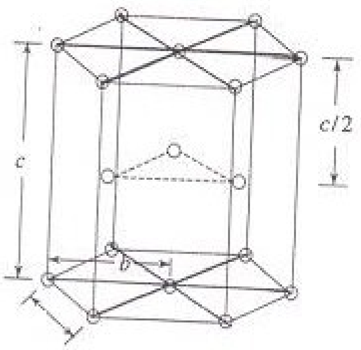
HEXAGONAL CLOSED PACKED STRUCTURE



- It 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.
- Each and every corner atom contributes 1/6 of its part to one unit cell.
- The number of total atoms contributed by the corner atoms of both top and bottom layers is 1/6   12 = 2.
- The face centred atom contributes 1/2 of its part to one unit cell.
- Since there are 2 face centred atoms, one in the top and the other in the bottom layers, the number of atoms contributed by face centred atoms is 1/2 2 = 1.
- Besides these atoms, there are 3 full atoms in the middle layer.
- Total number of atoms present in an HCP unit cell is 2+1+3 = 6.

CO-ORDINATION NUMBER (CN)

- The face centered atom touches 6 corner atoms in its plane.
- The middle layer has 3 atoms.

- There are three more atoms, which are in the middle layer of the unit cell.
- Therefore the total number of nearest neighbours is 6+3+3=12.

ATOMIC RADIUS (R)

- Consider any two corner atoms.
- Each and every corner atom touches each other. Therefore a = 2r.

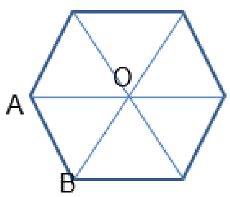
i.e., The atomic radius, r = a/2

ATOMIC PACKING FACTOR (APF)

APF = v/V

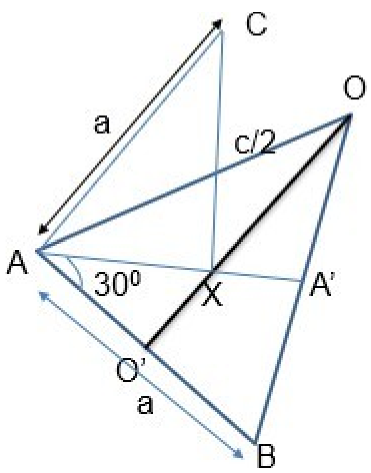
$v = 6 \quad 4/3 \quad r^3$

Substitute r = a/2



$v = 6 \quad 4/3 \quad \frac{a^3}{8}$

$v = a^3$



AB = AC = BO = 'a'. CX = c/2 where c height of the hcp unit cell.

Area of the base = 6 area of the triangle ABO = 6 1/2 AB OO

Area of the base = 6 1/2 a OO

In triangle O'OB

|O'OB 30

$\cos 30^o = \frac{OO'}{BO} \quad \frac{OO'}{a}$

$OO = a \cos 30^o = a \sqrt{3/2}$

Now, substituting the value of OO ,

$\sqrt{3/2} \qquad \frac{3\sqrt{3}a^2}{}$

Area of the base = 6 1/2 a

V = Area of the base × height

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

$$\therefore APF = \frac{v}{V} = \frac{\pi a^3}{\frac{3\sqrt{3}\ a^2\ c}{2}}$$

$$\therefore APF = \frac{2\pi a^3}{3\sqrt{3}a^2 c} = \frac{2\pi}{3\sqrt{3}}\ \frac{a}{c}$$

Determination of c/a ratio:

In the triangle ABA ,

Cos 30º = A '

AB

30

AA = AB cos 30º = a 3/2

But AX = 2/3 AA = $\frac{2}{3}a\frac{\sqrt{3}}{2}$

i.e. AX = $\frac{a}{\sqrt{3}}$

In the triangle

AXC, AC^2 =

$AX^2 + CX^2$

Substituting the values of AC, AX and CX,

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

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

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

$$\frac{c^2}{4} = a^2\left(1 - \frac{1}{3}\right)$$

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

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

Now substituting the value of c/a to calculate APF of an hcp unit cell,

$$APF = \frac{2\pi}{3\sqrt{3}}\sqrt{\frac{3}{8}}$$

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

$$\therefore APF = \frac{\pi}{3\sqrt{2}} = 0.74$$