volume of one unit cell, $v = 8 \times \frac{4}{3}\pi r^3$

Where r is the atomic radius

$$\text{Atomic radius, } r = \frac{a\sqrt{3}}{8}$$

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,

$$PF = \frac{8 \times \frac{4}{3}\pi r^3}{a^3}$$

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

$$PF = \frac{\frac{32}{3}\pi(\frac{a\sqrt{3}}{8})^3}{a^3} = \frac{\frac{32}{3}\pi a^3\sqrt{3}^3}{8^3 a^3}$$

$$= \frac{\frac{32}{3}\pi 3\sqrt{3}}{8^3} = \frac{32\sqrt{3}\pi}{512}$$

$$= \frac{\pi\sqrt{3}}{16} = 0.34$$

$$PF = 34\ \%$$

Thus, 34% of the volume is occupied by the atoms and remaining 66% volume is vacant which implies that diamond structure can be termed as loosely packed structure.