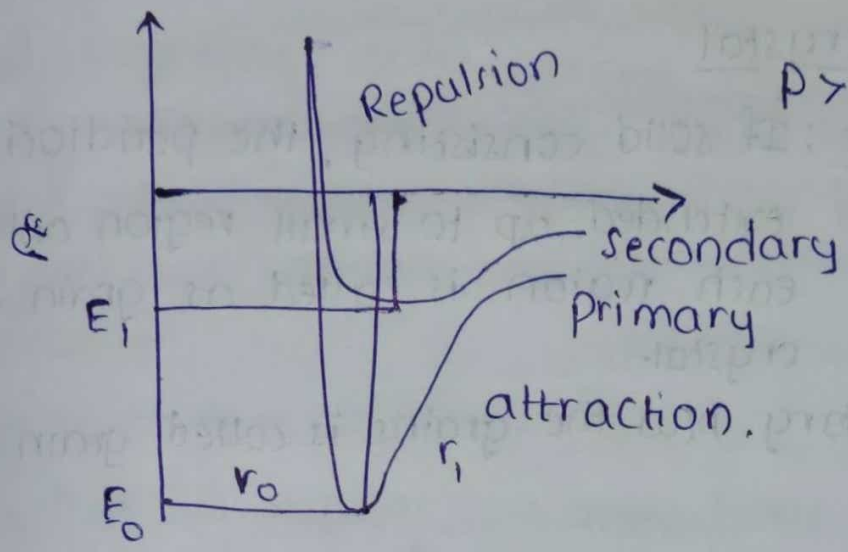
Hydrogen bond: (weak)

→ H^+ ion located b/w 2 ions

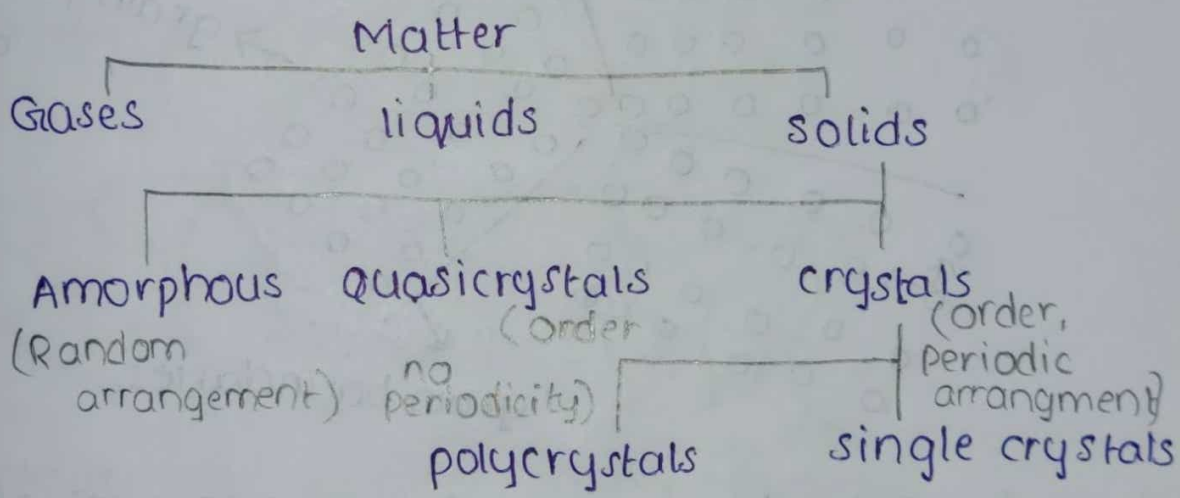
Interatomic Vs P.E curve



29/1/21 Friday

electronegitivity: Tendency to attract the e^-

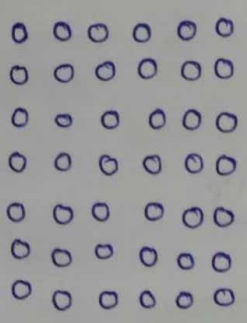
classification of matter



→ properties of molecules depends on the arrangment of the atoms.

*periodicity: regularly repeated (same distance in one direction)

Single crystal: If the periodic arrangement extended through out the crystalline material, it is called as single crystalline material.

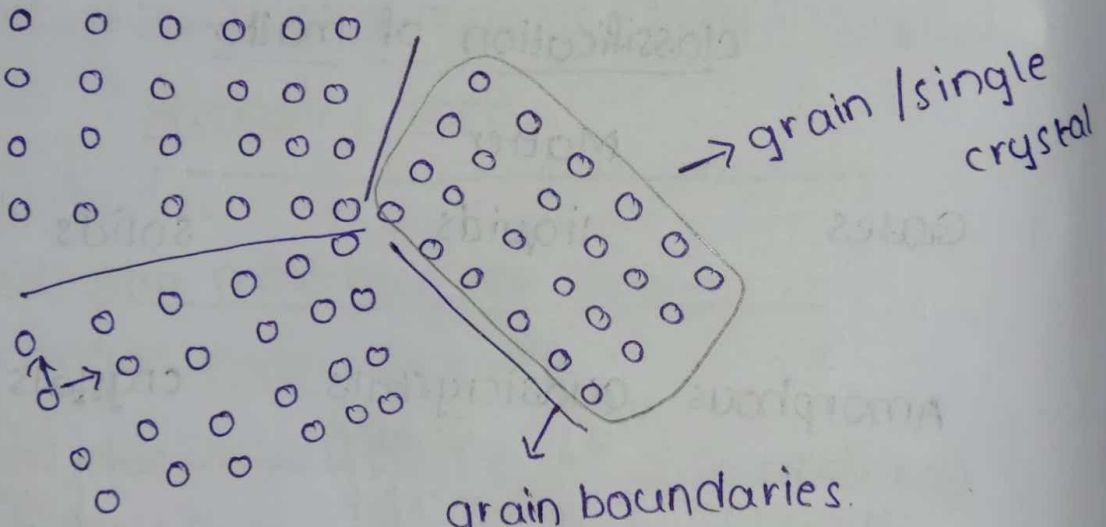


Single crystal

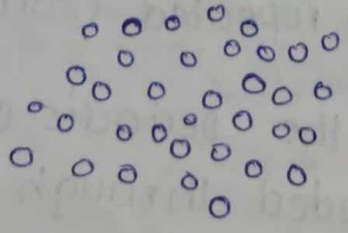
Poly crystalline : If solid consisting, the peridiocity extended up to small region only and each region is called as grain or single crystal.

→ The boundary blw the grains is called grain boundary.

→ If solid contains many no.of grains(single crystals) is also called as polycrystalline material



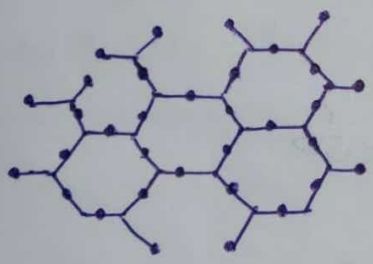
Amorphous: Random or irregular arrangement of atoms or ions or molecules is known as amorphous material.



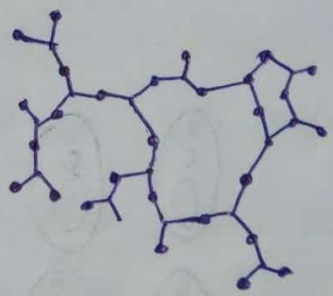
Amorphous / Non crystalline

Differences blw crystalline and Amorphous solids

Crystalline	Amorphous
→ Regular arrangement of atoms along the 3D.	→ NO regular arrangement of atoms.
→ Have long range order	→ Have short range order.
→ sharp melting point	→ NO sharp melting point
→ They are anisotropic (properties are different in different directions)	→ They are isotropic
→ They are most stable	→ they are most unstable
→ They have a regular cut	→ they have irregular cut
→ show all characters of solids.	→ Don't show all characters of solids.
Eg: Diamond, NaCl, KCl, copper, Iron etc.	Eg: Glasses, plastic, rubber.

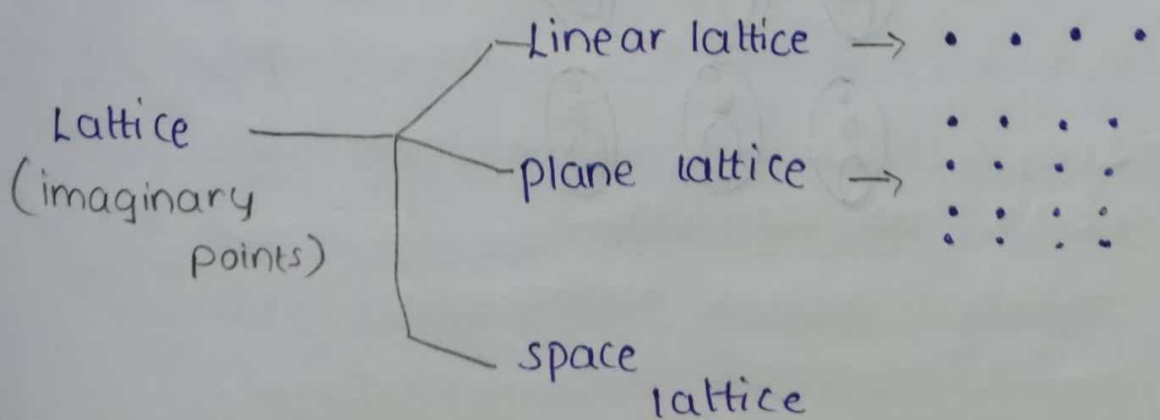


crystalline



Non crystalline

Basic definitions: Given by



Linear Lattice: Arrangement of points in one direction of (x-direction) is called linear lattice.

Space lattice: Infinite array of points (imaginary) periodically in 3-D and each and every point has identical environment is known as space lattice.

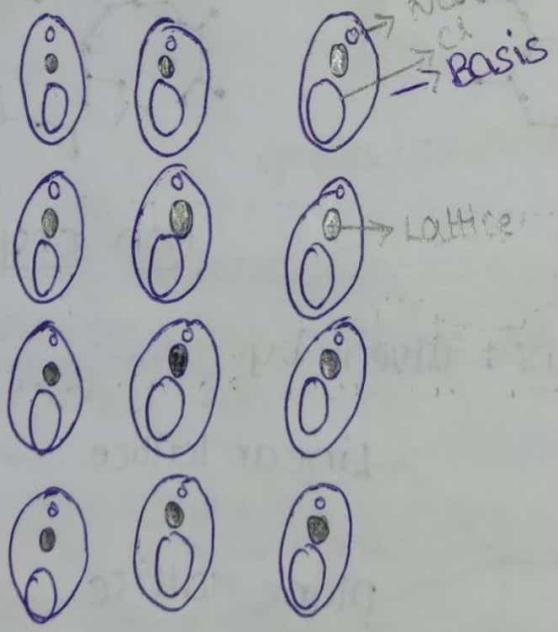
Plane lattice: Periodic arrangement in x and y directions (2D) is known as plane lattice

Basis (or) pattern (or) Motif:

A group of atoms (or ions) which when attached to every lattic points produces the crystal structure.

Basis is a group of atoms/molecules (or) which are identical in composition, arrangement and orientation.

Lattice + Basis = crystal structure



Unit Cell: It is a smallest geometrical figure (or) building block which is repeated along the 3 crystallography axis, it gives actual crystal structure.

→ The choice of unit cell is not unique.

→ Based on the no. of points (lattice) present in a unit cell, unit cells are classified into 2 types.

① primitive unit cell

② Non-primitive unit cell.

Primitive Unit Cell: If unit cell contains only 1 lattice point is called primitive unit cell.

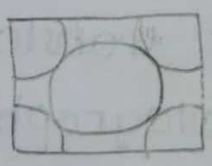
Eg: simple cubic cell.

Non-primitive unit cell: If unit cell contains more than 1 lattice point is called non primitive unit cell.

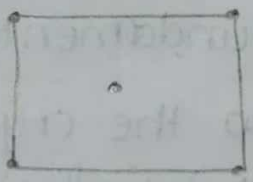
Eg: Body centered cubic, Face centered cubic and base centered structure.

→ Basis consisting
- 1 atom → monoatomic
- 2 atoms → Diatomic
- 3 atoms → Triatomic (polyatomic)

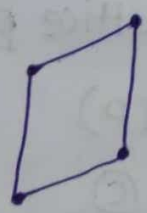
30/1/21
Saturday



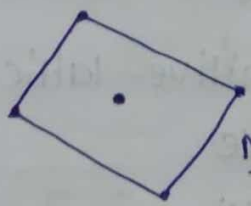
Face centered



Body structured



Primitive



Non primitive

Statement: All primitives unit cells are unit cells but all unit cells are not primitive

Crystallographic axes and lattice parameters

→ ~~Intersection~~ Let us consider, 3 non-coplanar planes and intersection of 3 non-coplanar planes is known as crystallographic axis named as x, y and z.

→ Let us consider a unit cell, unit cell intersects at a distance of a along the x-axis, at a distance of b along the y-axis, at a distance of c along the z-axis, a, b, c intersects are called primitives (or) fundamental translation vectors.

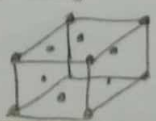
→ The angles b/w the crystallographic axis α, β and γ are called interfacial or interaxial angles.

→ so a, b, c, α, β and γ are called lattice parameters

→ Simple lattice (or) primitive lattice (P)

→ Base centered lattice (C)

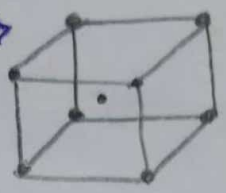
→ Body centered lattice →  (I)

→ Face centered lattice →  (F)

6/2/21
saturday → 7 crystal systems → 14 Bravis lattices.

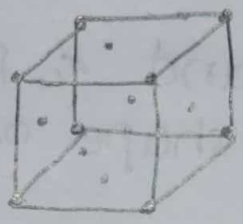
→ simple → 8 corner atoms

1/8 - each atom $n = 1/8 \times 8 = 1$.

→ Body centered → 

8 corner atoms + 1 atom completely inside.

$n = 1/8(8) + 1 = 2$.

→ Face centered → 

$n = 8 \times \frac{1}{8} + 6 \times \frac{1}{2}$

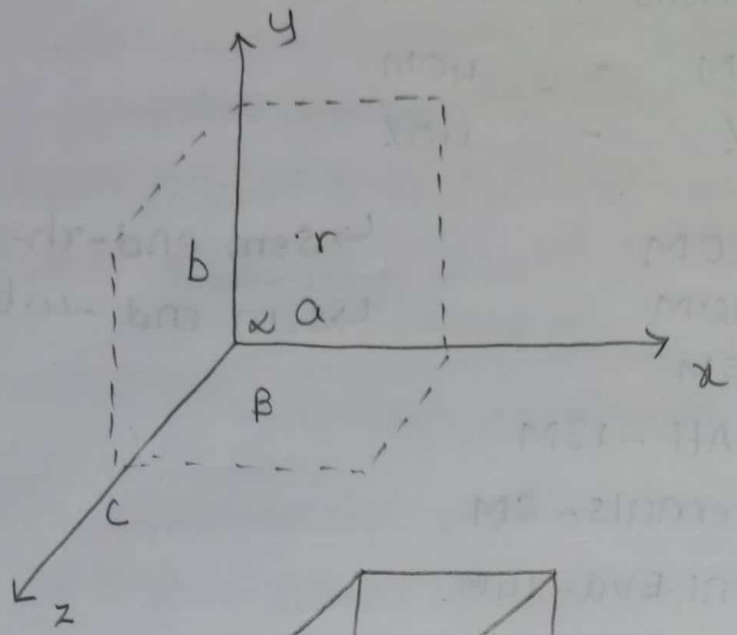
$= 1 + 3 = 4$.

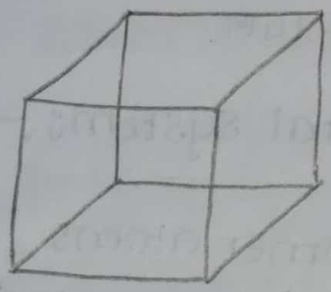
→ Base centered → 

$n = 8 \times 1/8 + 2\ 1/2 = 1 + 1 = 2$

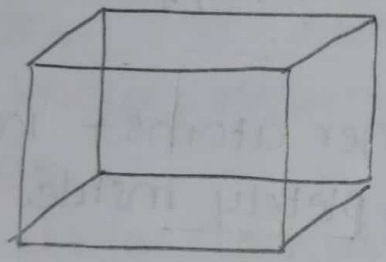
→ a, b, c are intercepts made by the planes in a unit cell. with crystallographic axes.

→ The size of unit cell can be determined with the help of a, b, c. (α, β, γ)





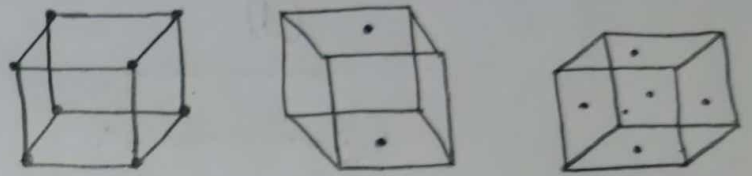
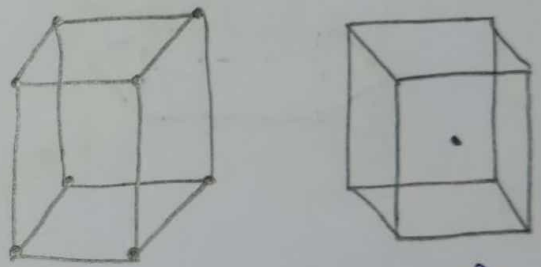
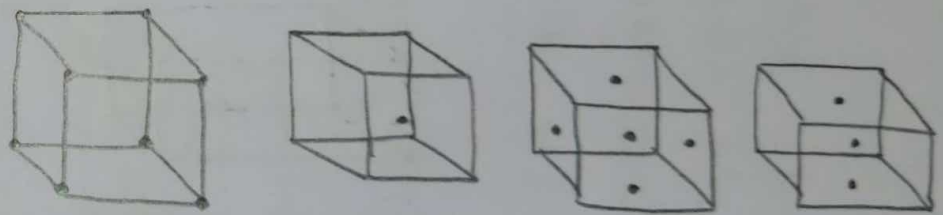
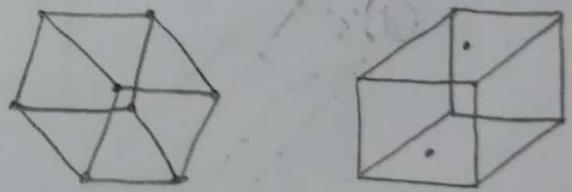
$a = b = c = 1$
$\alpha = \beta = \gamma = 90°$



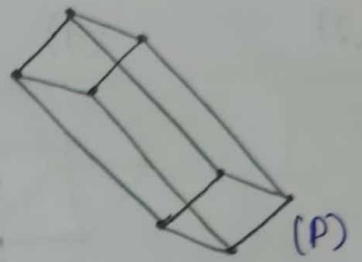
$a = b = 1$
$c = 3.$
$\alpha = \beta = \gamma = 90°.$

→ Based α, β, γ and a, b, c crystals are classified into 7 crystal systems and 14 bravis lattice.

→ If we know a, b, c and α, β, γ values we can assume the size and shape of the crystal structure.

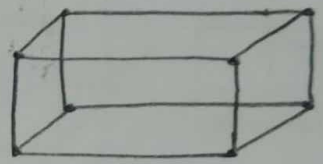
Name of the crystal system	a, b, c	α, β, γ	Diagram
cubic	$a=b=c$	$\alpha=\beta=\gamma=90^\circ$	 (P) (I) (F)
Tetragonal	$a=b\neq c$	$\alpha=\beta=\gamma=90^\circ$	 (P) (I)
orthorhombic	$a\neq b\neq c$	$\alpha=\beta=\gamma=90^\circ$	 (P) (I) (F) (C)
Monoclinic	$a\neq b\neq c$	$\alpha=\beta\neq\gamma=90^\circ$	 (P) (C)

Triclinic $a \neq b \neq c$ $\alpha \neq \beta \neq r = 90°$



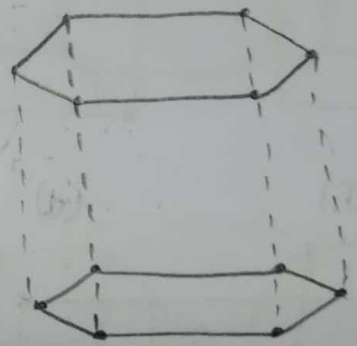
(P)

Rhombohedral $a = b = c$ $\alpha = \beta = r \neq 90°$ $< 120°$



(P)

hexagonal $a = b \neq c$ $\alpha = \beta \neq r = 90°$ $r = 120°$



(P)

Parameters

(i) no.of lattice points in unit cell (no.of atoms present inside the unit cell)

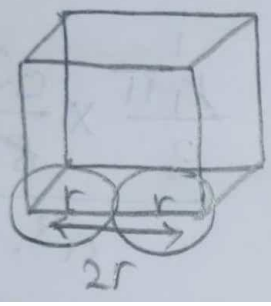
simple centered → n = 1

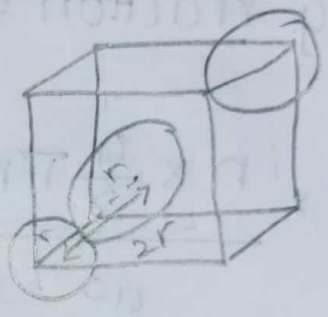
Body centered → n = 2

Face centered → n = 4

Base centered → n = 2

(ii) Nearest neighbour distance (Distance blw any two nearest neighbour atoms)





(iii) Atomic Radius: $\frac{N.N.D}{2} = \frac{2r}{2} = r$.

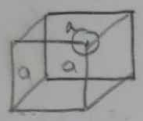
(iv) Co-ordination number: The no. of equidistant nearest neighbour atoms.

(v) Atomic packing fraction: It is the ratio of volume occupied by the atoms in the unit cell to volume of the unit cell.

$$Apf = \frac{\text{volume occupied by the atoms in unit cell}}{\text{volume of unit cell.}}$$

$$= \frac{\text{no. of atoms in unit cell} \times \text{vol. of each atom}}{\text{vol. of unit cell.}}$$

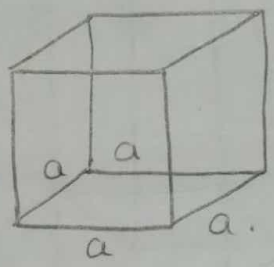
→ If unit cell is having crystal structure



Vol. of U.C = a x a x a

$= a^3$

Vol. of atom $= \frac{4}{3}\pi r^3$



$a = b = c$

$\alpha = \beta = \gamma = 90°$

$$Apf = \frac{n \times \frac{4}{3}\pi r^3}{a^3}$$

(Cubic cells)

10/2/21 Wednesday

→ Atomic packing fraction of simple cubic (sc) structure. (Explain the structure of sc).

No. of atoms in sc unit cell $= 8 \times \frac{1}{8} = 1$.

*Nearest neighbour distance $= 2r = a$.

* packing fraction $= \frac{\text{vol. of atoms}}{\text{vol. of uc}}$

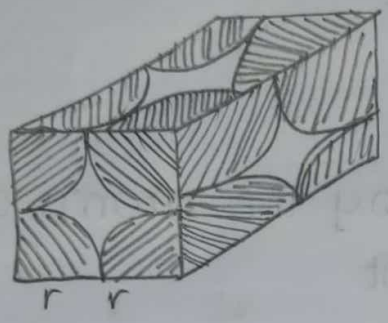
$$= \frac{n \times \frac{4}{3}\pi r^3}{a^3} = \frac{1 \times \frac{4}{3}\pi \left(\frac{a}{2}\right)^3}{a^3} = \frac{\frac{\cancel{4}^{1}\pi}{3} \times \frac{a^3}{\cancel{8}^{2}}}{a^3}$$

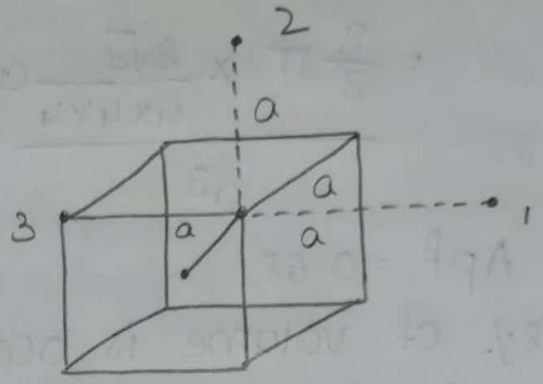
$= \frac{\pi}{6} = 0.52.$

→ Atomic packing fraction = 52%.

→ 52% space is occupied by atoms in sc and 48% of empty space is there.

co-ordinate number = 6.





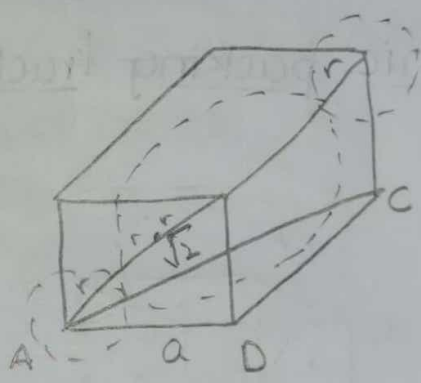
$2r = a.$

Atomic packing fraction for Body centered cubic Structure:

NO. of atoms in unit cell

$= 8 \times \frac{1}{8} + 1 = 2.$

- Nearest neighbour distance



From ΔACD

$AC^2 = AD^2 + CD^2$

$AC^2 = a^2 + a^2$

$AC^2 = 2a^2$

$AC = \sqrt{2}a$

From ΔABC

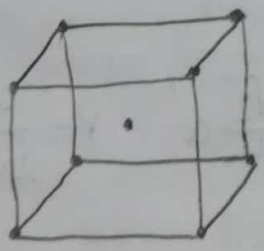
$AB^2 = AC^2 + BC^2$

$(4r)^2 = (\sqrt{2}a)^2 + a^2$

$(4r)^2 = 2a^2 + a^2 = 3a^2$

$4r = \sqrt{3}a$

$r = \frac{\sqrt{3}}{4}a$



$NND = 2r = \frac{\sqrt{3}}{2}a.$

Atomic radius $r = \frac{\sqrt{3}}{4}a.$

$$APF = n \times \frac{4}{3}\pi r^3$$

$$= 2 \times \frac{4}{3}\pi \times \left(\frac{\sqrt{3}}{4}a\right)^3$$

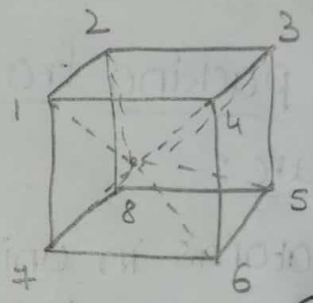
$$= 2 \times \frac{4}{3}\pi \times \left(\frac{\sqrt{3}}{4}a\right)^3$$

$$= \frac{8}{3}\pi \times \frac{3\sqrt{3}}{4\times4\times4}\frac{a^3}{a^3} = \frac{\sqrt{3}}{8}\pi$$

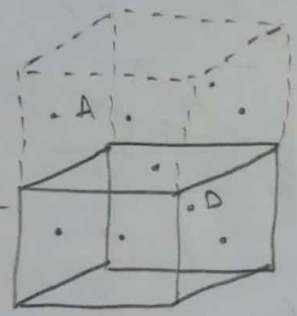
$$APF = 0.68$$

→ 68% of volume is occupied by the atoms and 32% of empty space is present.

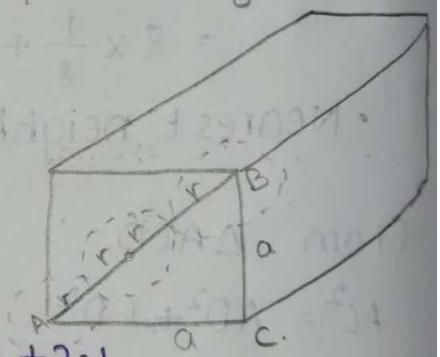
Co-ordination numbers - 8.



Atomic packing fraction of fcc:



above = 4
Within plane = 4
Below = 4



No. of atoms $n = 8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 1 + 3 = 4.$

Nearest neighbouring dist = $2r$

from ΔABC

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

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

$(4r)^2 = 2a = 4r = \sqrt{2}a.$ $\quad r = \frac{\sqrt{2}}{4}a \quad r = \frac{a}{2\sqrt{2}}$

$NND = 2r = \frac{a}{\sqrt{2}}$

Atomic value $r = \frac{a}{2\sqrt{2}}$

$APF = n \times 4/3\,\pi r^3 \,/ a^3.$

$= 4 \times \frac{4}{3}\pi\left(\frac{a}{2\sqrt{2}}\right)^3 / a^3.$

$= \frac{16}{3}\pi \frac{a^3}{8 \times \sqrt{2} \times \sqrt{2} \times \sqrt{2}} = \frac{16\pi}{3} \times \frac{1}{8 \times 2\sqrt{2}} = \frac{\pi}{3\sqrt{2}}$

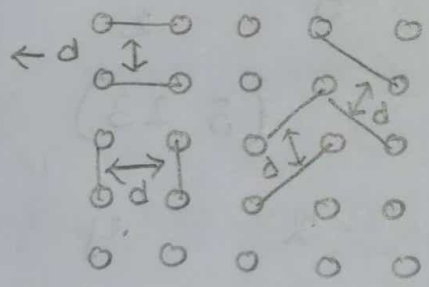
Apf = 0.74.

→74% of space is occupied by atoms and 26% is left empty. Co-ordination number = 12.

Structure	n	NND	r	Apf	E	Co-ordination
SC	1	2r	a/2	0.52	48%	6
BC	2	2r	$\frac{\sqrt{3}}{4}$ a	0.68	32%	8
FCC	4	2r	$\frac{a}{2\sqrt{2}}$	0.74	26%	12.

13/2/21
Saturday

Crystal planes: The imaginary planes passing through the lattice which are having large concentration of atoms.



Interplanar d: The distance b/w any two successive parallel planes is known as interplanar distance

Miller indices:

→ Miller indices gives the position and orientation of crystal planes in the lattice.

→ Miller indices are the 3 smallest integers whose ratios are the reciprocals of interceps made by the crystallographic planes with crystallographic axes.