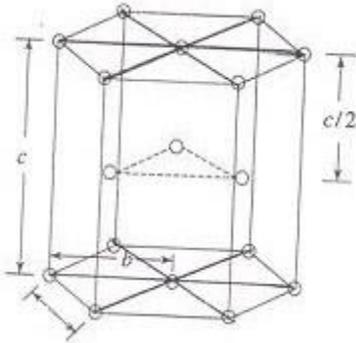




## HEXAGONAL CLOSED PACKED STRUCTURE



- 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  $a = 2r$ .

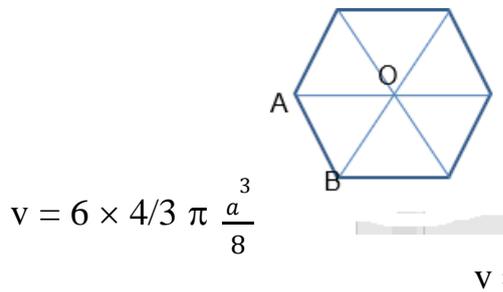
i.e., The atomic radius,  $r = a/2$

### ATOMIC PACKING FACTOR (APF)

$$\text{APF} = v/V$$

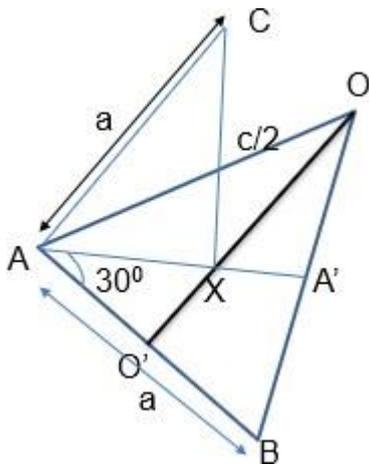
$$v = 6 \times \frac{4}{3} \pi r^3$$

Substitute  $r = a/2$



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

$$v = \pi a^3$$



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

Area of the base =  $6 \times$  area of the triangle  $ABO = 6 \times \frac{1}{2} \times AB \times OO'$

Area of the base =  $6 \times \frac{1}{2} \times a \times OO'$

In triangle  $O'OB$

$\angle O'OB = 30^\circ$

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

$$\therefore OO' = a \cos 30^\circ = a \frac{\sqrt{3}}{2}$$

Now, substituting the value of  $OO'$ ,

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



Area of the base =  $6 \times \frac{1}{2} \times a \times$   
 $V = \text{Area of the base} \times \text{height}$

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

**Determination of c/a ratio:**

In the triangle ABA',

$$\cos 30^\circ = \frac{A'A}{AB}$$
$$= \frac{30^\circ}{c}$$



$$\therefore AA' = AB \cos 30^\circ = a\sqrt{3}/2$$

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

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

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,

$$\begin{aligned} \text{APF} &= \frac{2\pi}{3\sqrt{3}} \sqrt{\frac{8}{3}} \\ &= \frac{2\pi}{3\sqrt{3}} \frac{\sqrt{3}}{2\sqrt{2}} \end{aligned}$$

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