

# Crystal Structure:-

## Structure of metals -

As Metallic bonds are non-directional, each metal atom in a crystal tends to surround itself with as many neighbours as possible, for minimizing the pot. energy.

Approximation for metal atom

1. Spherical atom
2. Hard & incompressible
3. Non-directional bonds.

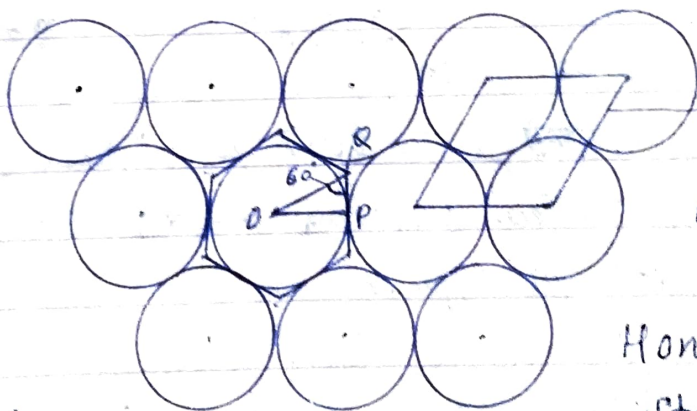
To consider some of the ways that spheres can be packed together in 3-D arrays.

first consider the arrangement of sphere in a plane

this is the array in which max<sup>m</sup> available space is occupied.

This array is called

hexagonal ~~closed~~ closest-packed layer or simply closest-packed layer

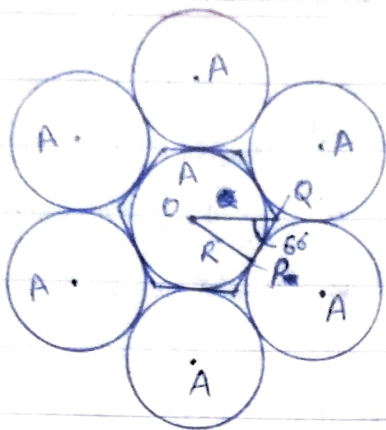


unit cell  
Rhombic-  
dral  
Rhombus

Honey-Comb  
Structure

no. of nearest  
neighbours = 6

$$\text{packing fraction} = \frac{\text{Volume Occupied}}{\text{Volume Available}}$$



$$\tan 60^\circ = \frac{R}{PQ}$$

$$PQ = \frac{R}{\tan 60^\circ} = \frac{R}{\sqrt{3}}$$

$$\text{Area } \Delta POQ = \frac{1}{2} \cdot R \cdot \frac{R}{\sqrt{3}} = \frac{R^2}{2\sqrt{3}}$$

$$\text{Packing fraction} = \frac{\text{Area of circle}}{\text{Area of Hexagonal}}$$

$$\text{Area of Hexagonal} = 12 \times \frac{R^2}{2\sqrt{3}} = 2\sqrt{3} R^2$$

$$\text{Area of circle} = \pi R^2$$

$$\therefore P.f = \frac{\pi R^2}{2\sqrt{3} R^2} = \frac{\pi}{2\sqrt{3}} = 0.907$$

$$= \frac{90.7}{100} = 90.7\% \text{ space occupied}$$

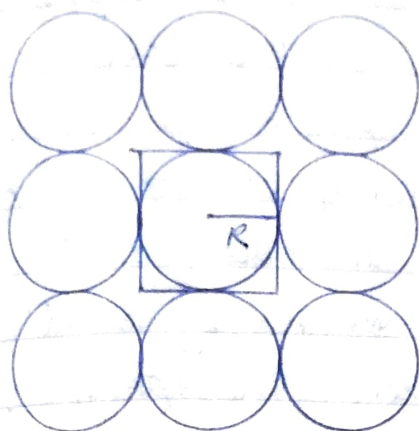
ie. the circles occupy max<sup>m</sup> 90.7% of available space.

The unit cell of the plane lattice of this array is shown in fig.

$$a = b \quad \gamma = 120^\circ \quad \text{Rhombus}$$

Rhombohedral

each unit cell contains two void spaces, B & C the three alternative placements of spheres can be distinguished, namely A, B or C each of which results in a closed closest-packed layers of spheres



Packing fraction

$$= \frac{\text{Area of circle}}{\text{Area of square}}$$

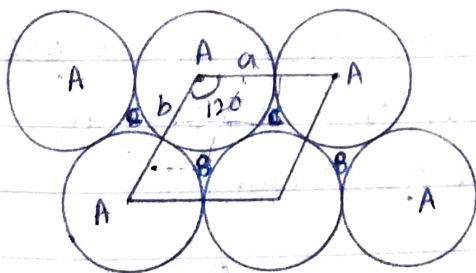
$$= \frac{\pi R^2}{4R^2} = \frac{\pi}{4}$$

$$= 0.785$$

$$= 78.5\% \text{ space occupied.}$$

nearest neighbour: 4.

In square lattice unit cell - square.



Center A	0	0
center B	$\frac{1}{3}$	$\frac{2}{3}$
Center C	$\frac{2}{3}$	$\frac{1}{3}$

B layer displaced by  
 $\frac{1}{3} \vec{a} + \frac{2}{3} \vec{b}$

C layer displaced by  
 $\frac{2}{3} \vec{a} + \frac{1}{3} \vec{b}$

