5.5 Hexagonal Closed Packed Structure (HCP)

The hexagonal closed packed (HCP) structure consists of three layers of atoms. The bottom layer has six corner atoms and one face centred atom. The middle layer has three full atoms. The upper layer has six corner atoms and one face centred atom.

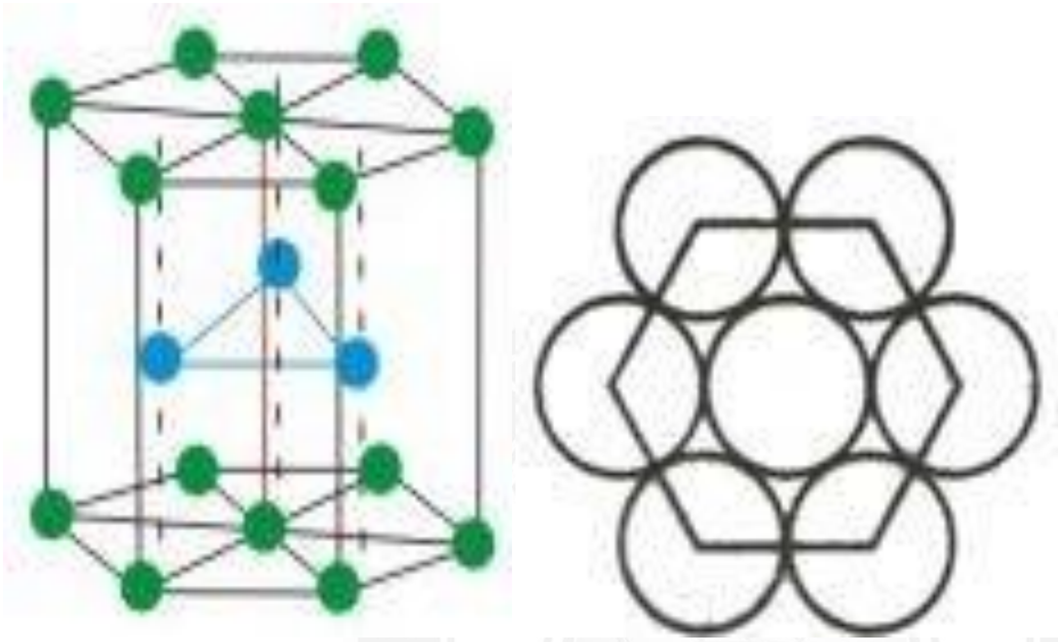


Fig:5.5.1- Hexagonal Closed Packed Structure

Number of atoms per unit cell

In order to calculate the total number of atoms in the hcp structure, let us consider the bottom layer of atoms. The bottom layer consists of six corner atoms and one face centred atom. Each and every corner atom contributes 1/6 of its part to one unit cell. Thus,

Hence,

the total number of atoms contributed by the face centred atom is = $\frac{1}{6}$ X 6 = 1

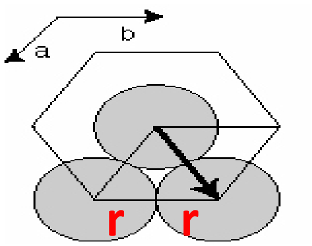
The face centred atom contributes ½ of its part to one unit cell. Therefore, the total number of atoms present in the case of the bottom layer is = $1 + \frac{1}{2} = \frac{3}{2}$

Similarly, the upper layer also has 3/2 number of atoms. The middle layer has three full atoms. Therefore, the total number of atoms present in a unit cell is = $\frac{3}{2} + \frac{3}{2} + 3 = 6$

The total number of atoms present in the case of hcp crystal structure is six.

Atomic Radius

To find the atomic radius of HCP structure, consider any two corner atoms. It has to be noted that, each and every corner atom touches



each other; therefore they are the nearest neighbours.

From figure,

We can write $a = 2r$

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

Co-Ordination Number

The HCP structure is considered to have three layers via. (i) Bottom layer (B_L), (ii) Top layer (T_L), (iii) Middle layer (M_L) as shown in figure.

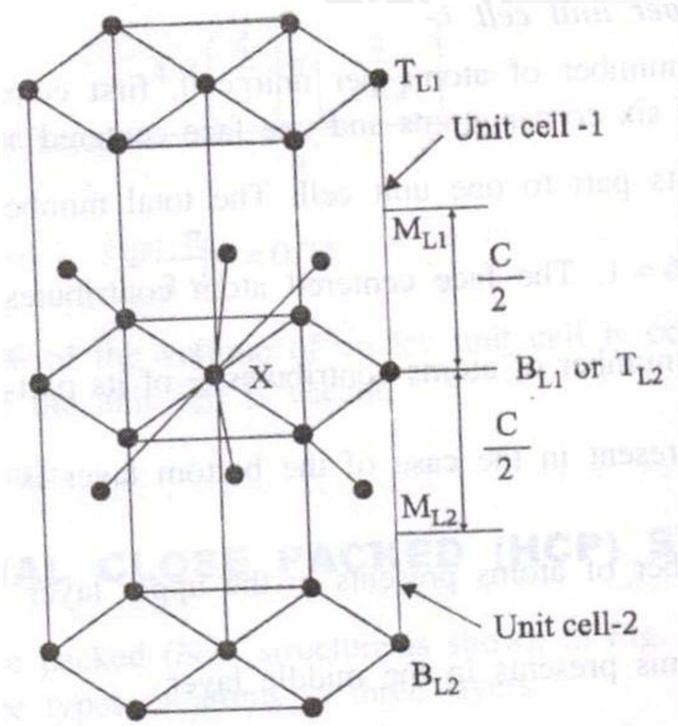


Fig:5.5.2- Hexagonal Closed Packed Structure

In the top and bottom layers, the base centred atom is surrounded by six corner atoms. In the middle layer we have 3 atoms stacked inside the unit cell as shown in figure.

Let us consider two unit cells as shown in figure. Let ‘X’ be the reference atom taken in the bottom layer (BL_1) of unit cell – I (or top layer [TL_2] of unit cell 2). This atom has 6 neighbouring atom in its own plane. Further at a distance of $c/2$ it has 3 atoms in the middle layer (ML_1) of unit cell-I and 3 more atoms in the middle layer (ML_2) of unit cell-2. Therefore, the total numbers of neighbouring atoms are 6+3+3=12.

Relation between ‘*c*’ and ‘*a*’ [*c*/*a* ratio]

In hexagonal system, ‘*c*’ is the height of the unit cell of HCP structure and ‘*a*’ is the distance between two neighbouring atoms. Now

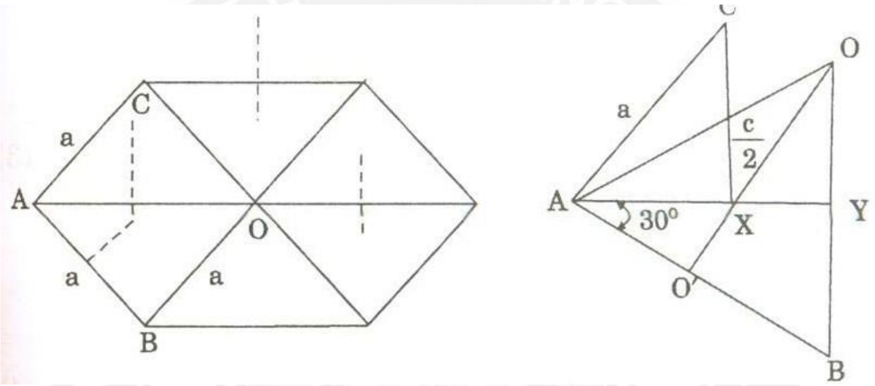


Fig:5.5.3- layer of HCP Structure

consider the triangle ABO in the bottom layer. Here A, B and O are the lattice points and exactly above these atoms at a perpendicular distance ‘$c/2$’ the next layer atom lies at C.

In Δ ABY,

$$\text{Cos } 30^0 = \frac{AY}{AB}$$

(or) $AY = AB \text{ Cos } 30^0$

Since, AB = a and $\text{Cos } 30^0 = \frac{\sqrt{3}}{2}$

$$AY = a\frac{\sqrt{3}}{2} \text{---------------------}(1)$$

But from figure, $AX = \frac{2}{3}\text{AY}$

Substituting the AY value in the above equation, we get

$$\text{AX } = \frac{2}{3}\, a\frac{\sqrt{3}}{2}$$

AX = $\frac{a}{\sqrt{3}}$-----------------(2)

In Δ AXC

$$AC^2 = AX^2 + CX^2$$

Substituting the given values in the above equation we get,

AC = a;AX $= \frac{a}{\sqrt{3}}$ and CX $= \frac{c}{2}$, we get

$$a^2 = \left(\frac{a}{\sqrt{3}}\right)^2 + \left(\frac{c}{2}\right)^2$$

$$a^2 = \frac{a^2}{3} + \frac{c^2}{4}$$

$$\frac{c^2}{4} = a^2 - \frac{a^2}{3}$$

$$\frac{c^2}{4} = \frac{3a^2 - a^2}{3}$$

$$\frac{c^2}{4} = \frac{2a^2}{3}$$

$$\frac{c^2}{a^2} = \frac{8}{3} \text{-----------------(3)}$$

Taking square root on both sides of equation (3) we get,

$$\sqrt{\frac{c^2}{a^2}} = \sqrt{\frac{8}{3}}$$

$$\frac{c}{a} = \sqrt{\frac{8}{3}} = 1.633 \text{-----------(4)}$$

Atomic Packing Factor (APF)

We know that,

APF = $\frac{u}{v}$-------------------(5)

Where

u = Total number of atoms per unit cell X volume of one atom

v = Total volume of the unit cell

The number of atoms per unit cell in HCP structure = 6

Volume of one atom (spherical) is = $\frac{4}{3}\pi r^3$

We know that, the atomic radius of HCP is $r = \frac{a}{2}$--------*(6)*

Therefore,

Volume occupied by the total number of atoms per unit cell is, U=6x$\frac{4}{3}\pi r^3$……………..(7)

Substitute equation (6) in (7) we get

U= $\frac{24}{3}\pi\left(\frac{a}{2}\right)^3$

$= \frac{24\pi a^3}{24}$

$= \pi a^3$-----------(8)

For HCP,

The volume of the unit cell is

$= Area\ of\ the\ base\ \times Height$……….(9)

Area of the base = Area of six triangles

Area of the base = 6 × area of the one triangle (AOB)
From figure,
The area of the triangle AOB =$\frac{1}{2}$(BO) X (AY)

Substituting the value of BO = a and $AY = \frac{a\sqrt{3}}{2}$ we have

Area of triangle AOB =$\frac{1}{2}$(a) $\frac{a\sqrt{3}}{2}$

$= \frac{a^2\sqrt{3}}{4}$ Area of the base = $6 \times \frac{a^2\sqrt{3}}{4}$

Area of the base $= \frac{3a^2\sqrt{3}}{2}$------------(10)
We know that,

The height of the hcp structure = c............. (11)

Substituting equations (10) and (11) in equation (9) we get

Volume of the unit cell is (v) $= \frac{3a^2\sqrt{3}}{2}$ c
Substituting equations (8) and (12) in equation (5), we get

Atomic packing factor $= \frac{\pi a^3}{\frac{3a^2\sqrt{3}c}{2}}$

$$= \frac{2\pi}{3\sqrt{3}} \left[\frac{a}{c}\right]$$

since $\frac{a}{c} = \left[\frac{3}{8}\right]^{\frac{1}{2}}$ we get

Atomic packing factor $= \frac{2\pi}{3\sqrt{3}} \left[\frac{3}{8}\right]^{\frac{1}{2}}$

Atomic packing factor $= \frac{2\pi}{3\sqrt{3}} \frac{\sqrt{3}}{2\sqrt{2}}$

$$= \frac{\pi}{3\sqrt{2}}$$

Atomic packing factor = 0.74

Therefore we can say that 74% volume of the unit cell of HCP is occupied by atoms and remaining 26% volume is vacant. Thus, the packing density is 74%, which is the same as that of FCC structure. Hence, HCP structure is also termed as tightly or closely packed structure.