SNS COLLEGE OF ENGINEERING

Coimbatore-641 107

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Affiliated to Anna University, Chennai

DEPARTMENT OF PHYSICS

COURSE NAME :19PY101-ENGINEERING PHYSICS

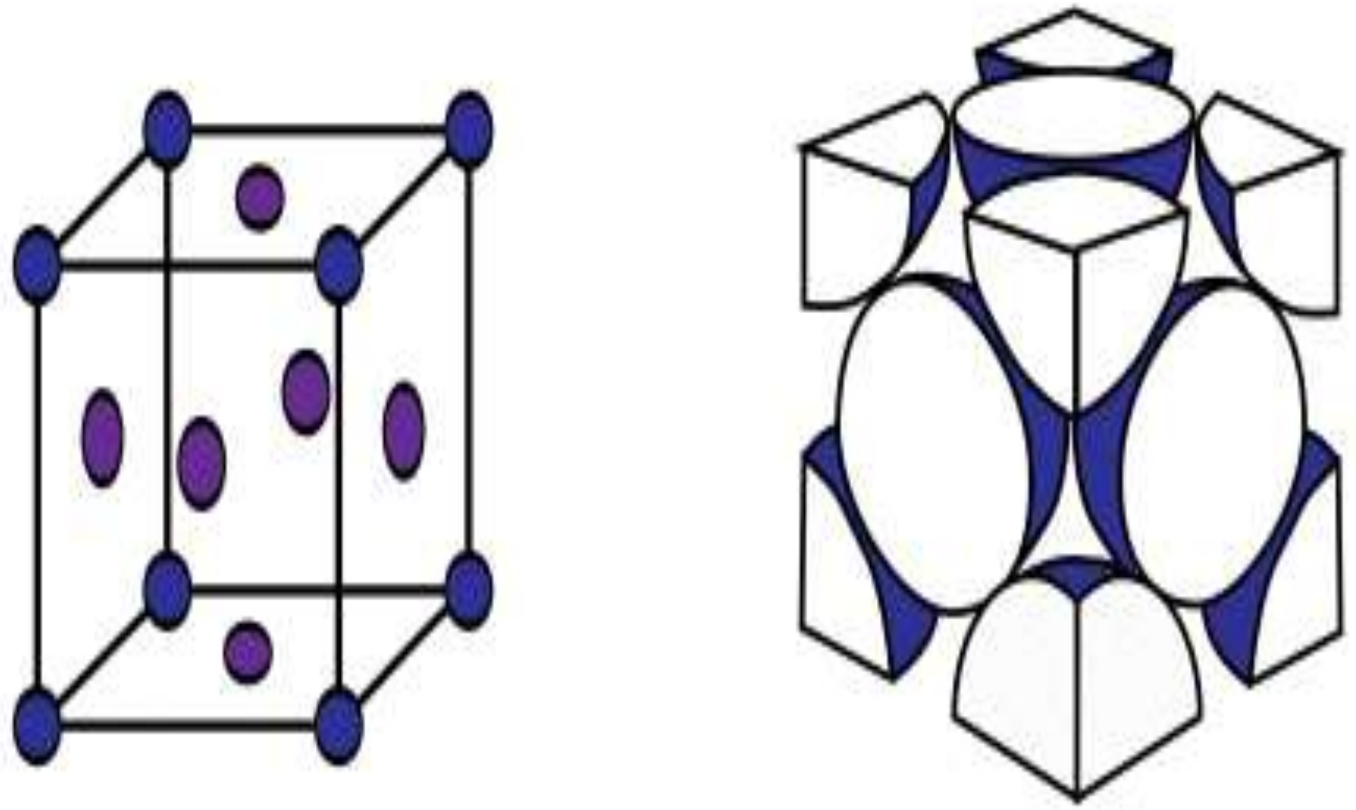
I YEAR / I SEMESTER

UNIT 4 – CRYSTAL PHYSICS

TOPIC 5 – CRYSTAL STRUCTURES - FCC & HCP

- FCC arrangement, again there are eight atoms at corners of the unit cell and one atom centered in each of the faces.
- The atom in the face is shared with the adjacent cell.
- FCC unit cells consist of four atoms, eight eighths at the corners and six halves in the faces.

Two representations of FCC Crystal Structure



FACE CENTERED CUBIC STRUCTURE

There are two types of atom 1.Corner atom, 2.Face center atom

There are 8 corner atom one at each corner of unit cell and six atoms at centers of six face of unit cell.

Number of corner atoms per unit cell = 1/8 X 8=1

Number of face centered atom per unit cell = ½ X6=3

Since by each face centered atom shared by two unit cells.

Total number of atoms per unit cell in FCC =

Total number of corner atoms + Total number of face centered atoms

= 1 + 3 = 4

ATOMIC RADIUS

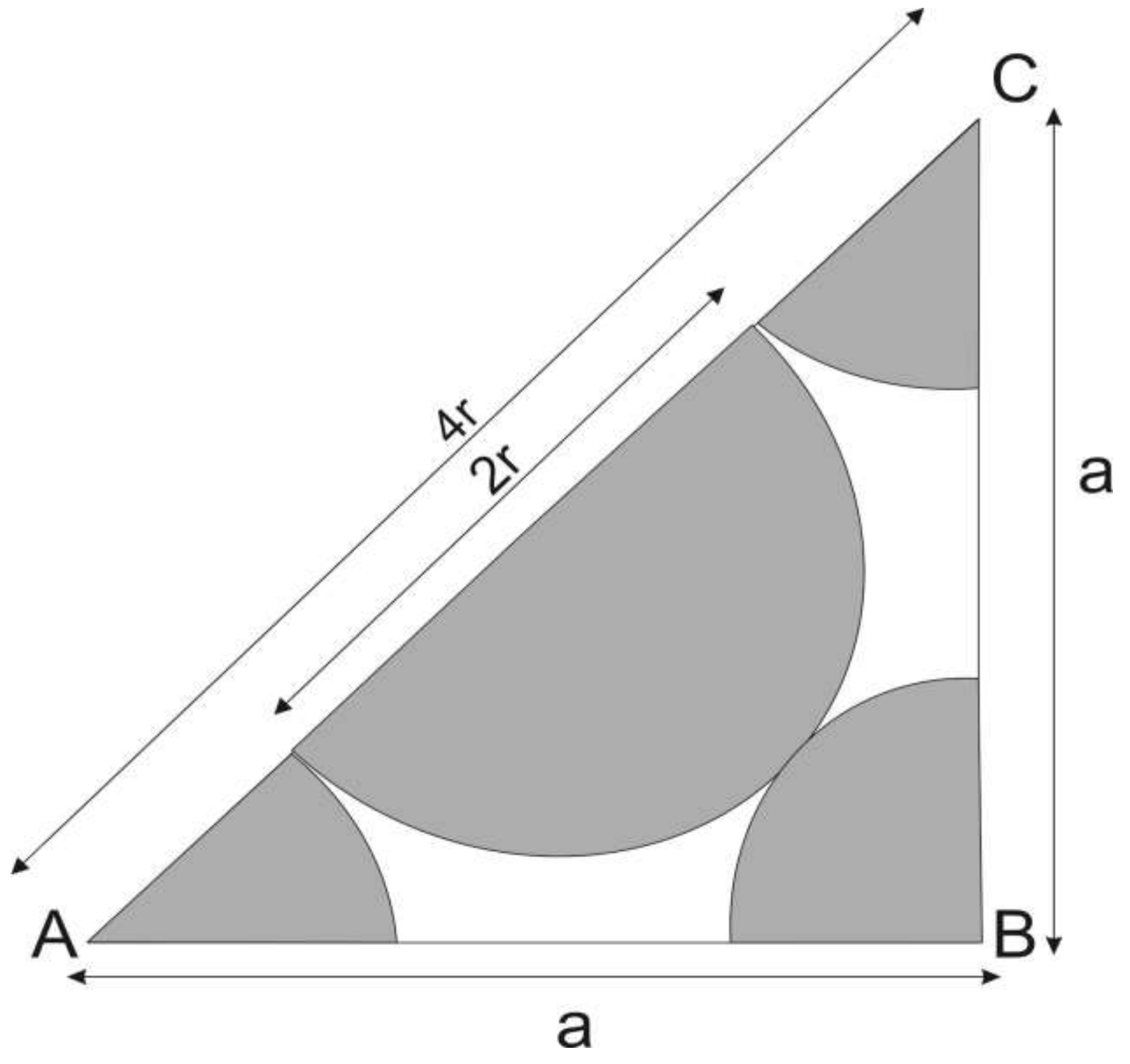
In Δ ABC,

$AC^2 = AB^2 + BC^2$

$(4r)^2 = a^2 + a^2$

$16r^2 = 2a^2$; $r^2 = 2a^2/16$;

$r = a\sqrt{2}/4$



ASSESSMENT - 1

Find the answers

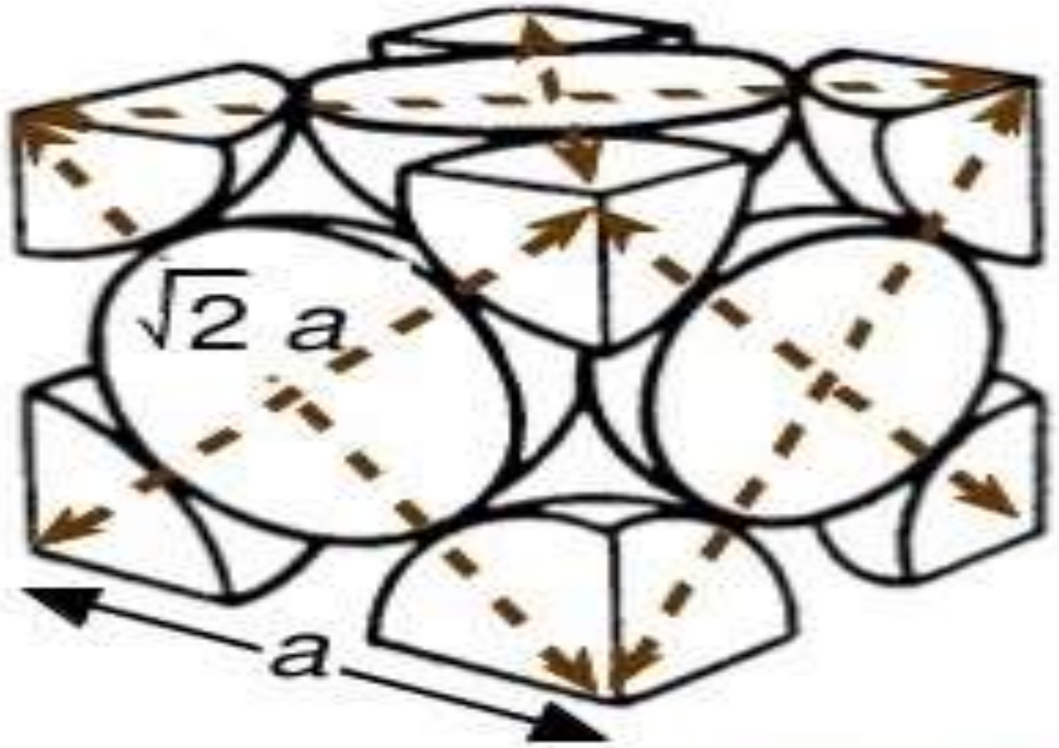
1.Why the atomic radius is change from BCC and FCC.

2. Compare the coordination number for BCC and FCC.

Atomic Packing Factor: FCC

- APF for a face-centered cubic structure = 0.74

maximum achievable APF



Close-packed directions:
length = $4R = \sqrt{2}\,a$

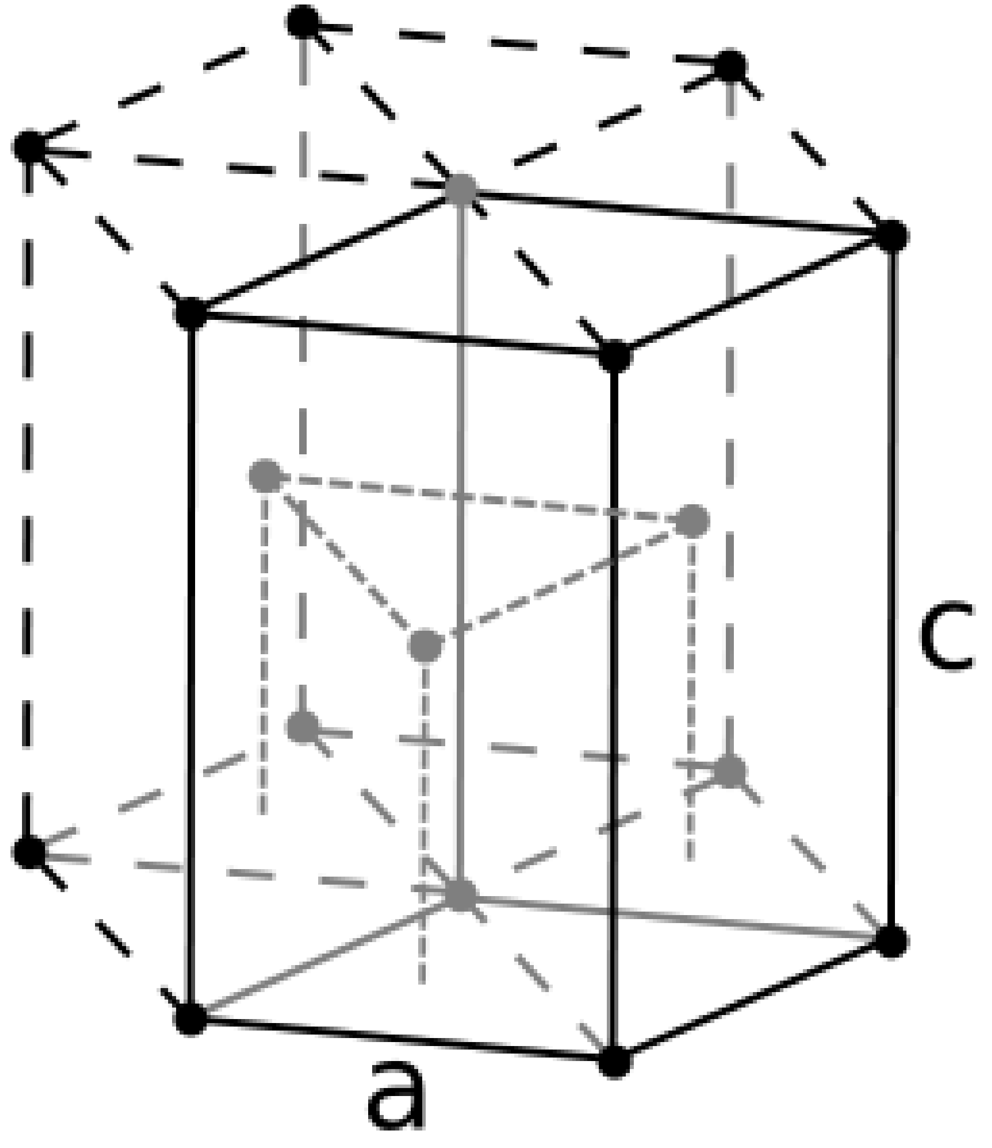
Unit cell contains:
$6 \times 1/2 + 8 \times 1/8$
= 4 atoms/unit cell

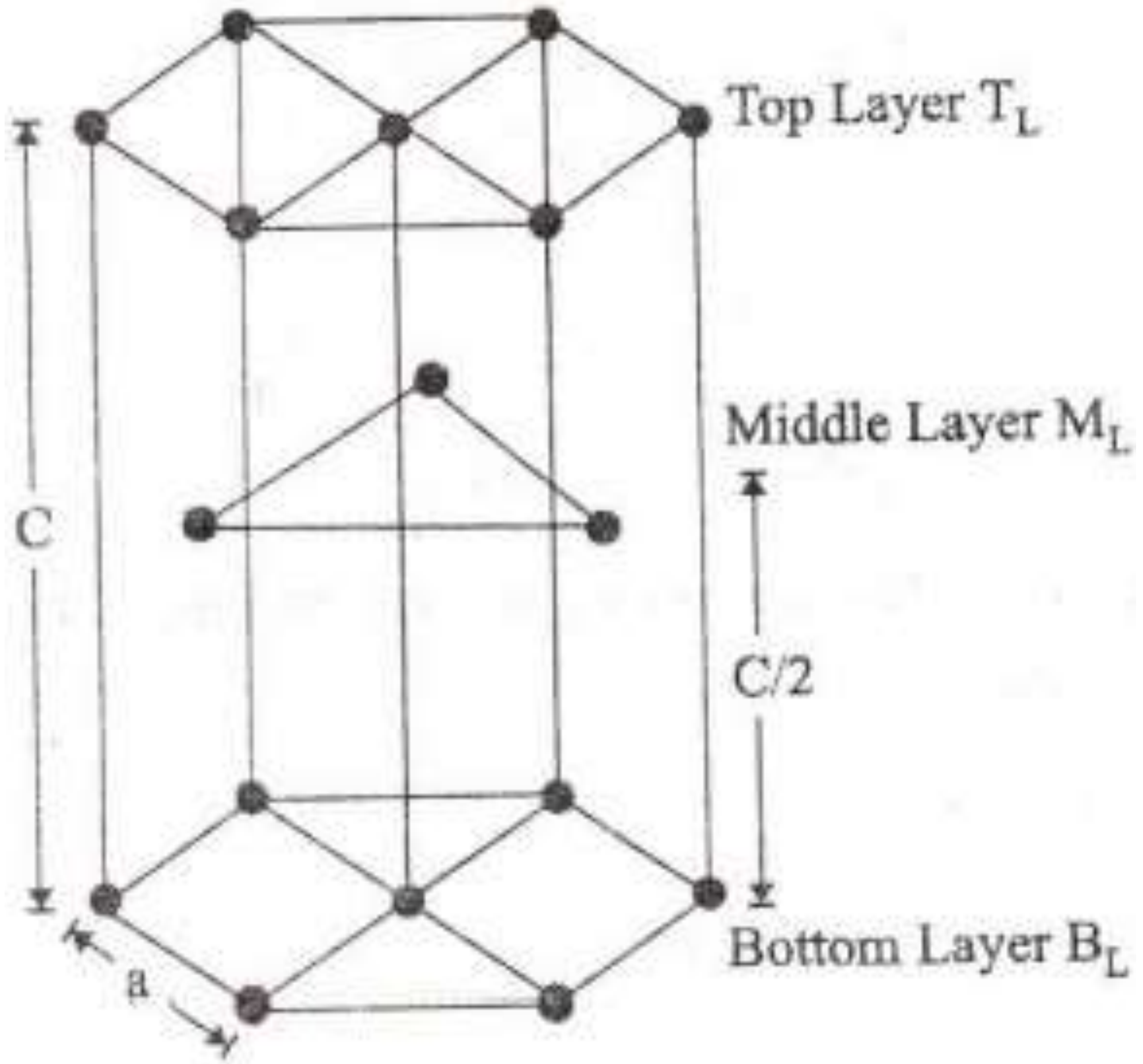
$$\text{APF} = \frac{4 \cdot \frac{4}{3}\pi\left(\sqrt{2}a/4\right)^3}{a^3}$$

- 4: atoms / unit cell
- $\frac{4}{3}\pi\left(\sqrt{2}a/4\right)^3$: volume / atom
- a^3: volume / unit cell

Properties of hexagonal closest packed (HCP)

1. The hexagonal closest packed (hcp) has a coordination number of 12 and contains 6 atoms per unit cell.
2. Covalent bond structure crystal.
3. Ionic crystal
4. excellent corrosion behavior,
5. creep stability, and
6. Tensile properties


c
a


Top Layer T_L
Middle Layer M_L
C
C/2
Bottom Layer B_L
a

1. Coordination number

There are three types of atom

1.Corner atom,

2.Base atom,

3.Middle layer atom

1. Number of corner atoms per unit cell =1/6 X12=2 .

This by each corner atom shared by six hexagon unit cell and we have 12 corners.

2. Number of Base centered atom per unit cell = 1/2 X 1 = 1/2

This by each base atom shared by two unit cell and we have 2 base atoms.

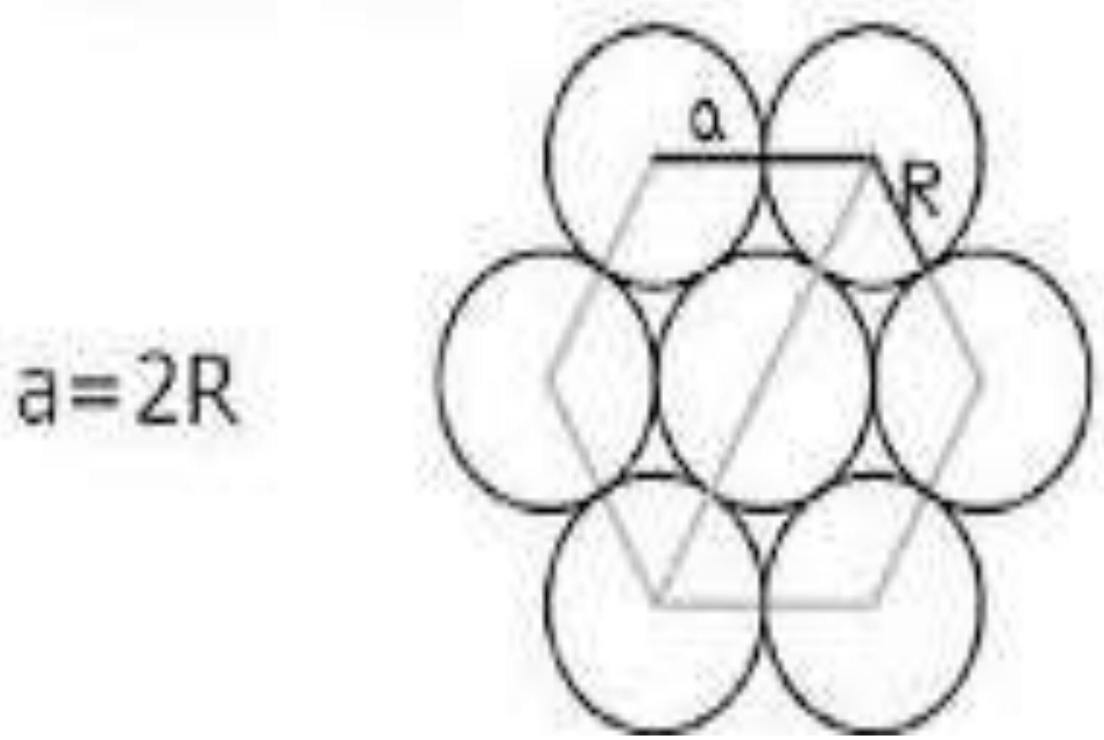
3. Number of middle layer atoms per unit cell = 3

This is by three atoms form a triangle in middle layer.

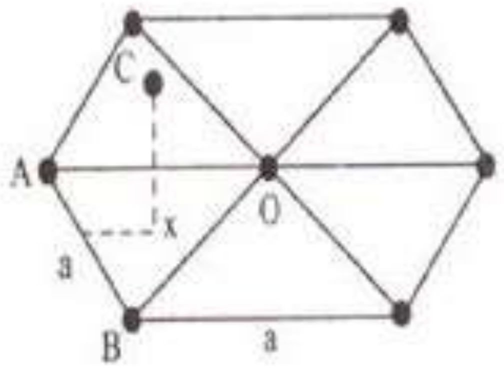
Total number of atoms per unit cell in HCP =Total number of corner atoms +Total number of base atoms + Total number of middle layer atoms = 2 + 1 + 3 = 6.

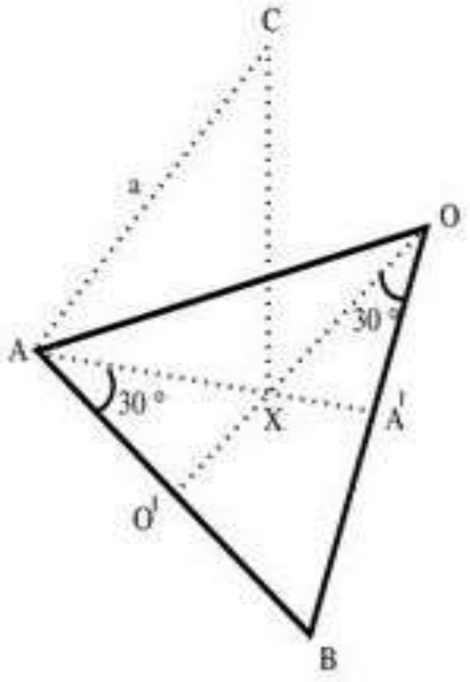
2. Atomic Radius

A hexagonal edge length “a” and the atomic radius ‘r’



Calculation of c/a ratio





In the triangle ABA′,

$$\angle A'AB = 30^\circ$$

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

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

But $\quad AX = \frac{2}{3}AA' = \frac{2}{3}\, a\frac{\sqrt{3}}{2}$

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,

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

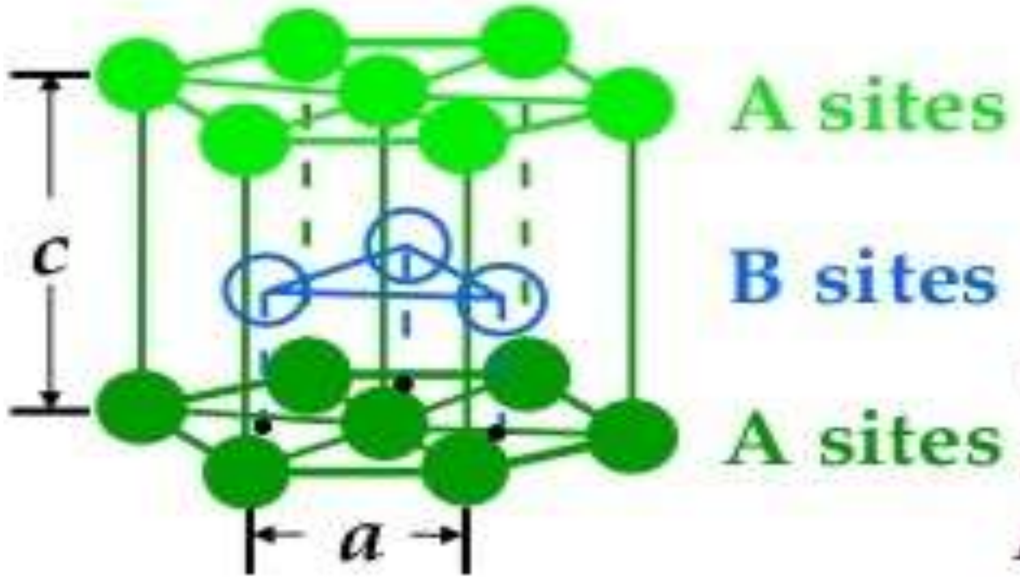
$$a^2 = \frac{a^2}{3} + \frac{c^2}{4}$$

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

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

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

APF for HCP



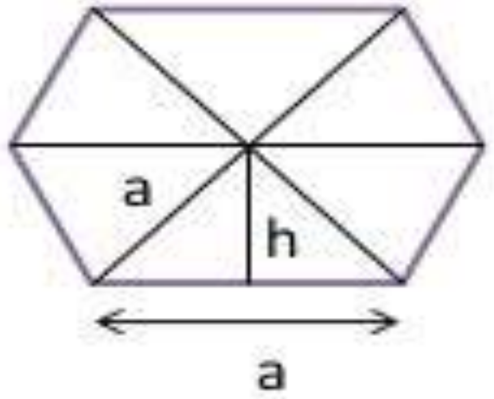
C=1.633a

Number of atoms in HCP unit cell=
(12*1/6)+(2*1/2)+3=6atoms

Vol.of HCP unit cell=
area of the hexagonal face X height of the hexagonal

Area of the hexagonal face=area of each triangle X6

a=2r



Area of triangle $= \frac{bh}{2} = \frac{ah}{2} = \frac{1}{2}a.\frac{a\sqrt{3}}{2}$

Area of hexagon $= 6.\frac{a^2\sqrt{3}}{4}$

Volume of HCP= $6.\frac{a^2\sqrt{3}}{4}.C = 6.\frac{a^2\sqrt{3}}{4}.1.633a$

APF= $6*\frac{4\pi r^3}{3}/(\frac{\sqrt{3}}{4}*6*1.633*a3)$

APF =0.74

SUMMARY

Structure	a_0 vs. r	Atoms per cell	Coordination Number	Packing factor	Examples
SC	$a_0 = 2r$	1	6	0.52	Polonium (Po),α-Mn
BCC	$a_0 = \frac{4}{\sqrt{3}} r$	2	8	0.68	Fe,Ti,W,Mo, Nb,Ta,K,Na, V,Zr,Cr
FCC	$a_0 = \frac{4}{\sqrt{2}} r$	4	12	0.74	Fe,Cu,Au,Pt ,Ag,Pb,Ni
HCP	$a_0 = 2r$ $c_0 \approx 1.633 a_0$	2	12	0.74	Ti,Mg,Zn,Be ,Co,Zr,Cd

References

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- https://depts.washington.edu/matseed/mse_resources/Webpage/Metals/metalstructure.htm
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