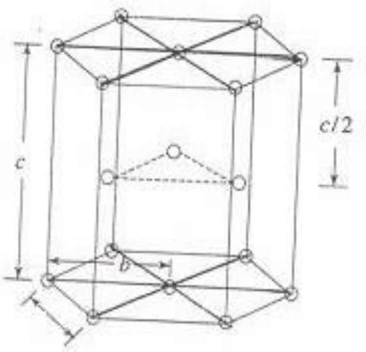
HEXAGONAL CLOSED PACKED STRUCTURE



- 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 $1/6 \times 12 = 2$.
- 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 $1/2 \times 2 = 1$.
- 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.

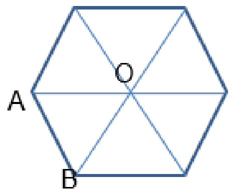
i.e., The atomic radius, $r = a/2$

ATOMIC PACKING FACTOR (APF)

APF = v/V

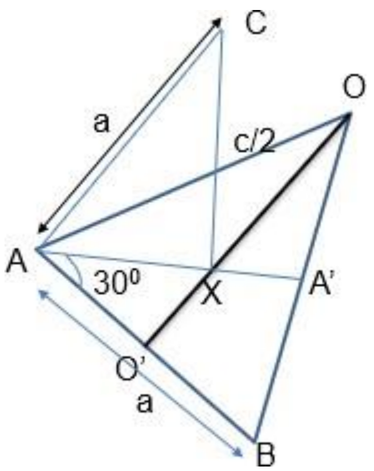
$v = 6 \times 4/3\ \pi r^3$

Substitute r = a/2



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

$v = \pi a^3$



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

$\underline{|O'OB} = 30°$

$\cos 30° = \frac{OO'}{BO} = \frac{OO'}{a}$

$\therefore\ OO' = a \cos 30° = a\sqrt{3/2}$

Now, substituting the value of OO′,

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

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 = $\underline{|A'AB}$

$= 30°$

$\therefore$ 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,

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

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

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