AIR-1 Notes

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Handwritten notes by

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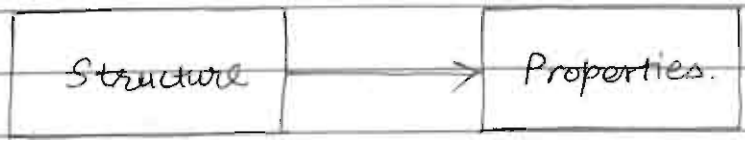
Material Science

→ It is a branch of science which deals with the investigation of relationship that exist between structure and property.



→ Property - It is a characteristic of a material which can be measured.
→ Property can be observed by applying external stimulus and hence a response can be measured.
→ Stimulus can be electrical, magnetic, optical, mechanical force etc.

→ Following are the different types of structure:

1) Macrostructure - External shape and forms such as shape and size by naked eye.

Mechanical POV:

2) Microstructure - In it we study shape and size of grains by optical microscope

3) Sub-structure - In it we study defects in the grains by ~~magnifi~~ scanning electron microscope.

4) Crystal structure - In it we study arrangement of atoms by X-Ray Diffraction technique.

Electronics and Electrical POV:

5) Electronic structure - In it we study electrons distribution around an atom by Electron spectroscopy.

6) Nuclear structure - In it we study about the nucleus by nuclear magnetic Resonance or Moss-Bauer Spectroscopy

→ Following are the important engineering materials:

1) Metals and Alloys - Aluminium, Iron, Copper, Magnesium, Zinc, Titanium, Nickel, Tin and Lead.

2) Polymers
   (a) Thermoplastic polymers
   (b) Thermo-setting plastic polymers

3) Composite

4) Ceramics - Oxides, Carbides, Nitrites, glasses etc.
~~Depending upon the atomic arrange~~

→ Depending upon the atomic arrangement of the above materials are classified into 2 groups.

Crystalline	Non-crystalline / Amorphous
1) Atoms are regularly arranged over large atomic distances.	1) Atoms are irregularly or randomly arranged.
2) Long range order exist.	2) No long range order exist.
3) Since Bond length is same everywhere, hence sharp melting point exists.	3) No sharp melting point exists.
4) Mechanical property depends on no. of atoms on a given line hence crystalline materials are anisotropic in nature	4) Since no. of atoms on each and every line is same, hence property is isotropic in nature.
5) It is true solid having fixed external shape and size.	5) It is called super cooled liquids which doesn't have fixed shape and size.
eg- All metals, many ceramics and some polymers. (Crystalline materials are hard and brittle)	eg- charcoal, glass, many polymers and some ceramics

⇒ Crystal Structure

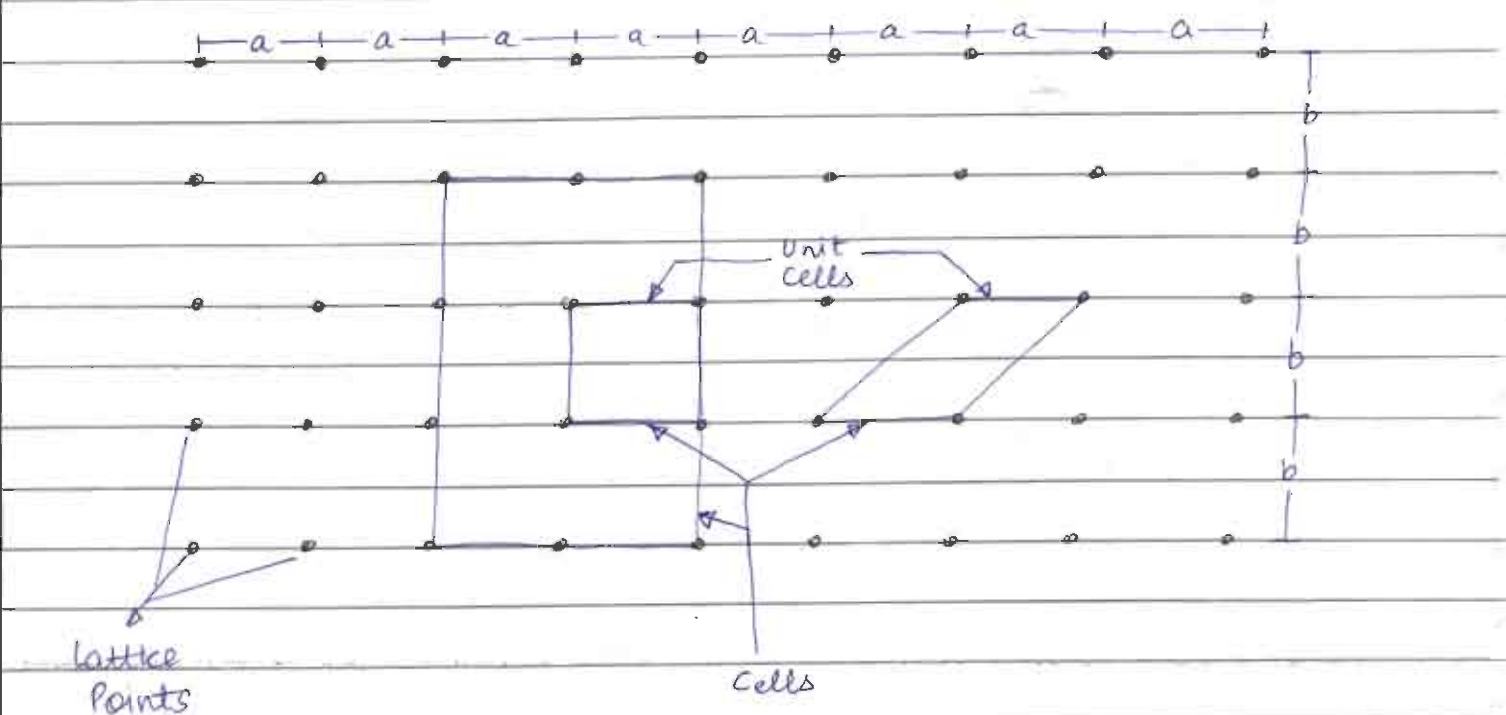
In it we study arrangement of atoms and the science involved is called crystallography.

→ In this we assume atoms to be having some well defined diameter i.e. It is assumed to be sphere. This model is called Hard Sphere Model.

→ Assumptions of Hard Sphere Model

1) Cation is always smaller than its respective anion.
2) Cations and Anions always are in contact with each other.
3) Since cation has higher charge Density (charge per unit Surface area) hence it is always surrounded by maximum no. of anions as permitted by geometry.

→ Space Lattice - It is an infinite array of points arranged in 3-dimensional space which is periodically repeated and has identical surroundings.

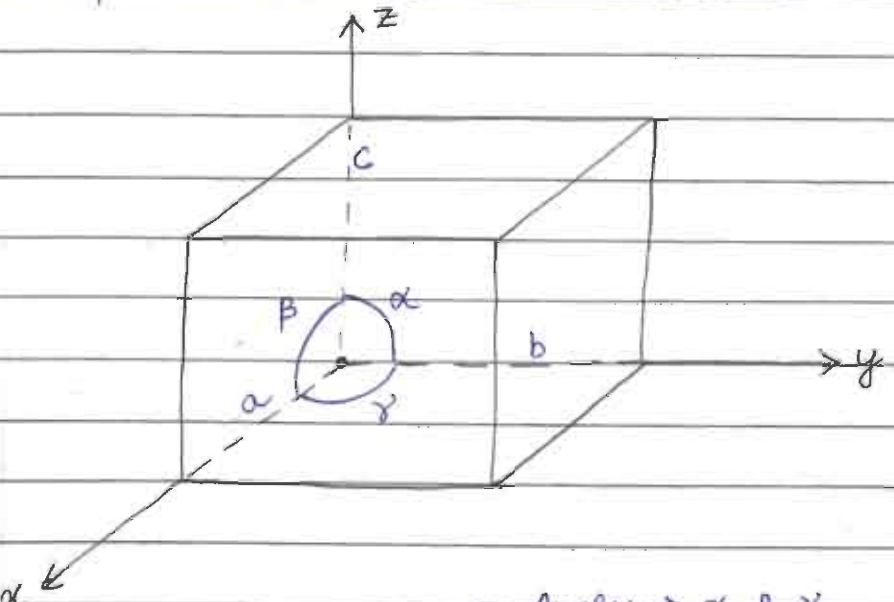


→ These space lattice are periodically repeating in three directions (x, y, z) and the periodic distance along those directions are called Lattice Parameter (a, b, c).

→ With the help of these 3 Lattice parameter, we can create a volume which is called cell.

→ A cell can be said to be unit cell if it has smallest size, maximum symmetry and if it is repeated in space lattice then it can cover entire space lattice.

→ There can be ∞ number of unit cell possible and out of them some important unit cells will be studied.



6 Lattice Parameters → Angles → α, β, γ
6 Lattice Parameters → length → a, b, c

→ With the help of 6 Lattice Parameters there are large no. of unit cell possible but we have to study only those unit cells which have smallest size and maximum possible symmetry and Bravais found out that there are only such 14 unit cell available which is called crystal class and they can be grouped into 7 crystal systems.

⇒ Following are the 7 crystal systems:

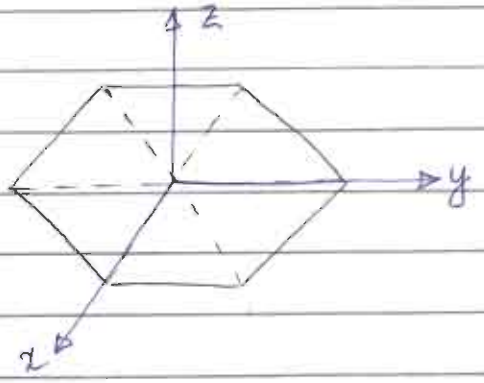
1) Cubic Crystal → $a = b = c$, $\alpha = \beta = \gamma = 90^\circ$

2) Rhombohedral → $a = b = c$, $\alpha = \beta = \gamma \neq 90^\circ$
(Cube + Shear on all faces)

3) Tetragonal → $a = b \neq c$, $\alpha = \beta = \gamma = 90^\circ$
(Duster)

4) Orthorhombic → $a \neq b \neq c$, $\alpha = \beta = \gamma = 90^\circ$
(CPU)

5) Hexagonal → $a = b \neq c$, $\alpha = \beta = 90^\circ$ and $\gamma = 120^\circ$

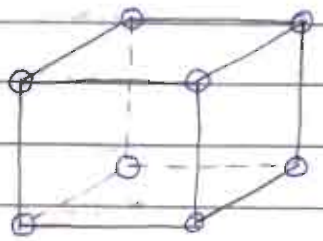


6) Triclinic → $a \neq b \neq c$, $\alpha \neq \beta \neq \gamma$
(Highly unsymmetrical)

7) Monoclinic → $a \neq b \neq c$, $\alpha = \gamma = 90^\circ \neq \beta$.

⇒ Cubic crystal system

1) Simple Cubic Crystal



→ No. of Lattice Points = 8

→ Contribution of each corner atom $= \frac{1}{8}$

→ Atoms per unit cell $= 8 \times \frac{1}{8} = 1$

→ Geometrical relationship $\boxed{a = 2r}$

Lattice Parameter — Radius of atom.

→ Coordination Number → No. of nearest neighbour atoms.

$\boxed{CN = 6}$ (2×3)

↳ No. of axes.

→ Atomic packing factor / efficiency → It represents the fraction of volume of unit cell that is filled by atoms and is given by a ratio as:

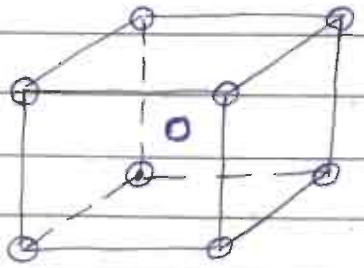
$$APF = \frac{n \times \text{Volume of atom}}{\text{Volume of unit cell}} = \frac{1 \times \frac{4}{3}\pi\left(\frac{a}{2}\right)^3}{a^3}$$

$n \rightarrow$ no. of atoms per unit cell.

$\boxed{= 0.52}$

eg - Manganese (Mn)

2) Body Centered cubic



No. of Lattice points $= 8 + 1$

Corner — Body centre.

→ Contribution of each corner atom = $\frac{1}{8}$

→ Contribution of body centered atom = 1

→ No. of atoms per unit cell = $\frac{1}{8} \times 8 + 1 \times 1 = 2$

→ CN = 8

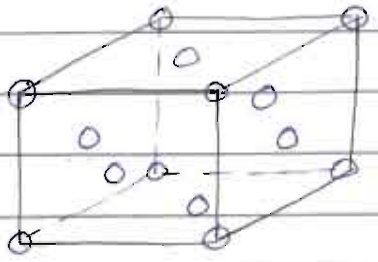
→ Geometrical Relationship → $\sqrt{3}a = 4r$

→ $\boxed{a = \frac{4r}{\sqrt{3}}}$

→ APF = $\frac{2 \times \frac{4}{3} \pi \times \frac{3}{16} a^3 \frac{\sqrt{3}}{4}}{a^3} = \frac{\sqrt{3}\pi}{8} \boxed{= 0.68}$

→ eg- Iron (α), Chromium, Tungsten, Molybdenum

3) Face Centered Cubic (FCC)



→ No. of Lattice points = 8 + 6 = 14
(8 ↙ Corner, 6 ↘ Face centered)

→ Contribution of each corner atom = 1/8

→ Contribution of each face centered atom = 1/2

→ No. of atoms per unit cell = 1/8 × 8 + 1/2 × 6 = 4

→ CN = 12 = 4 × (3) (→ No. of planes.)

→ Geometrical Relationship ⇒ $\sqrt{2}a = 4r$

→ APF = $\frac{4 \times \frac{4}{3} \pi \left(\frac{\sqrt{2}a}{4}\right)^3}{a^3} = \boxed{0.74}$

→ eg- Iron, copper, Aluminium, Silver, nickel, gold, platinum.

Allotrops – When 2 elements exist in more than 1 form at different temperature and pressure then they are called Allotrops and this phenomena is called Allotropy.

eg – Carbon → Graphite, Diamond.

Iron → α-Iron (BCC), γ-Iron (FCC), δ-Iron (BCC)

Tin → α-Tin and β-Tin

⇒ As atomic packing factor increases, ductility increases.

Simple Cubic < BCC < FCC

Ductility ↑↑ →

4) Hexagonal Closed Packed Structure (HCP)

→ No. of lattice points = 6X2 + 2 + 3

→ Contribution of corners = 1/6

→ Contribution of face atom = 1/2

→ Contribution of centre atom = 1

→ $N = 12 \times \frac{1}{6} + 2 \times \frac{1}{2} + 3 \times 1 = 2 + 1 + 3 = 6$

→ CN = 12

→ APF = 0.74

→ Eg – Titanium, Zinc#, Cobalt Cadmium, Graphite#

⇒ Difference b/w FCC and HCP

→ Although FCC and HCP have same coordination no. and same APF and both are called closed packed structure (voids are low) but arrangement of atom sequence is different.

→ Stacking sequence of FCC structure is ABC ABC

→ Stacking sequence of HCP is ABABAB

⇒ Closed Packed structure

→ These are those structures which creates minimum empty space and these empty spaces are called voids or interstitial or holes.

Q- What is the diameter of largest sphere in terms of lattice parameter a which will fit the void at the centre of the cube edge of a BCC crystal.

$\sqrt{3}a = 4r$

$d = a - 2r$

$= a - 2 \times \frac{\sqrt{3}a}{4} = a - 0.866a$

$\boxed{d = 0.134a}$

Q- Repeat the above question for FCC structure.

$\sqrt{2}a = 4r$

$d = a - 2r$

$= a - \frac{a}{\sqrt{2}} = (1 - 0.707)a = 0.293a$

$\boxed{d = 0.293a}$

Since size of voids in FCC > size of voids in BCC

→ more carbon can be alloyed with FCC Iron to form steel.

⇒ Types of Void

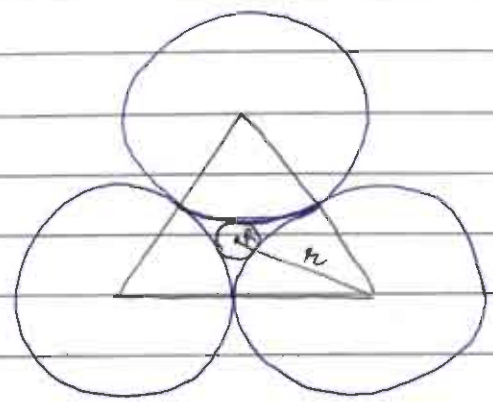
There are 3 types of void:

1) Trigonal void

Formed by 3 spherical atoms.

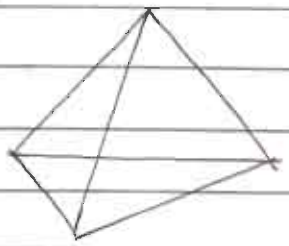
Size of void, $R = 0.155\, r$

(R: Radius of void; r: Radius of atom)



⇒ Tetragonal / Tetrahedral void

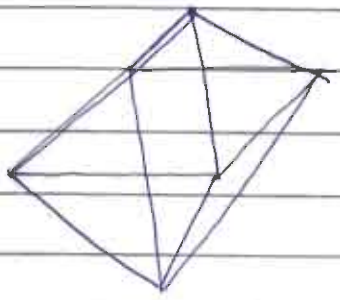
Formed by 3 atoms in one plane and one atom above that plane.



$R = 0.225r$

⇒ Octahedral void

Formed by 4 atoms in one plane, 1 atom above and one atom below that plane.



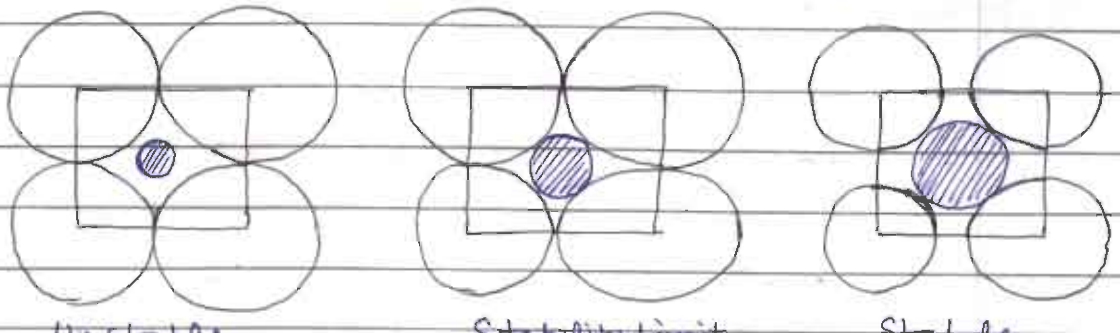
$R = 0.414r$

Examples

1) Tetragonal → Zinc Sulphide (ZnS) → Zinc Blende
2) Trigonal → Boron Oxide.
3) Octahedral → Sodium Chloride (NaCl)

⇒ Rules of stacking cations and anions for stable configuration

① Cation and anion must touch each other.
② Cation is surrounded by maximum number of anions.



For stable configuration | Size of atom which fits in the void > Size of void.

⇒ Density of crystal

Avagadro No: 6.022×10^{23} ← N atoms weigh A gms. (A → Atomic weight.)

n atoms weigh $\frac{A}{N} \times n$ gms.

(n ← no. of atoms per unit cell.)

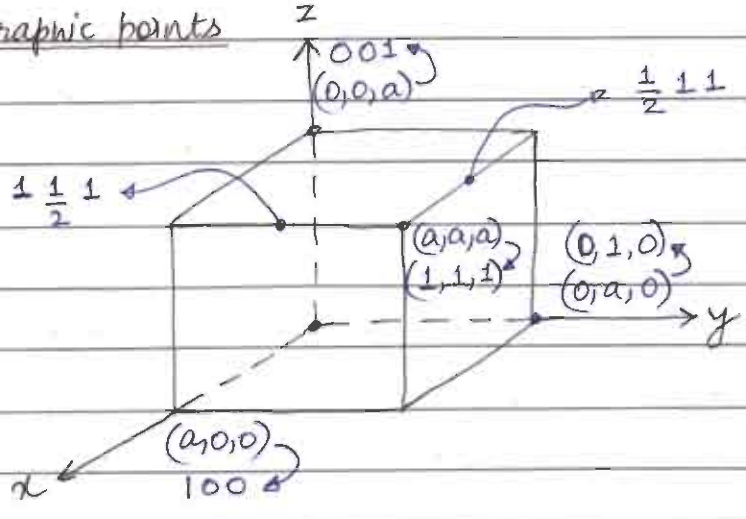
$$\therefore \quad \rho_{Crystal} = \frac{A \times n}{N \times a^3}$$

Q- Find the density of γ-Iron (FCC) if atomic weight is 56 gm/mole and length of unit cell is 10 Å. (in kg/m^3)

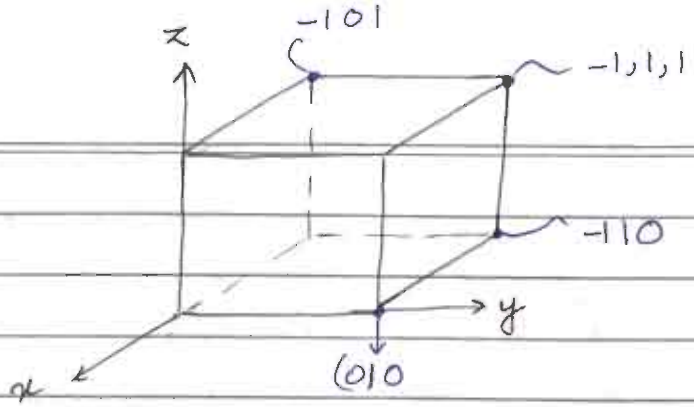
$$\rho_{Crystal} = \frac{\frac{56}{6.022 \times 10^{23}} \times 4 \times 10^{-3}}{(10 \times 10^{-10})^3} = 372 \ kg/m^3.$$

⇒ Crystallographic points, directions and planes

1) Crystallographic points



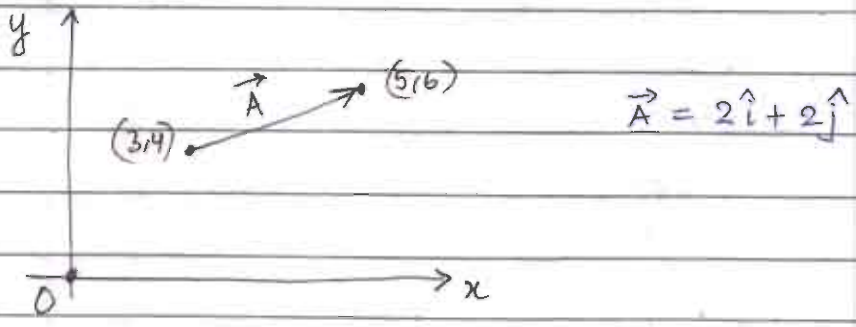
→ Point coordinates are represented as p q r without any comma (,) and bracket [()] as a fraction of a, b, c respectively



⇒ Crystallographic direction

→ Since it is a vector quantity and it can be represented by an arrow. and that arrow has a tail and head.

→ Head represents the direction.



→ In order to find a vector quantity it's tail and head coordinate is desired but if tail of vector passes through origin, then only head coordinate is desired. Therefore, in order to find a direction vector, we shift the origin to the tail.

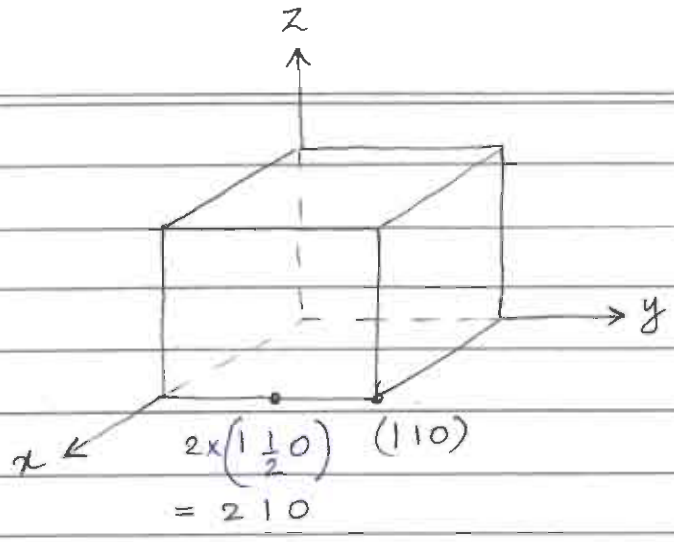
#

→ Rules for finding direction vector

Rule 1 → Check whether the direction vector is passing through origin or not.

→ If the tail of vector is not passing through Origin then shift the origin to it's tail.

Rule 2 → Find the head coordinate as a fraction of a, b, c.



Rule 3 - The indices obtained in step 2 is converted into nearest integer values.

Rule 4 - The obtained indices after reduction is written as

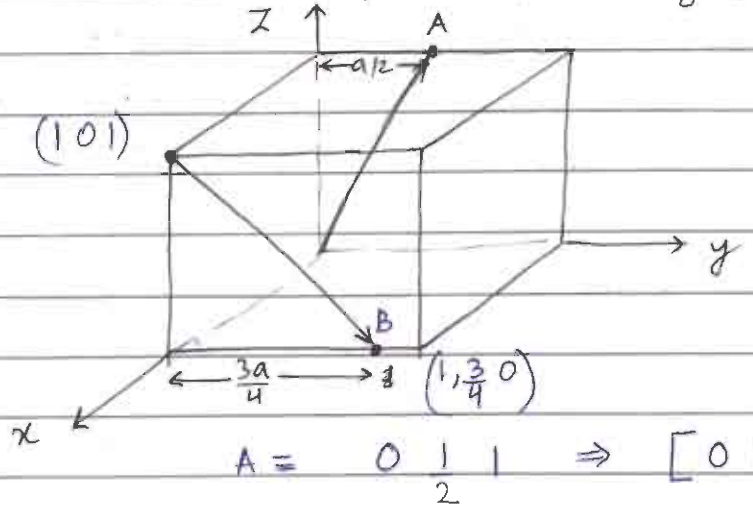
$$[u\ v\ w]$$

without any comma in square bracket

If any value comes out to be negative, we put a bar over it eg- $[u\ \bar{v}\ w]$ → v is negative.

	x	y	z
Intercept of head	1	1	0
Reduction	1	1	0
Direction.		[1 1 0]	

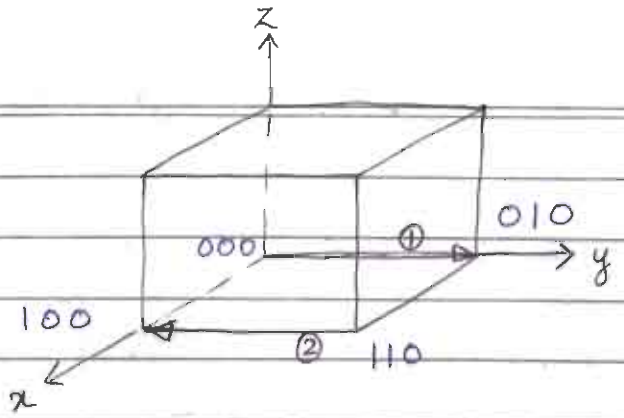
Q- Find the direction vector for the following figure.



$\vec{B} \equiv 0\ \frac{3}{4}\ -1$

$\Rightarrow [0\ 3\ \bar{4}]$

$A \equiv 0\ \frac{1}{2}\ 1 \Rightarrow [0\ 1\ 2]$



① ≡ [0 1 0]

② ≡ 0 → 1 0 ≡ [0 $\bar{1}$ 0]

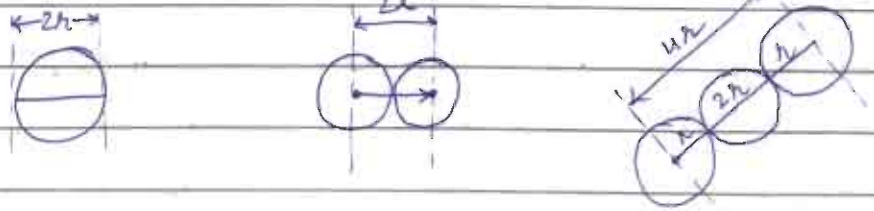
NOTE:

① When a direction vector [u v w] is multiplied by -1 then it will give an antiparallel direction vector

② The indices u, v, w in direction vector [u v w] is proportional to lattice parameters a, b, c respectively.

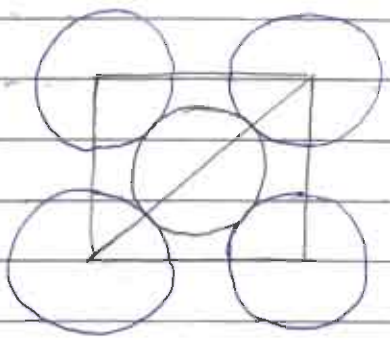
⇒ Linear Density

→ It is defined as the number of atoms centered on a given direction vector per unit length of that direction vector.



2r ≡ 1 atom 2r ≡ 1 atom 4r ≡ 2 atoms.

FCC



LD along [0 1 0]

$LD_{[010]} = \frac{1}{a}$

~~LD along~~ [0 1 1]

$LD_{[011]} = \frac{2}{\sqrt{2}a} = \frac{\sqrt{2}}{a}$