

- Definition of Physical metallurgy :-

→ It is a studying within metallurgy, where the focus is on the physical properties & structure (micro structure) of the materials.

- Chapter-1 Crystal structure of metals

- Solids may be classified into two groups on the basis of their structure :-

(I) crystalline

(II) Non-crystalline
(or)
Amorphous

- Crystalline :-

→ Crystalline Solids have orderly arranged of atoms in three dimensions.

→ ex :- Ice, Sugar, quartz.

- Non-Crystalline (or) Amorphous :-

→ Amorphous Solids have randomly arrangement of atoms.

→ ex :- glass, plastic, rubber, polymer.

- Characteristics of crystalline materials :-

→ Solids have orderly arrangement of atoms.

→ Individual crystals are bonded by planes.

→ Crystalline solid, exhibit 'anisotropic'.

→ Solid to liquid transition always distinct

- Crystalline solid are further classified into 'single crystalline' and 'polycrystalline'.

→ Single crystal find extensive use as semiconductors in field of electronics engineering.

→ Most of the engineering materials are polycrystalline in nature. They are made up of millions of tiny crystals.

- Different between isotropic and anisotropic

Isotropic

→ when properties of material is 'same' in all crystallography direction of materials is said to be 'isotropic'.

Anisotropic

→ If properties of materials is different in all crystallography direction of materials is said to be 'An-isotropic'.

→ It is independent of direction.

→ It exhibits consistent and uniform chemical bond.

→ Example :-

- Glass.
- Plastic
- Diamond.

→ It is dependent in direction.

→ It exhibit inconsistent and uniform chemical bond.

→ Example :-

- Wood
- Graphite.
- Composite materials

• Crystallography :-

It is a branch of science in which the internal structure of crystals, their properties, external and internal symmetry of crystals are studying.

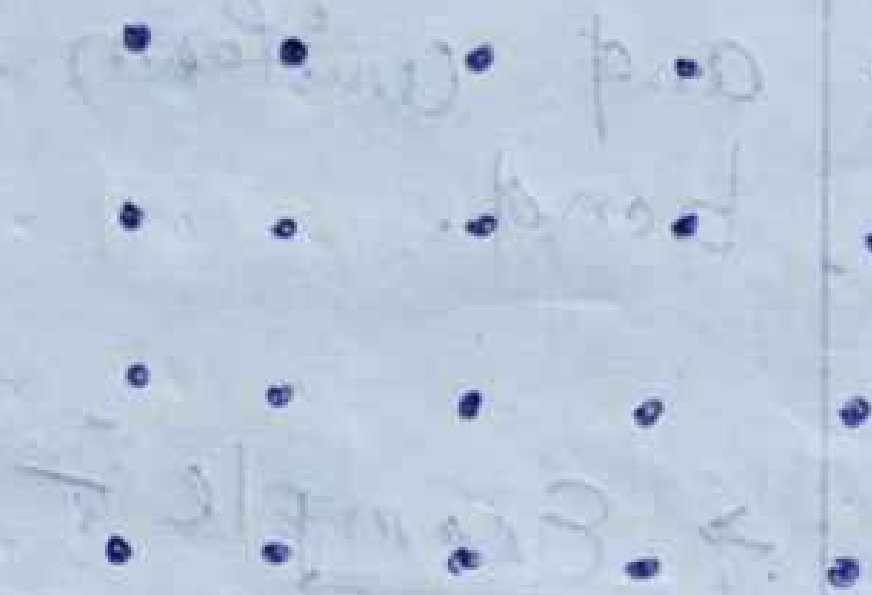
• Crystal structure :-

→ A metal is composed of several atoms which are arranged in a regular repeated three dimensional pattern.

→ These arrangement is known as 'Crystal structure'.

- Lattice :-

→ Three dimensional regular arrangement of points in space is called 'Lattice'.



(Lattice)

- Space Lattice :-

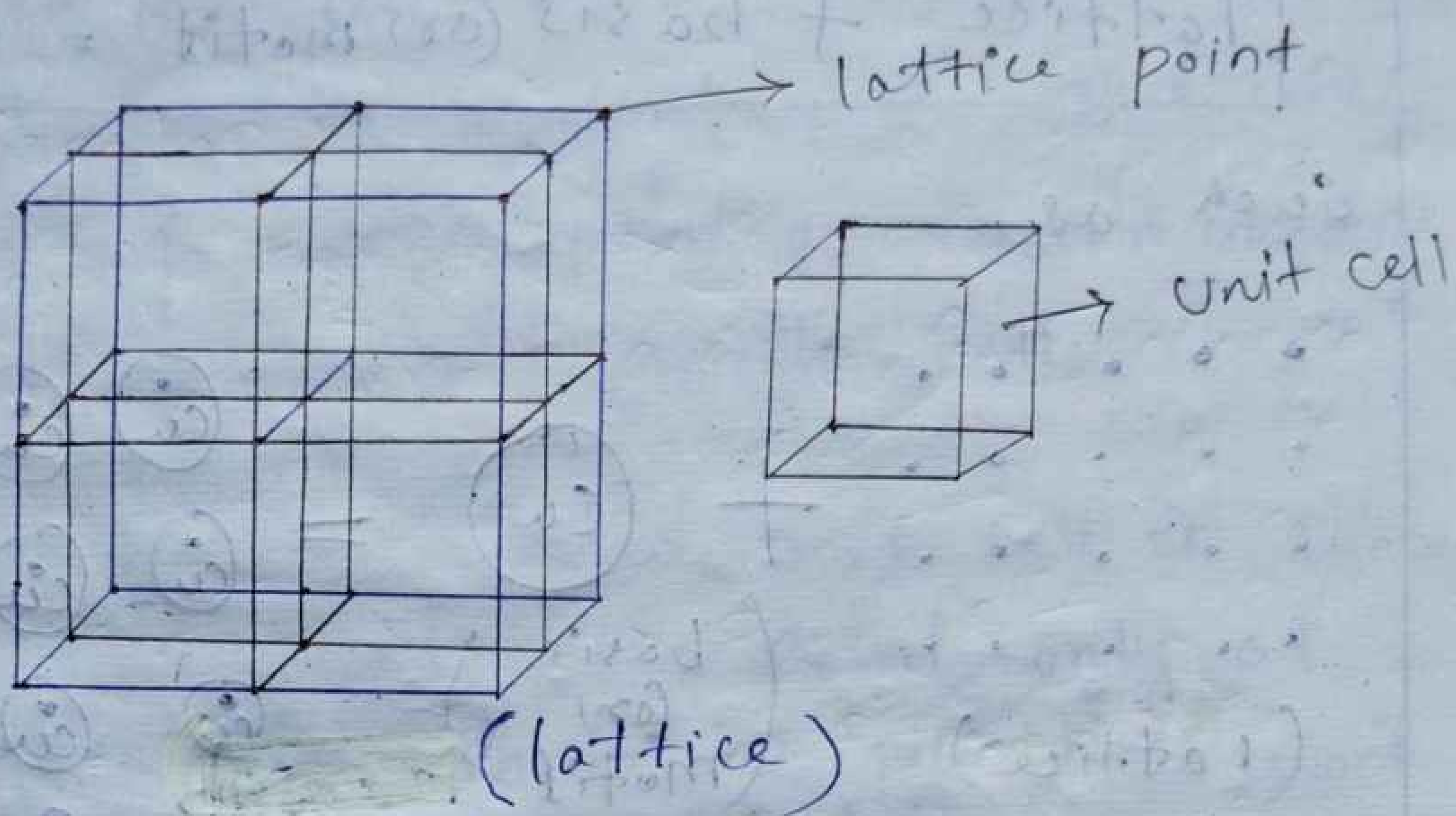
→ Three dimensional periodic or regular arrangement of infinite number of points in space is called as 'space lattice'.

→ The points in the space lattice are known as 'Lattice point'.

→ Space Lattice provides the frame work with reference to which the crystal structure can be described.

→ The lattice is imaginary while crystal structure is real.

→ Crystal is also called 'space lattice'.
(But not directly).



• Basis (or) motif :-

→ From a lattice, to represent a crystal structure with associated every lattice point with one or more atoms.

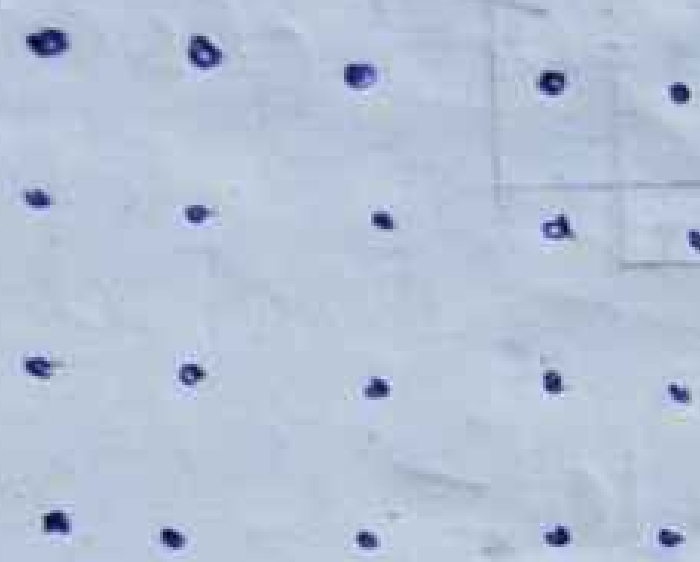
→ The way of 'filling up' of lattice points by the atoms is known as 'basis' (or) 'motif'.

→ Repeating unit to be placed at each lattice point is called as 'motif' (or) 'basis'.

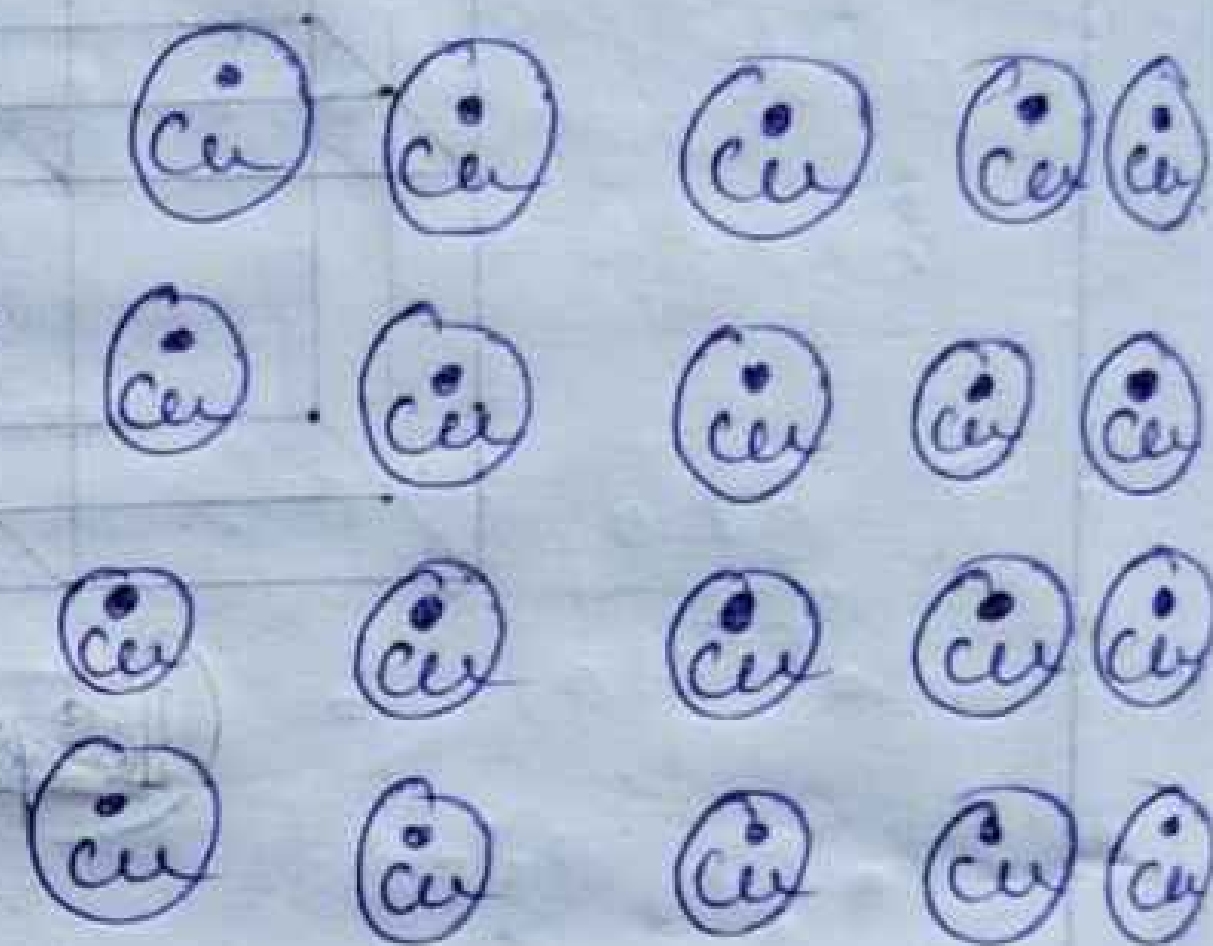
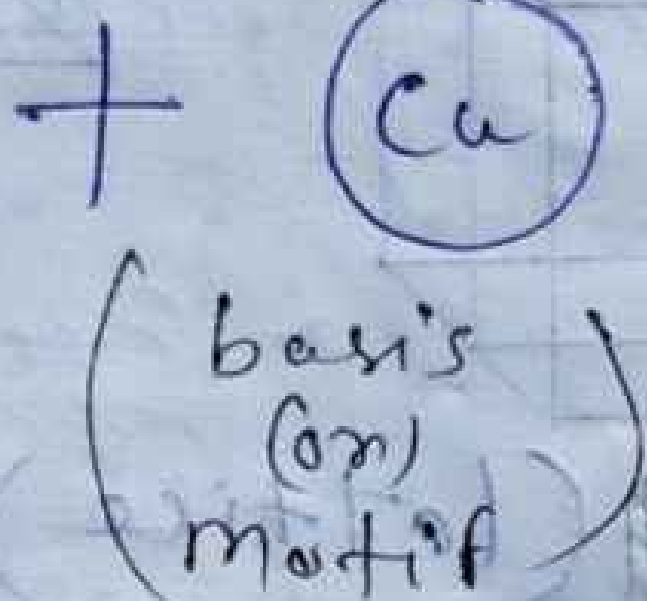
→ It can be a single atom, group of atoms, single molecule (or) group of molecules.

Lattice + basis (or) motif = Crystal

Such as,



(Lattice)



(Crystal)

Unit cell

→ 3 dimensional repeating 'group of lattice' in space is called 'unit cell' (or)

→ Unit cell is the smallest group of atoms possessing the symmetry of the crystal. (shape)

→ Unit cell is the subdivision of space lattice that still retains the overall characteristics of space lattice (or) crystal lattice.

→ Unit cell is the basic structural unit (or) building block of the crystal.

- Primitive unit cell:-

→ Primitive unit cell is a smallest unit cell that contains exactly one lattice point per corner of unit cell.

→ It is the smallest possible cell.

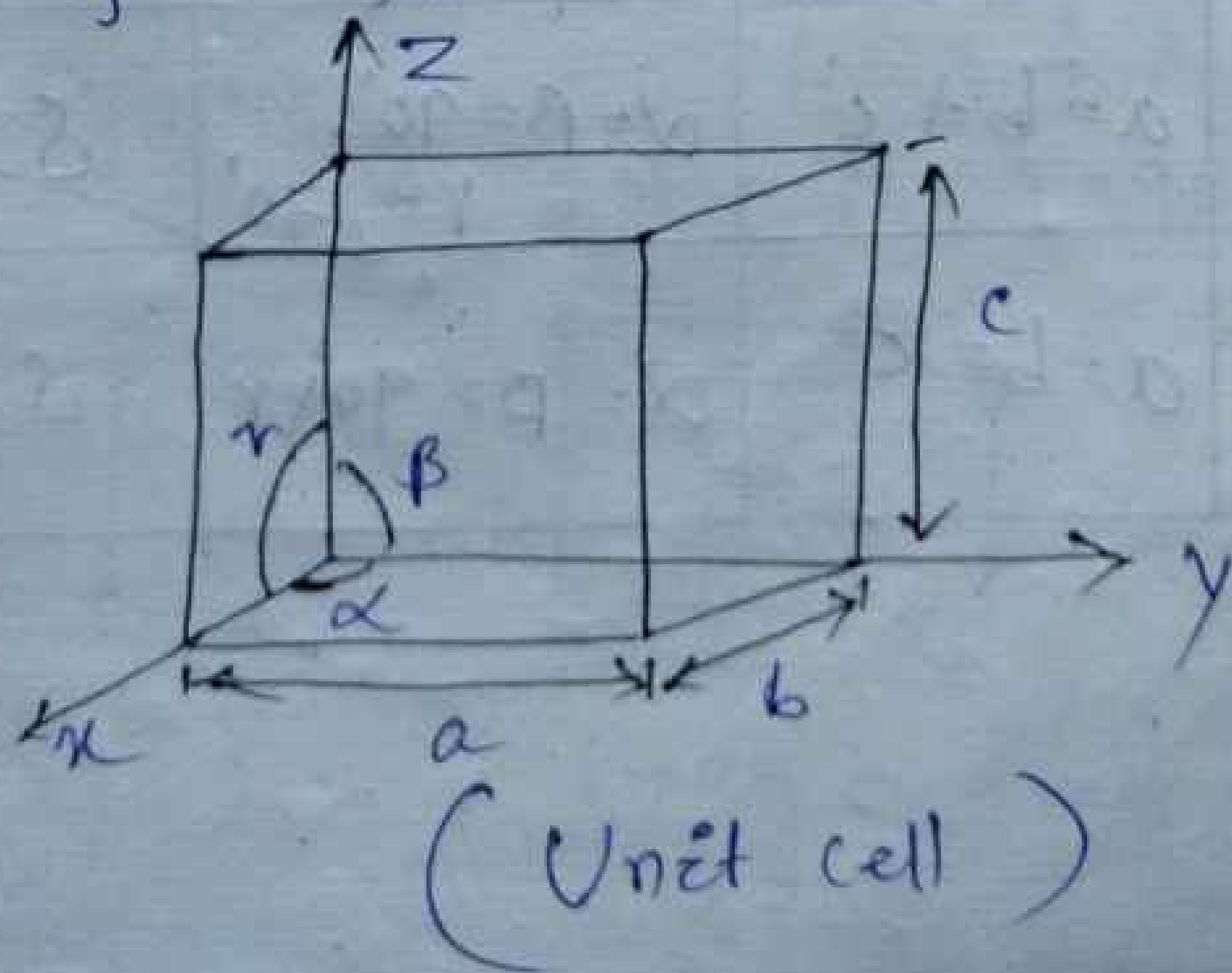
→ When a unit cell is chosen that contains lattice point only at its corner it is known as 'primitive unit cell'.

→ Example:- Simple monoclinic, triclinic, simple cubic.

- Lattice parameter:-

→ Lattice parameter describe the size and shape of the unit cell.

→ The unit cell geometry is completely defined in term of six parameters. Three edge length ($a, b \& c$), Three inter axial angle ($\alpha, \beta \& \gamma$).



→ In a cubic crystal system only the length of the side of the cube is necessary to completely describe the unit cell.

→ This length measure at room temperature, is the lattice parameter (or) lattice constant (a_0).

• There are '14' space lattices which are arranged from 'seven' crystal systems.

Trick
↓

C

T

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M

T

H

R

Crystal system :	Axial length	Axial angle	Bravais lattice
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$	SC, BCC, FCC
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	ST, BCT
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	SO, BCO, ECO, FCO
Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90^\circ \neq \beta$	SM, ECM
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$	STr
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90^\circ, \gamma = 120^\circ$	SH
Rhombohedral	$a = b = c$	$\alpha = \beta = \gamma \neq 90^\circ$	SR

• Full form of all bravais :- (Total = 14)

1. SC - Simple Cubic.

2. BCC - Body centered cubic

3. FCC - face centered cubic

1. ST - Simple Tetragonal

2. BCT - Body centered Tetragonal

1. SO - Simple Orthorhombic

2. BCO - Body centered orthorhombic

3. ECO - End Centred orthorhombic

4. FCO - face centered orthorhombic

1. SM - Simple monoclinic

2. ECM - End Centred monoclinic

1. STR - Simple Triclinic

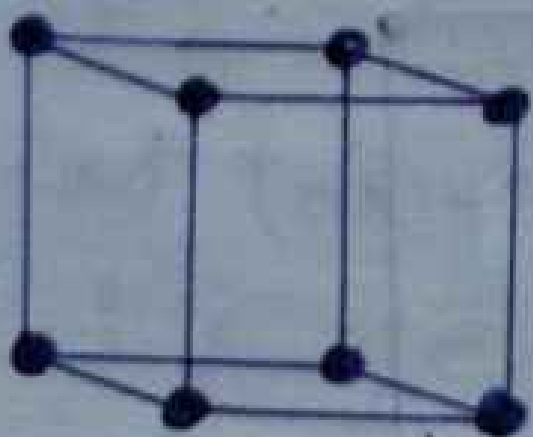
1. SH - Simple Hexagonal

1. SR - Simple Rhombohedral

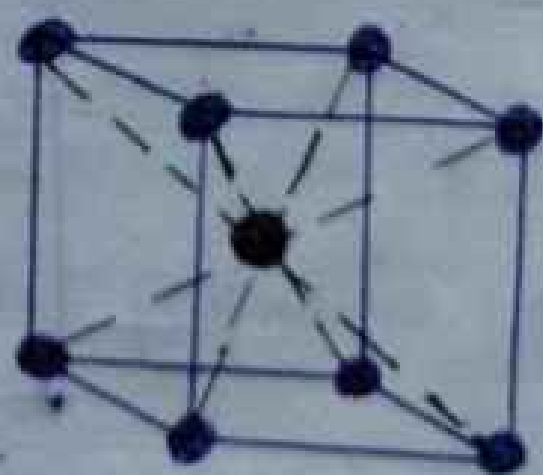
• 7 crystal system's Unit cell geometry :-

1. Cubic system :-

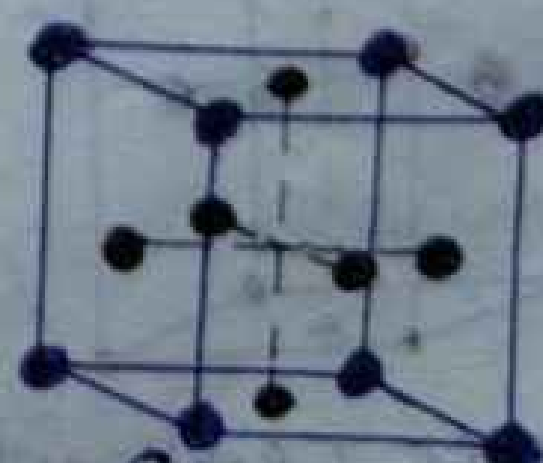
- $a = b = c$ $\div$ Axial length
- $\alpha = \beta = \gamma = 90^\circ$ $\div$ Axial angle



(Simple Cubic)



(Body centered cubic)

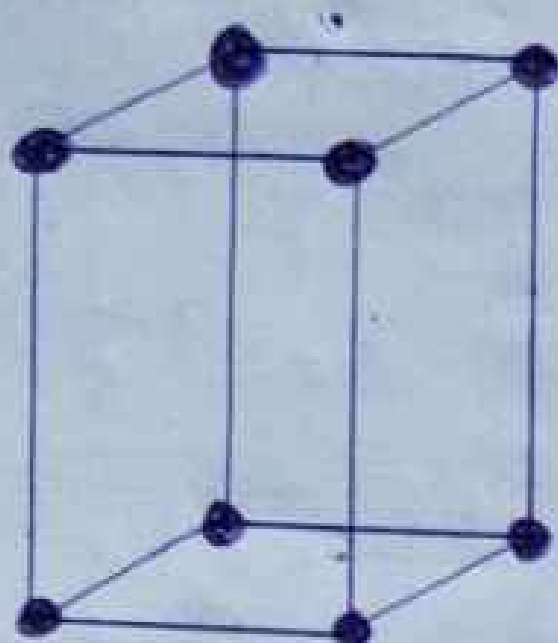


(face centered cubic)

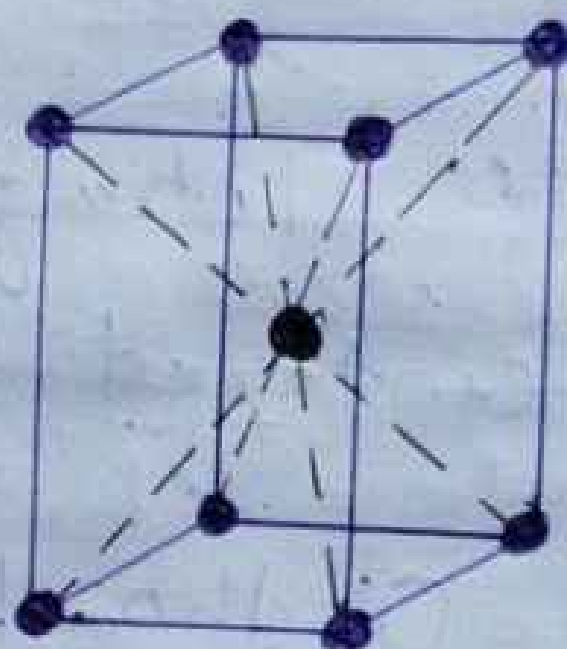
• Tetragonal system :-

→ Axial length :- $a = b \neq c$

→ Axial angle :- $\alpha = \beta = \gamma = 90^\circ$



(simple Tetragonal)

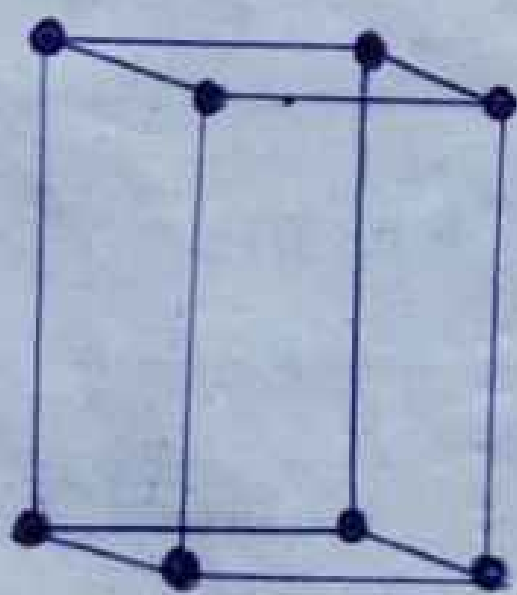


(Body centred Tetragonal)

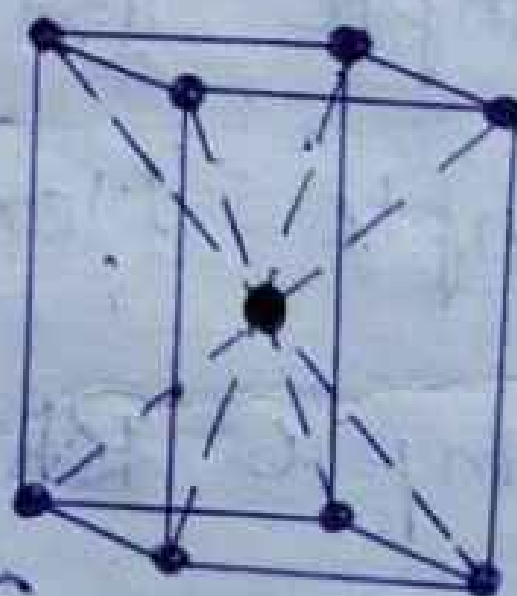
• Orthorhombic system :-

→ Axial length :- $a \neq b \neq c$

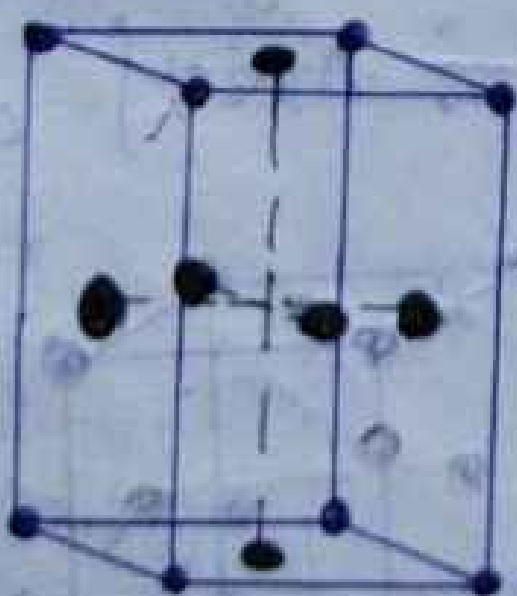
→ Axial angle :- $\alpha = \beta = \gamma = 90^\circ$



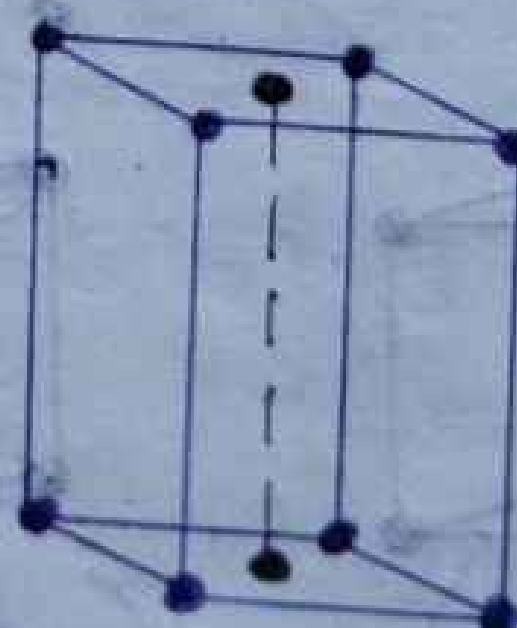
(simple orthorhombic)



(Body centred orthorhombic)



(face centred orthorhombic)

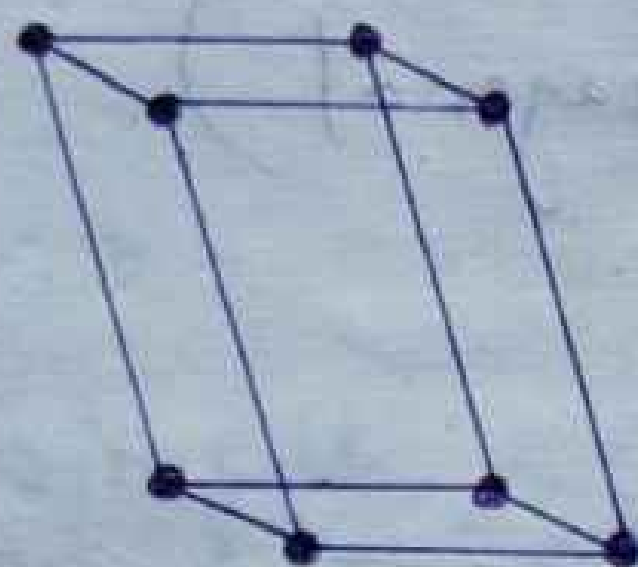


(end centred (or) base centred orthorhombic)

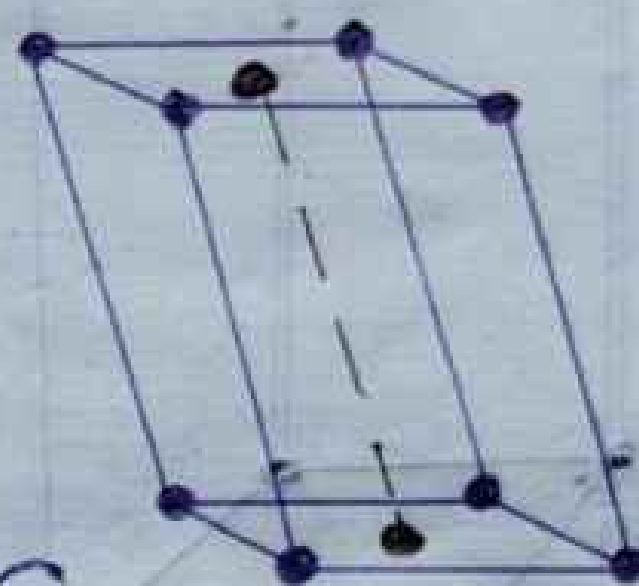
• Monoclinic System :-

→ Axial length :- $a \neq b \neq c$

→ Axial Angle :- $\alpha = \gamma = 90^\circ, \beta \neq 90^\circ$



(simple monoclinic)

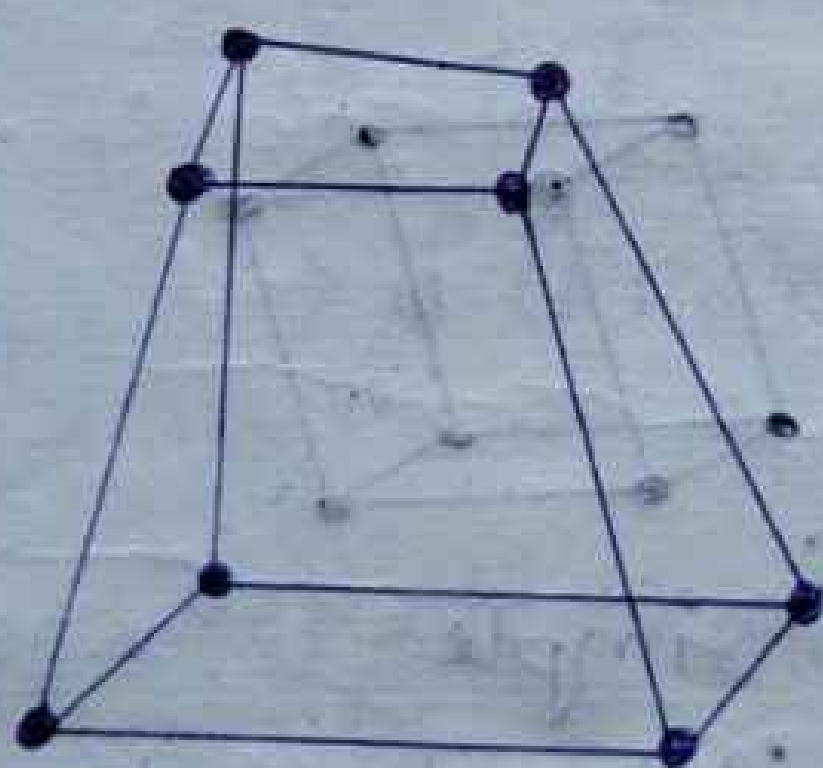


(End centred (or) base centred monoclinic)

• Triclinic system :-

→ Axial length :- $a \neq b \neq c$

→ Axial Angle :- $\alpha \neq \beta \neq \gamma \neq 90^\circ$

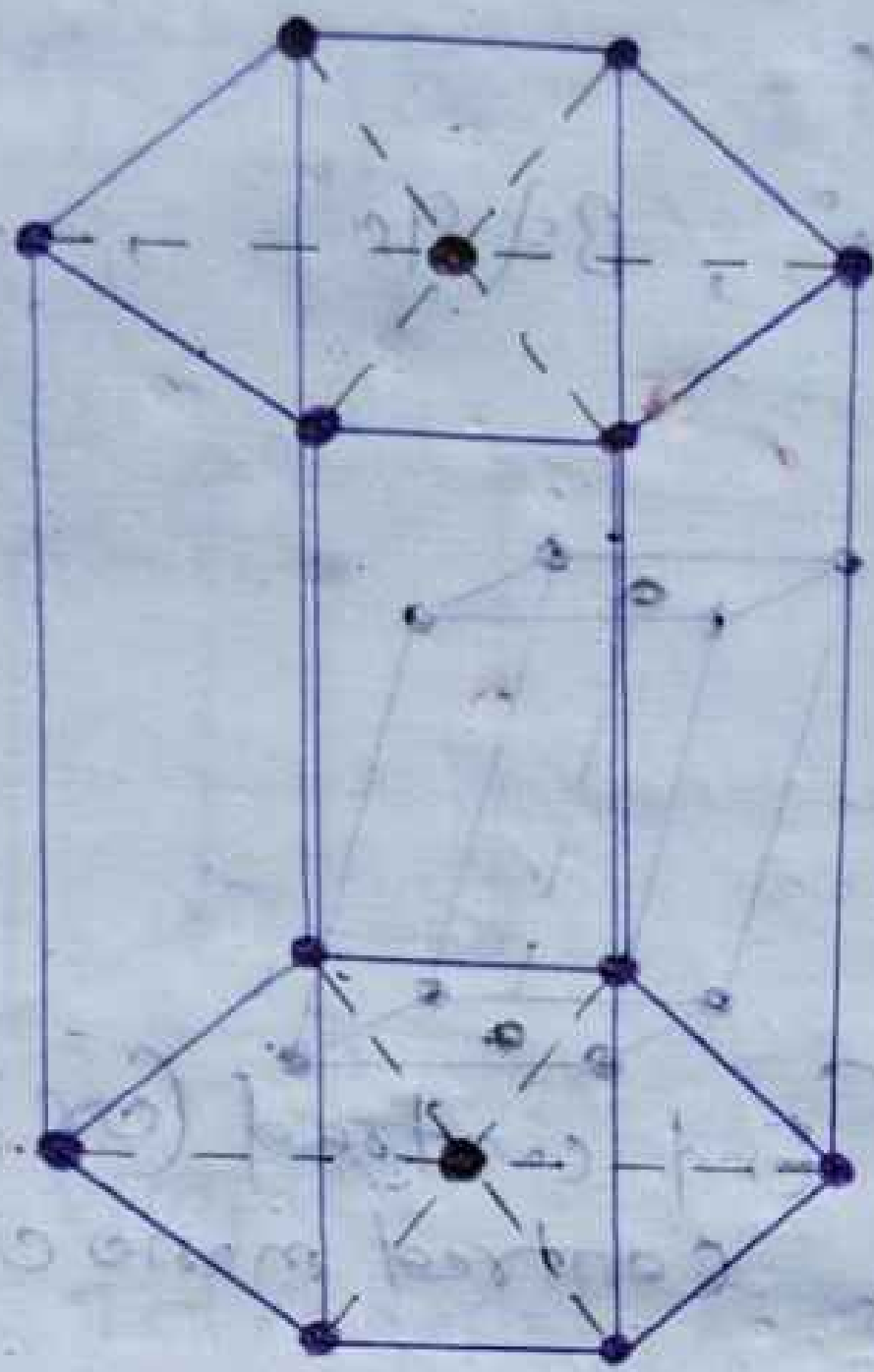


(simple Triclinic)

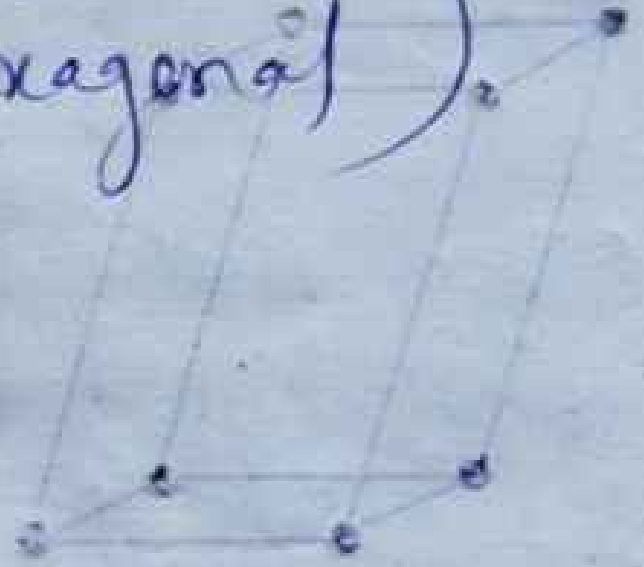
• Hexagonal System :-

→ Axial length :- $a = b \neq c$

→ Axial Angle :- $\alpha = \beta = 90^\circ, \gamma = 120^\circ$



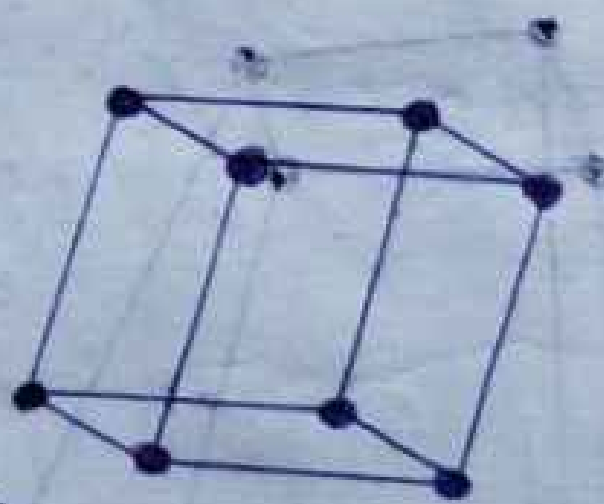
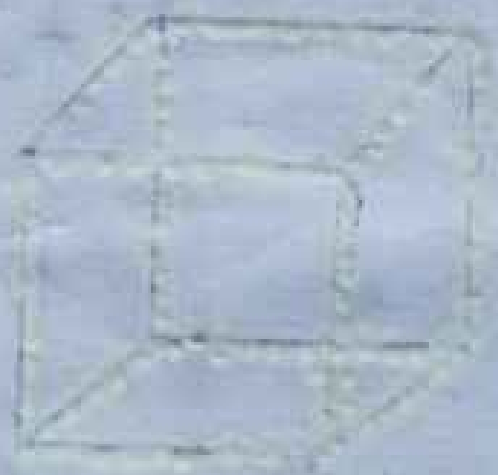
(simple hexagonal)



• Rhombohedral System

→ Axial length $a = b = c$

→ Axial Angle $\alpha = \beta = 90^\circ, \gamma \neq 90^\circ$



(simple Rhombohedral)

• Common Crystal structure in materials

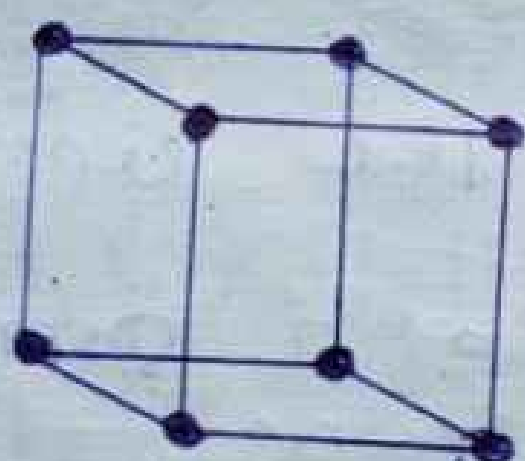
→ The most common crystal structure in common metals are

(1) Body Centred Cubic crystal structure.
(BCC crystal structure)

(i) face centred cubic Crystal structure.
(fcc Crystal structure):

(ii) Hexagonal closed packed Crystal structure.
(HCP crystal structure):

simple Cubic $\div$ (SC)



► we need to know,

→ Z = Coordination number of atom.

→ N = effective number of atom per unit cell.

→ r = atomic radius

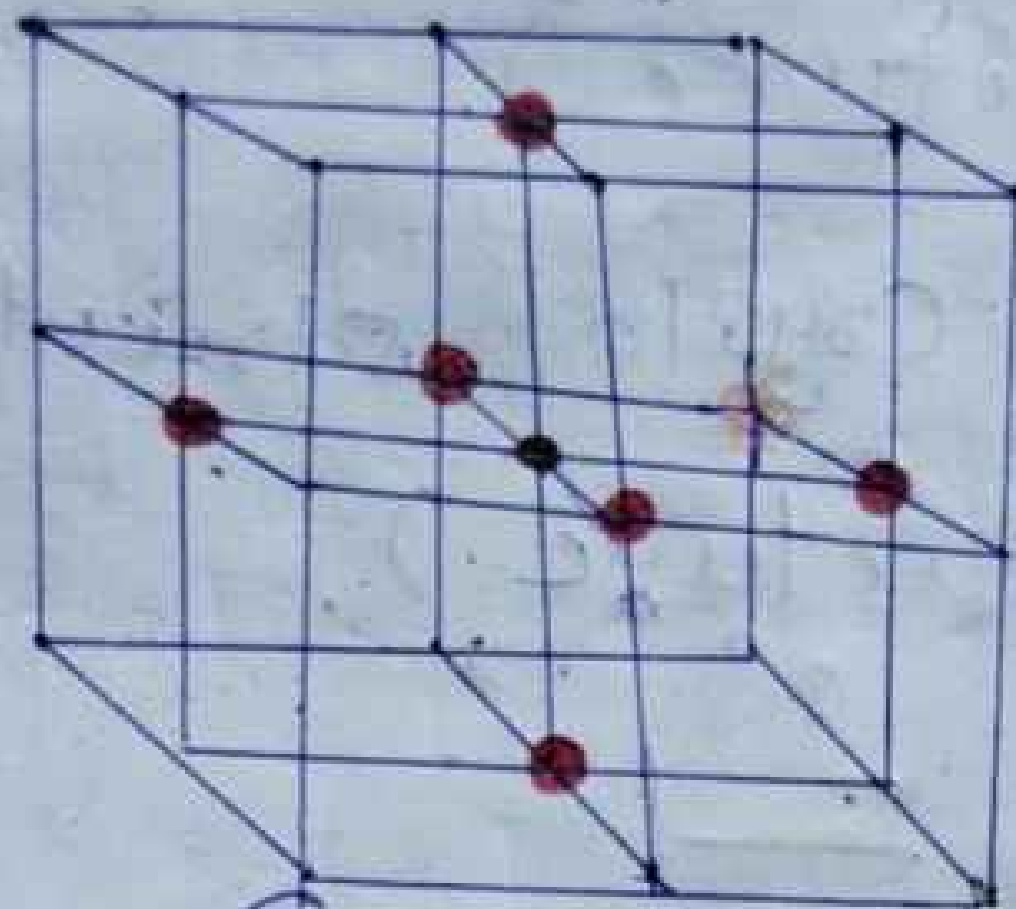
→ APF = Atomic packing factor.

→ ρ (Rho) = Theoretical density.

Z = Coordination number $\div$

→ It is defined as the number of nearest neighbour to a given atom in a crystal structure.

→ ' Z ' of simple cubic is '6'.



→ 6 coordination number of atom.

(space lattice)

• N = Effective number of atoms

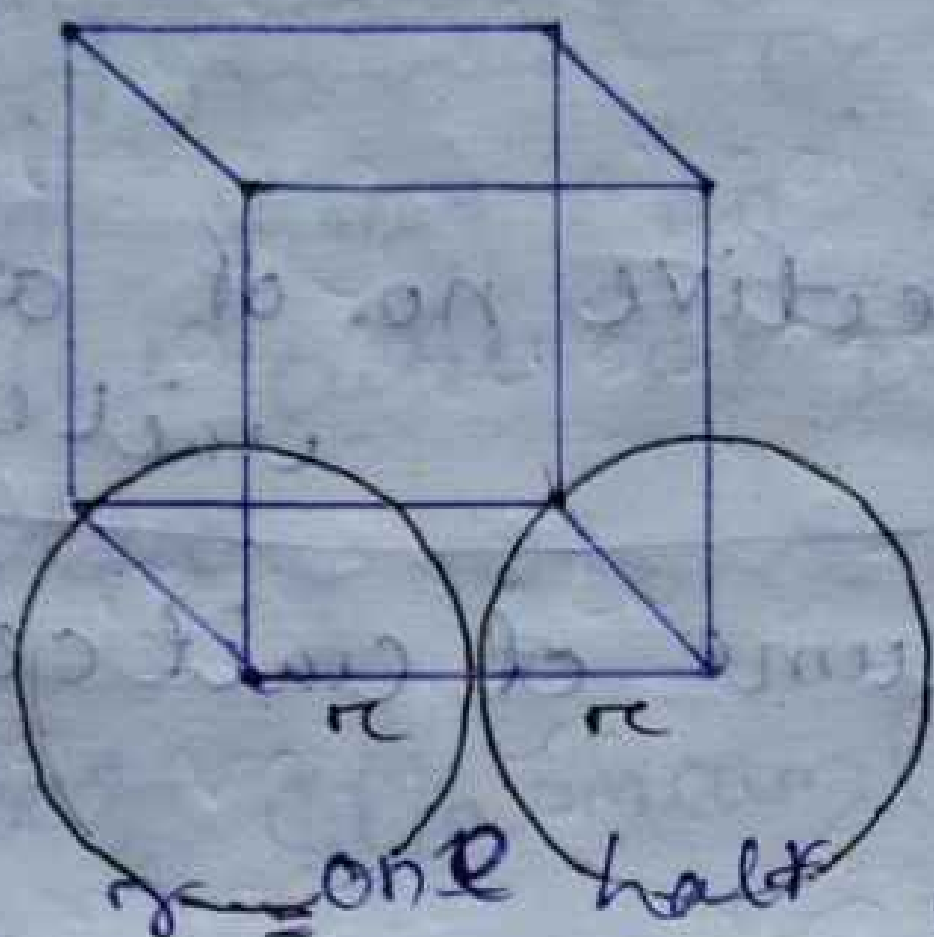
→ Total atom lies inside the unit cell.
In simple cubic, $\frac{1}{8}$ of each corner atom lies inside a unit cell.

→ $\frac{1}{8} \times 8 = 1$ (Primitive unit cell).



• r = atomic radius

→ we consider atoms are as being spherical



length = a

r = atomic radius

$$a = 2r$$

$$\Rightarrow r = \frac{a}{2}$$

r = one half of the inter atomic distance.
 $= (a/2)$

• APF = atomic packing factor

→ It is the fraction of volume occupied by the atoms in a crystal structure.

$$\text{APF} = \frac{\text{volume of effective atom Present in unit cell}}{\text{volume of unit cell}}$$

$$= \frac{1 \times \frac{4}{3} \pi r^3}{a^3} \rightarrow (\text{volume of sphere})$$

$$= \frac{1 \times \frac{4}{3} \pi r^3}{(2r)^3} = \frac{\frac{4}{3} \pi r^3}{8r^3} = \frac{\pi}{6} = 0.52$$

→ The atomic packing factor of a simple cubic

Structure is approximately '52%'. 

• ρ_{th} : Theoretical Density (ρ):

$$\text{Density} = \frac{\text{mass}}{\text{volume}}$$

mass of effective no. of atoms in unit cell

Volume of unit cell

$$= \frac{N \times A}{N_A \times V}$$

where

N = effective number of atoms

A = Atomic mass (or) weight of atom

N_A = Avogadro's Number

(value = 6.023×10^{23})

V = Volume of unit cell.

→ 6.023×10^{23} atoms have atomic weight/mass A .

→ 1 atom has atomic weight/mass

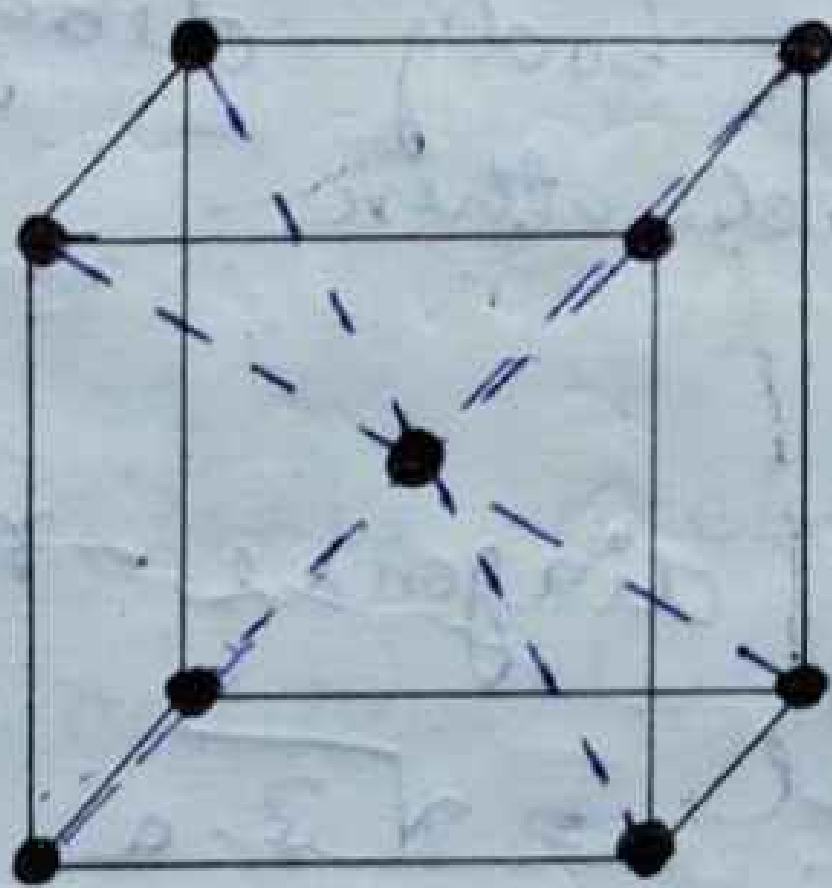
$$\frac{A}{6.023 \times 10^{23}}$$

→ (N) Effective numbers of atoms have $N \times A$
 6.023×10^{23}

• Body center cubic

→ It shows an atoms at each corner of the cube as well as at its body center.

→ ex: Chromium (Cr), Iron (Fe), Molybdenum (Mo), (W) Tungsten, (V) Vanadium, (Co) Cobalt, etc.

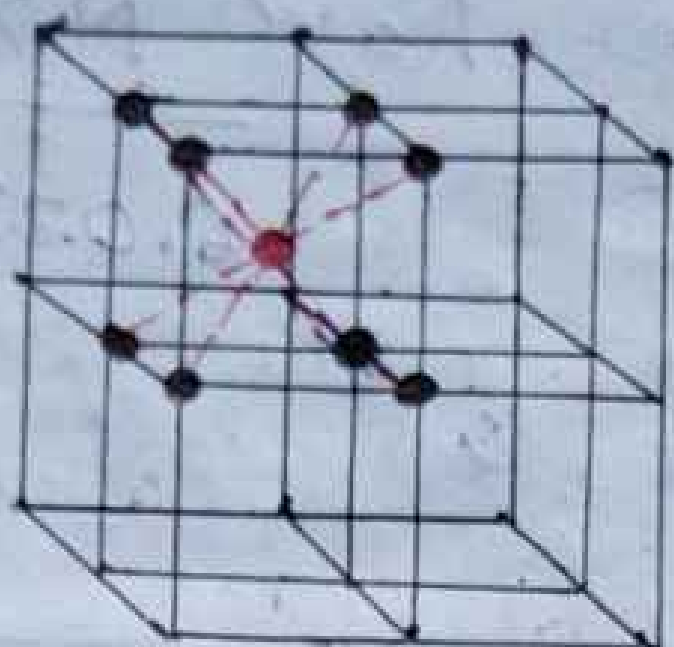


• Z = Coordination number

$$Z = 8$$

→ BCC crystal structure Each body center atom touches all the corner atoms.

$$Z = 8$$



→ 8 coordination number of atoms.

• Effective number of atoms $\frac{N}{6}$ (N)

$$\frac{1}{8} \times 8 + 1 = 2 \text{ (non-Primitive unit cell)}$$

$$N = 2$$

• r = atomic radius of

→ In 'Bcc' atoms on body diagonals are in contact with each other.

So,

$$\text{length of body diagonal} = r + 2r + r = 4r$$

$$\text{Also, body diagonal} = \sqrt{3} a$$

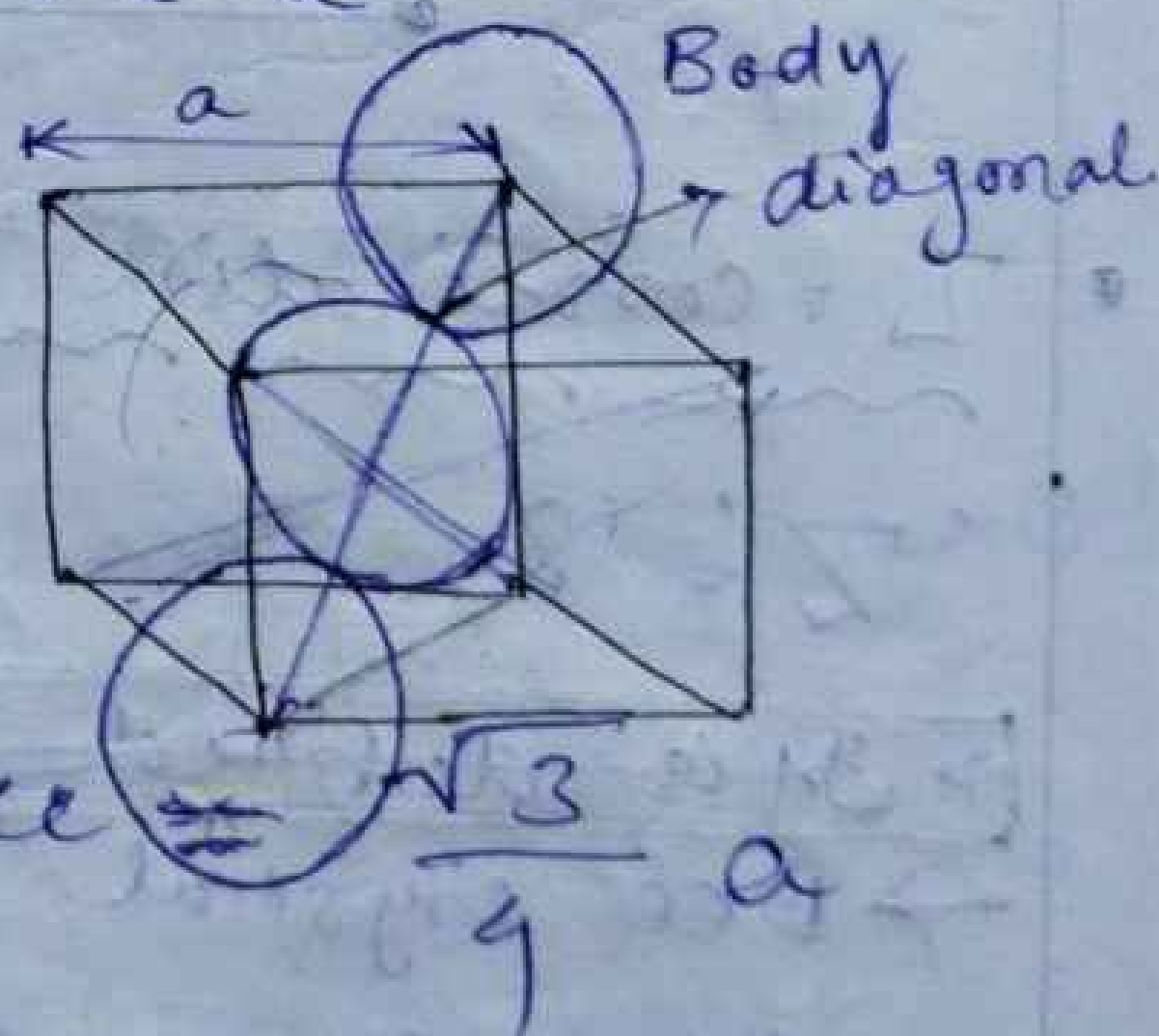
So,

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

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

∴ (i) atomic radius of Bcc = $\frac{\sqrt{3}}{4} a$

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



• APF = Atomic packing factor

$$\text{APF} = \frac{\text{Volume of effective atom present in unit cell}}{\text{volume of unit cell.}}$$

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

• For body centered cubic unit cell $N=2$
and $a = \frac{4}{\sqrt{3}} r$

$$= \frac{2 \times \left(\frac{4}{3}\right) \pi r^3}{\left(\left(\frac{4}{\sqrt{3}}\right) r\right)^3} = \frac{2 \times \left(\frac{4}{3}\right) \pi r^3}{\left(\frac{4}{\sqrt{3}}\right)^3 \times r^3} = 0.68$$

∴ The atomic packing factor of body centred cubic structure is approximately 68%.

• Theoretical density (ρ)

$$= \frac{\frac{\text{mass}}{\text{volume}}}{\text{mass of effective no. of atom in unit cell} / \text{volume of unit cell}}$$

$$= \frac{N \times A}{N_0 \times V}$$

where,

N = effective number of atoms

A = Atomic weight.

N_A = Avogadro's No.

V = vol^m of unit cell is

here,

$$N = 2$$

so,

$$\rho = \frac{2 \times A}{6.023 \times 10^{23} \times V}$$

- Face centred cubic

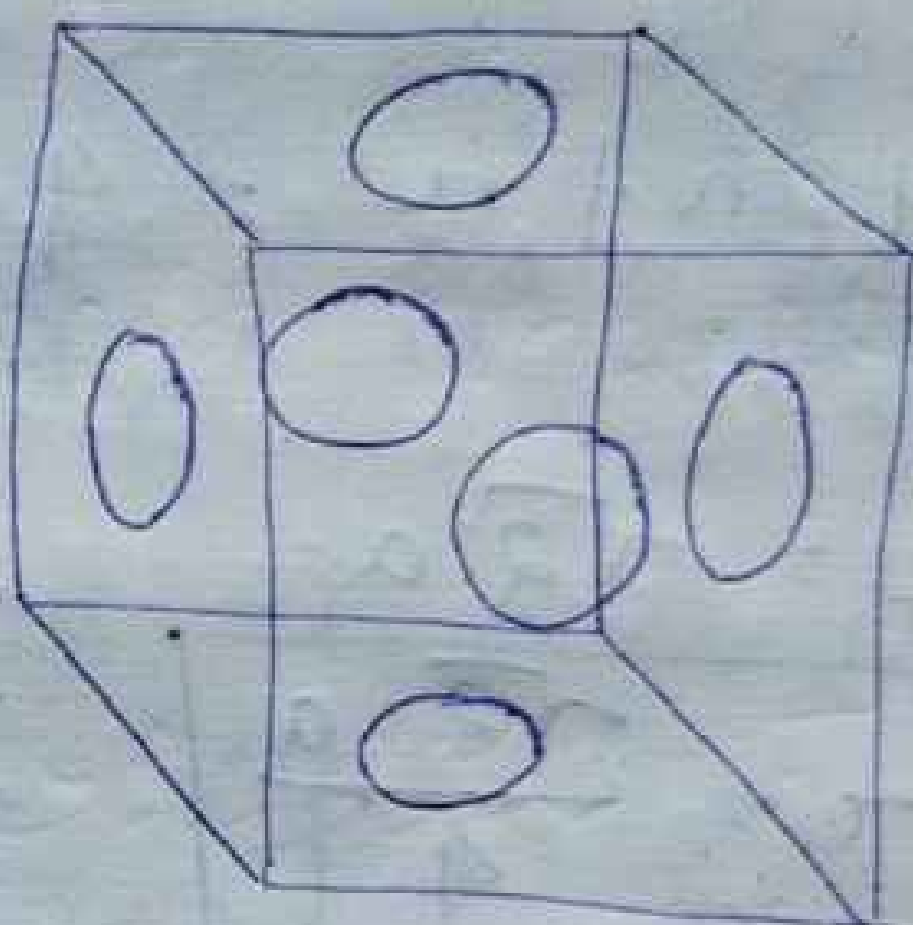
→ It has a cubic unit cell with atoms located at each of 8 corners and each of 6 faces.

→ Ex: (Pt) Platinum,

(Ag) silver, Gold (Au),

(Fe) iron, (Al) Aluminium,

(Cu) Copper, etc.



Effective number of atoms

$(N) \hat{=}$

$$N = \frac{1}{8} \times 8 + \frac{1}{2} \times 6 = 4$$

∴ Effective number of atoms $N = 4$.

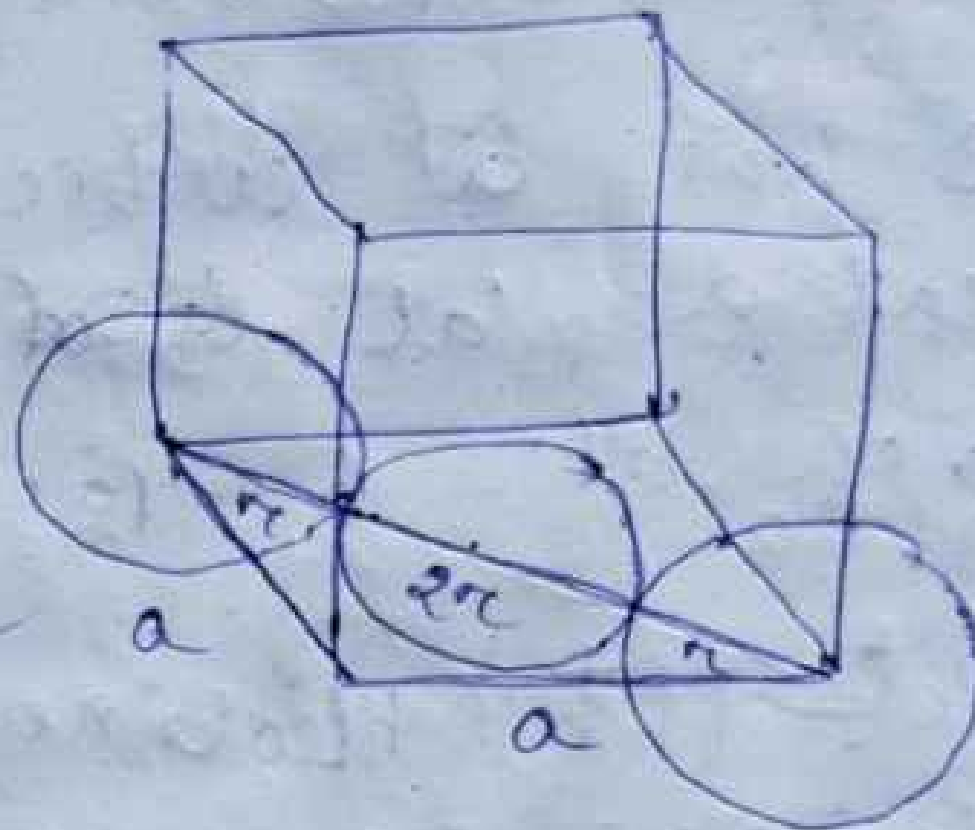
Z = Coordination Number

$$Z = 4 + 4 + 4 = 12$$

∴ Coordination Number $Z = 12$

• atomic radius (r)

$$\begin{aligned} \text{face diagonal} &= \sqrt{a^2 + a^2} \\ &= \sqrt{2a^2} \\ &= \sqrt{2} a \end{aligned}$$



length of face diagonal

$$= r + 2r + r = 4r$$

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

$$\Rightarrow r = \frac{\sqrt{2} a}{4}$$

$$\Rightarrow a = \frac{4r}{\sqrt{2}}$$

• Atomic packing factor (APF)

APF = $\frac{\text{volume of effective atom present in unit cell}}{\text{volume of unit cell}}$

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

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

$$= \frac{4 \times \frac{4}{3} \times \pi r^3}{\frac{64 r^3}{2\sqrt{2}}} = \frac{16 \times \pi \times r^3 \times 2\sqrt{2}}{64 \times r^3 \times 3} = \frac{\sqrt{2} \pi}{6}$$

$$= \frac{\sqrt{2} \pi}{6} = 0.74$$

∴ The atomic packing factor of face centered cubic structure is approximately 74%.

• Theoretical density $\hat{=}$ (f)

$$= \frac{\text{mass}}{\text{volume}} = \frac{\text{mass of effective no. of atom in unit cell}}{\text{volume of unit cell}}$$

$$= \frac{N \times A}{N_A \times V}$$

where, N = effective number of atoms

A = Atomic weight

N_A = Avogadro's No.

V = Vol^m of unit cell

Here, $N = 4$

- Hexagonal close packed (HCP)

→ Atoms are placed at the 6 regular corners of hexagonal along with 1 atom each at the center of the hexagonal basal plane.

→ Further there is another plane of atoms in the mid way between top and bottom surface position at the center of the alternative faces.

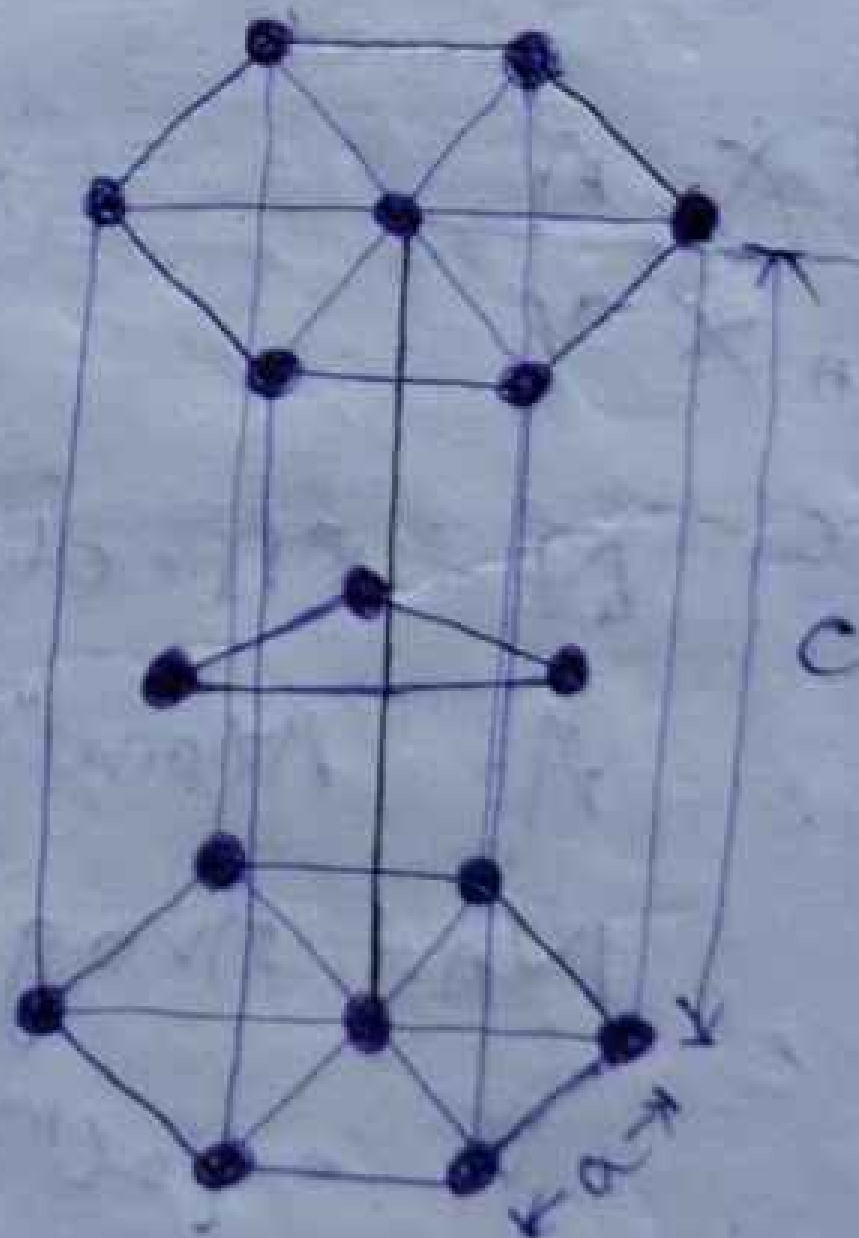
→ Ex^o (Mg) magnesium, Titanium (Ti), (Be) Beryllium, (Cd) cadmium, (Zn) zinc, etc.

- $Z = 12$

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

$= 6$

- $N = 6$



- atomic radius (r) $\frac{a}{2}$

$$a = 2r$$

$$\Rightarrow r = \frac{a}{2}$$

for most ideal metal,

$$\frac{c}{a} = 1.633$$

- (APF) Atomic packing-factor $\frac{V}{V_0}$

$$APF = \frac{6 \times \frac{4}{3} \times \pi r^3}{6 \times \frac{\sqrt{3}}{4} a^2 \times c}$$

$$= \frac{8 \times \frac{4}{3} \times \pi r^3}{6 \times \frac{\sqrt{3}}{4} a^2 \times a \times \frac{c}{a}}$$

$$= \frac{16\pi r^3}{3 \times \sqrt{3} \cdot a^3 \times 1.633}$$

$$= \frac{16\pi r^3}{3 \times \sqrt{3} \times (2r)^3 \times 1.633}$$

$$= \frac{16\pi r^3}{3 \times \sqrt{3} \times 8r^3 \times 1.633}$$

$$= \frac{2\pi}{3 \times \sqrt{3} \times 1.633}$$

$$= 0.74$$

$$\therefore \boxed{APF = 74\%}$$

Structure	a vs r	N	Z	APF	Typical metal
SC	$a = 2r$	1	6	0.52	Po, etc.
BCC	$a = \frac{4r}{\sqrt{3}}$	2	8	0.68	Fe, Ti, W, Mo
FCC	$a = \frac{4r}{\sqrt{2}}$	4	12	0.74	Ta, Cu, Al, etc.
HCP	$a = 2r$ $c/a = 1.633$	6	12	0.74	Ti, Mg, Zn, Cd, etc.

• Crystallographic points, planes and direction

When dealing with crystalline materials, it often becomes necessary to specify a particular point within a unit cell, a crystallographic direction or some crystallographic plane of atoms.

→ Three numbers (or) indices are used to designate point location, directions and planes.

→ Basic for determining index values unit cell consists of three axes (x, y, z) at one of the corners and coinciding with the unit cell edges.

(1) Point coordinate (lattice point)

→ The co-ordinate of a lattice point, or of an atom, centre within a unit cell are specified in terms of fractional multiplied of lattice parameters a, b, c .

Ex.

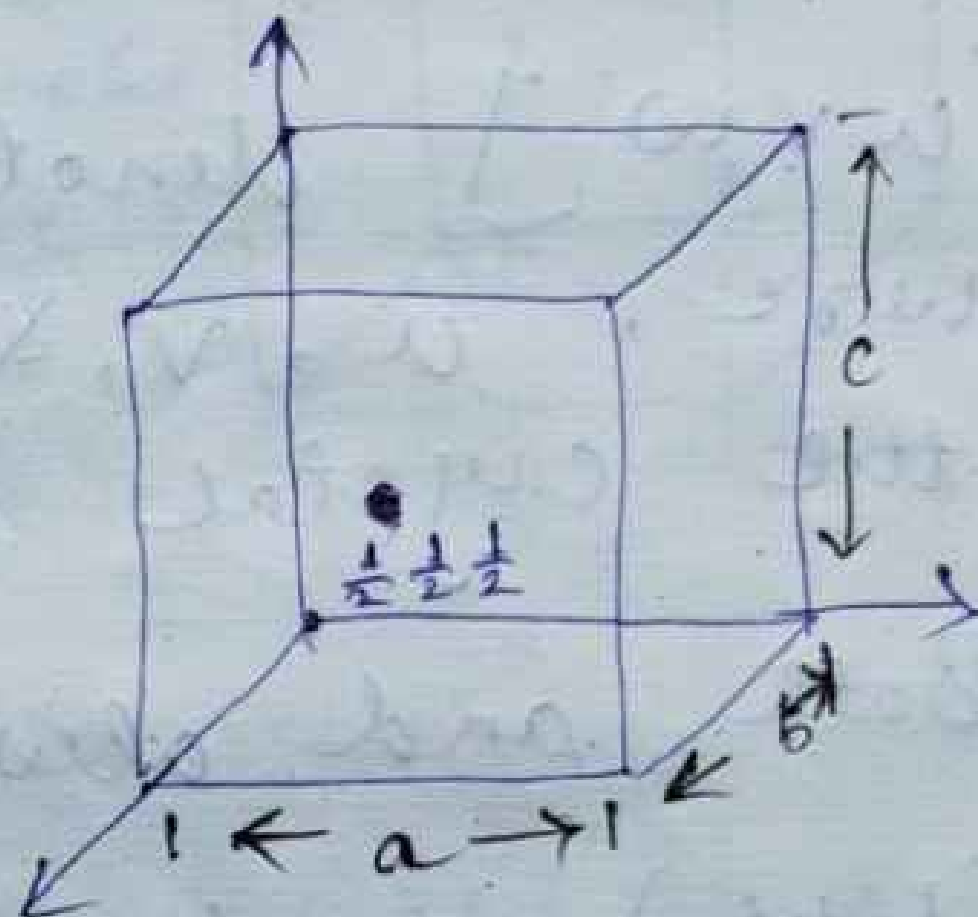
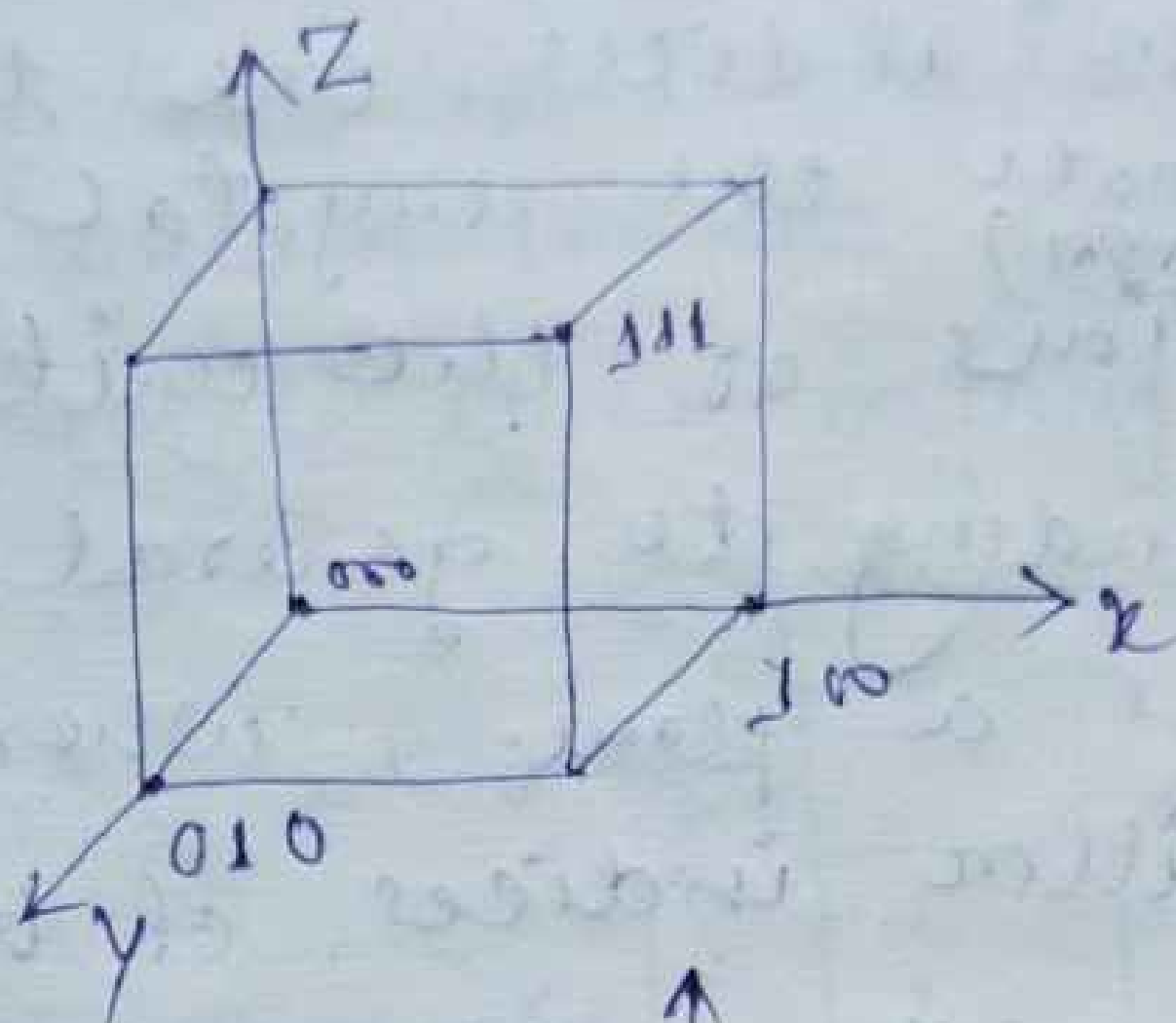
000 position

100 position

111 position

010 position

$\frac{1}{2} \frac{1}{2} \frac{1}{2}$ position



• Miller indices

It is useful to learn certain rules and notation to describe geometry in, and around a unit cell.

→ Lattice direction and planes in a metallic crystal structure play very important role in understanding the plastic deformation, the hardening and other aspects of the behaviour of metals.

→ Miller developed a concise and convenient quantitative description given by set of numbers that identify planes of atoms and directions.

→ These numbers are called 'Miller indices'.

→ miller indices are the nomenclatures to designate the crystal planes and directions of the unit cells.

→ According to general convention (hkl) denotes a plane, where $h, k, \& l$ are the miller indices of the crystal plane.

→ $[uvw]$ denotes crystal direction where, $u, v, \& w$ are miller indices of the crystal direction.

→ Both and always have integral value.

→ (hkl) denotes the plane.

further $\{hkl\}$ denotes a family of planes.

Ex:-

In $\{111\}$ family of plane there are 8 plane,

$$\{111\} = (111), (\bar{1}11), (1\bar{1}1), (11\bar{1}), (1\bar{1}\bar{1}), (\bar{1}\bar{1}1), (1\bar{1}\bar{1}), (\bar{1}\bar{1}\bar{1})$$

→ $[uvw]$ denotes the direction in unit cell. further $\langle uvw \rangle$ denotes family of ^{Direction}

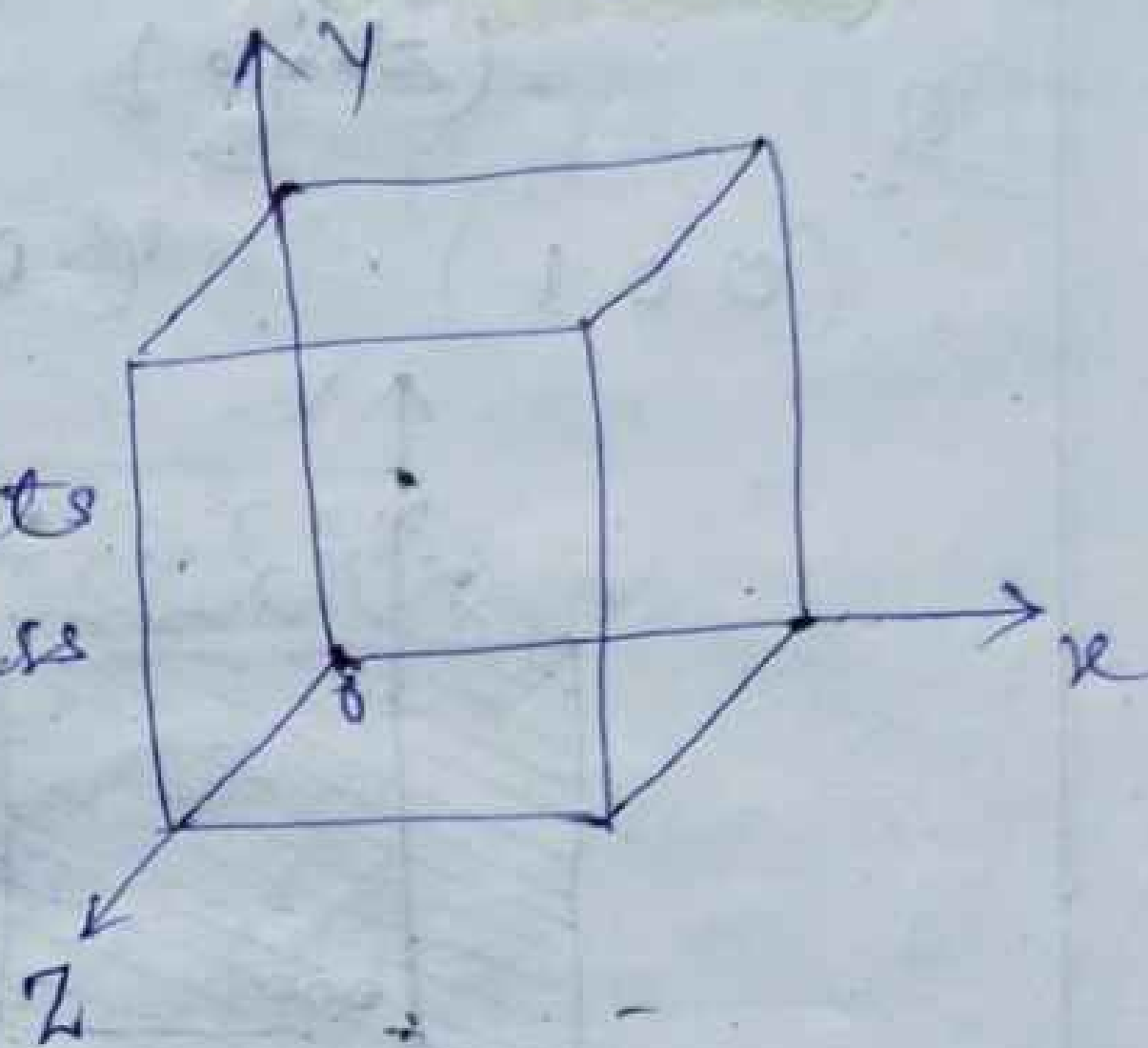
• miller indices for a plane

→ Sequential procedure for finding 'miller indices' for a plane is as follows.

→ A system of 3 coordinate axes indicating their origin is chosen for the unit cell.
→ for a cubic crystal it is orthogonal axis system x, y, z .

Step - I

Find out the intercepts of the plane that express in term of the lattice parameters a, b & c .



Step - II

Take reciprocal of these intercepts.

$$\left(\frac{1}{a}, \frac{1}{b}, \frac{1}{c} \right)$$

Step - III

Make the nearest integer of the reciprocals by multiplication (or) division by common factor.

(For this, multiplication of the reciprocals by the LCM of the number in the denominator is required).

→ The smallest integers / nearest integers generated are denoted as h, k & l .

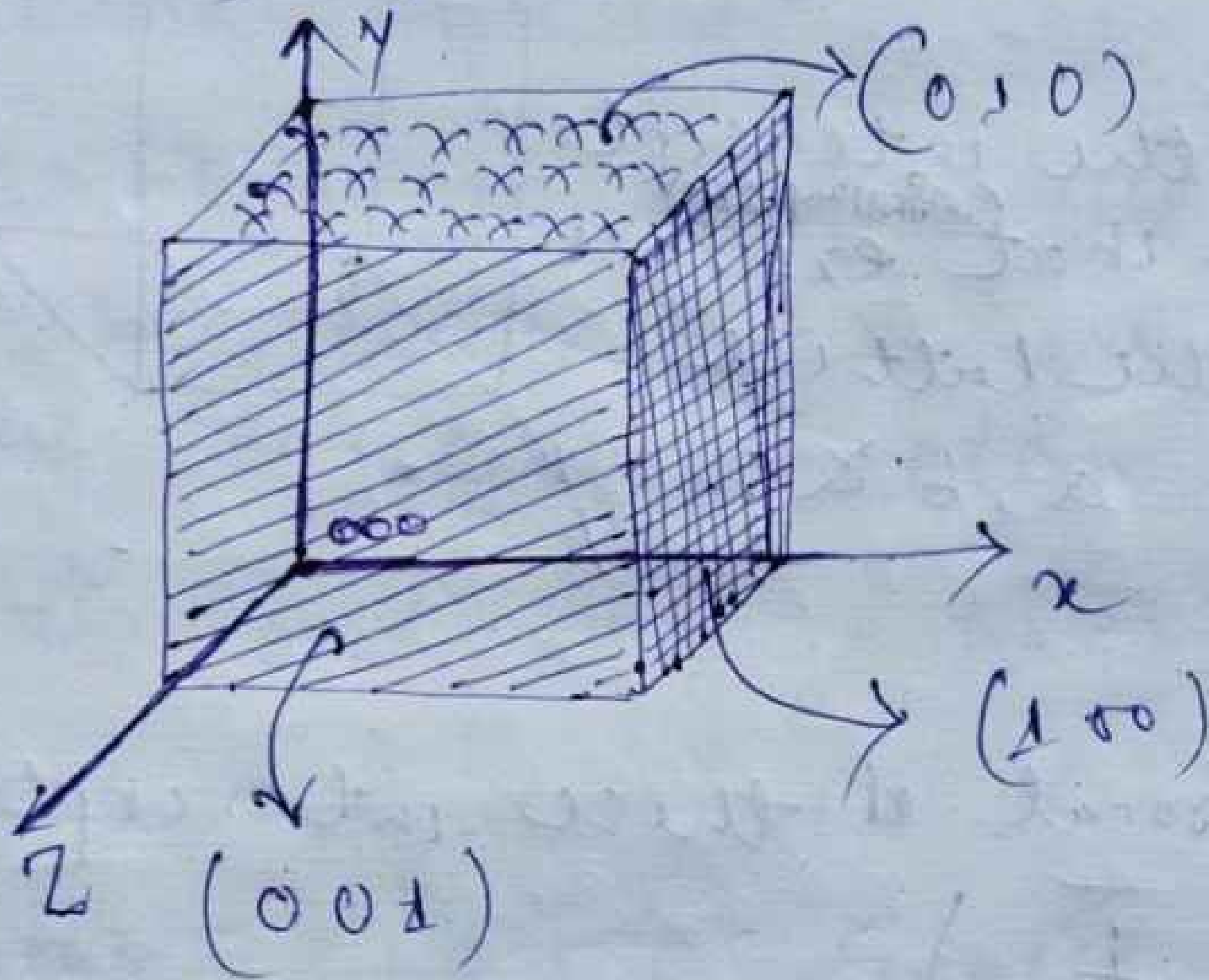
Step - IV

These integers are enclosed in bracket ().

without any comma, (hkl) .

$hkl \rightarrow$ This express the miller indices of the concerned crystallographic plane.

Q. (001) , (010) , (100) .



Q. $a=1$ $b=2$ $c=3$

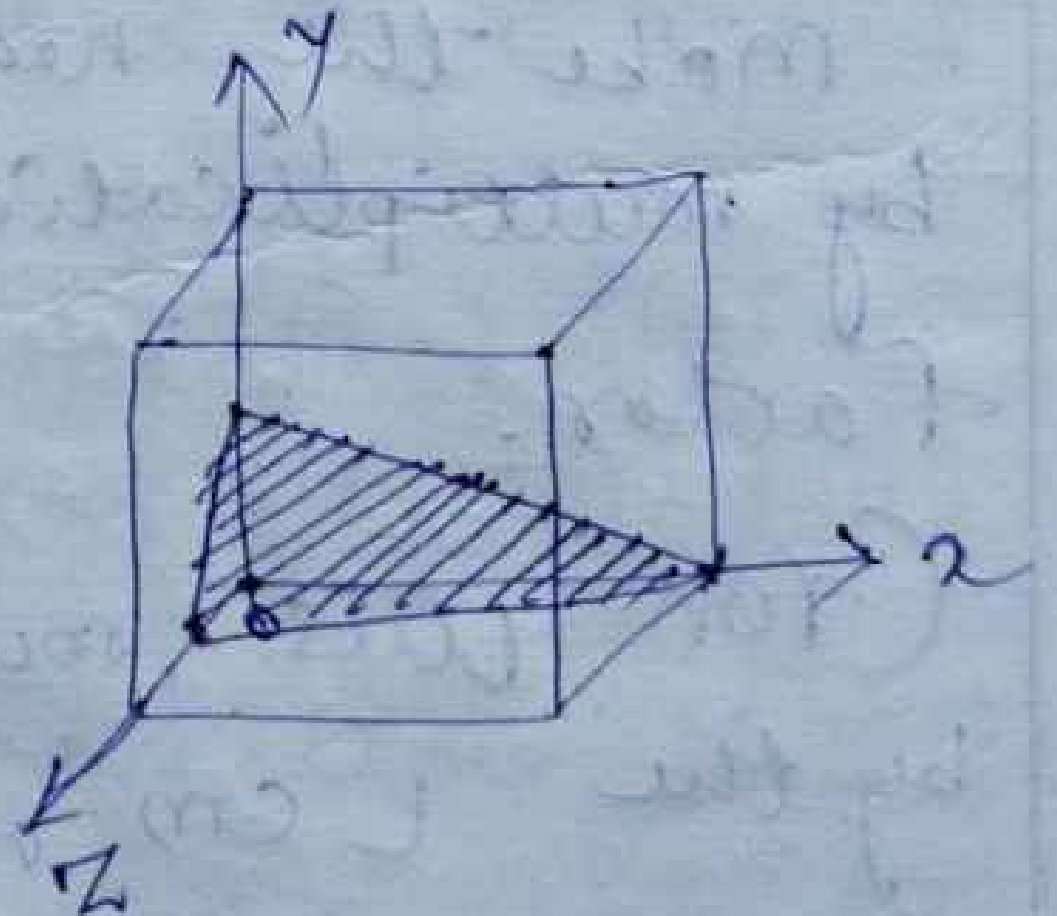
Miller indices:

(I) = 1, 2, 3

(II) = $\frac{1}{1}, \frac{1}{2}, \frac{1}{3}$

(III) = $6 \times \left(\frac{1}{1}, \frac{1}{2}, \frac{1}{3} \right)$

(IV) = 6, 3, 2



$\therefore$ miller indices for a plane $(6\ 3\ 2)$.

Q. if $a=1$ $b=0$ $c=2$ the miller indices;

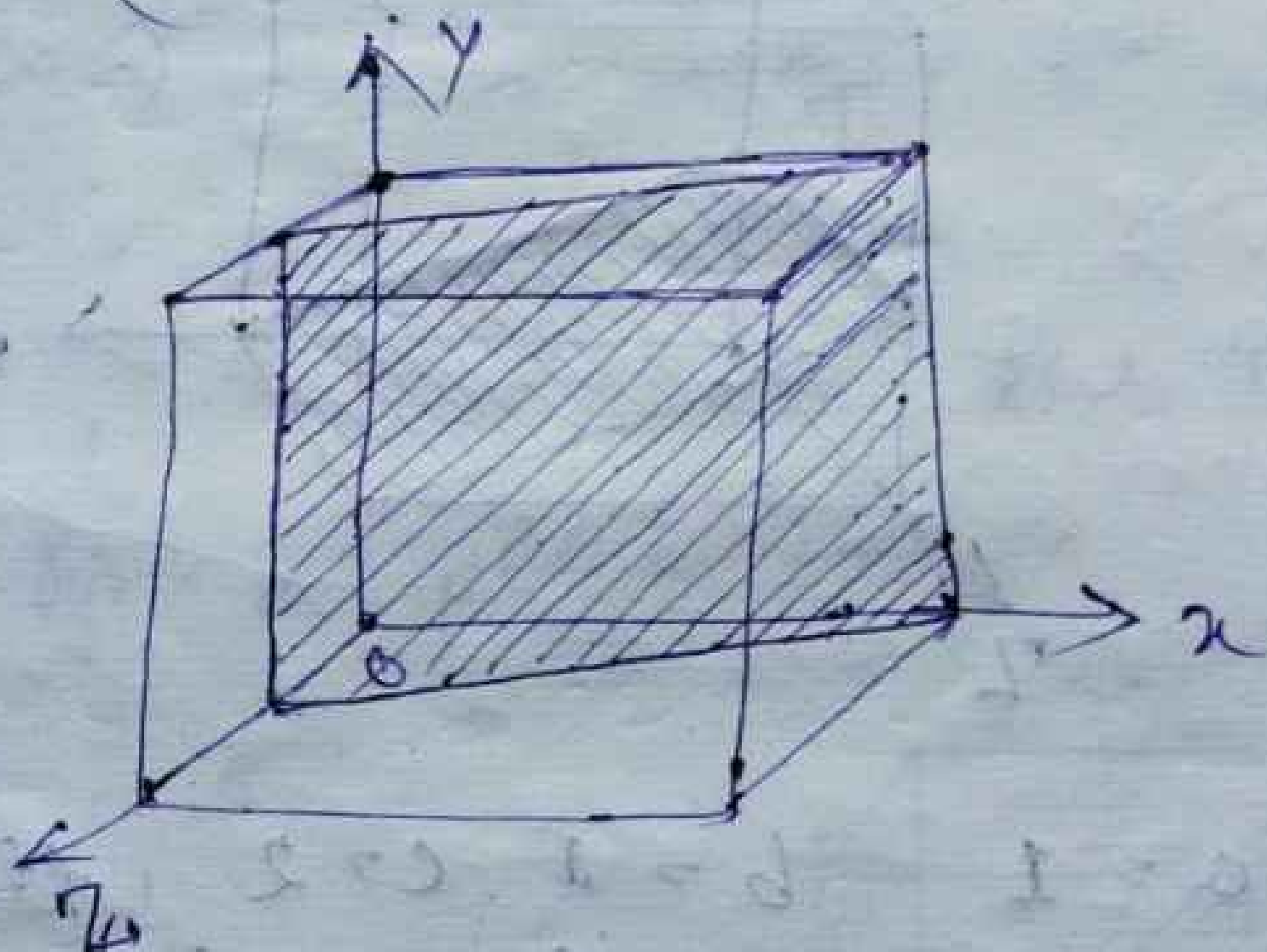
(I) = 1, 0, 2

$$(II) = \frac{1}{1}, \frac{1}{0}, \frac{1}{2}$$

$$(III) = 2 \left(\frac{1}{1}, \infty, \frac{1}{2} \right)$$

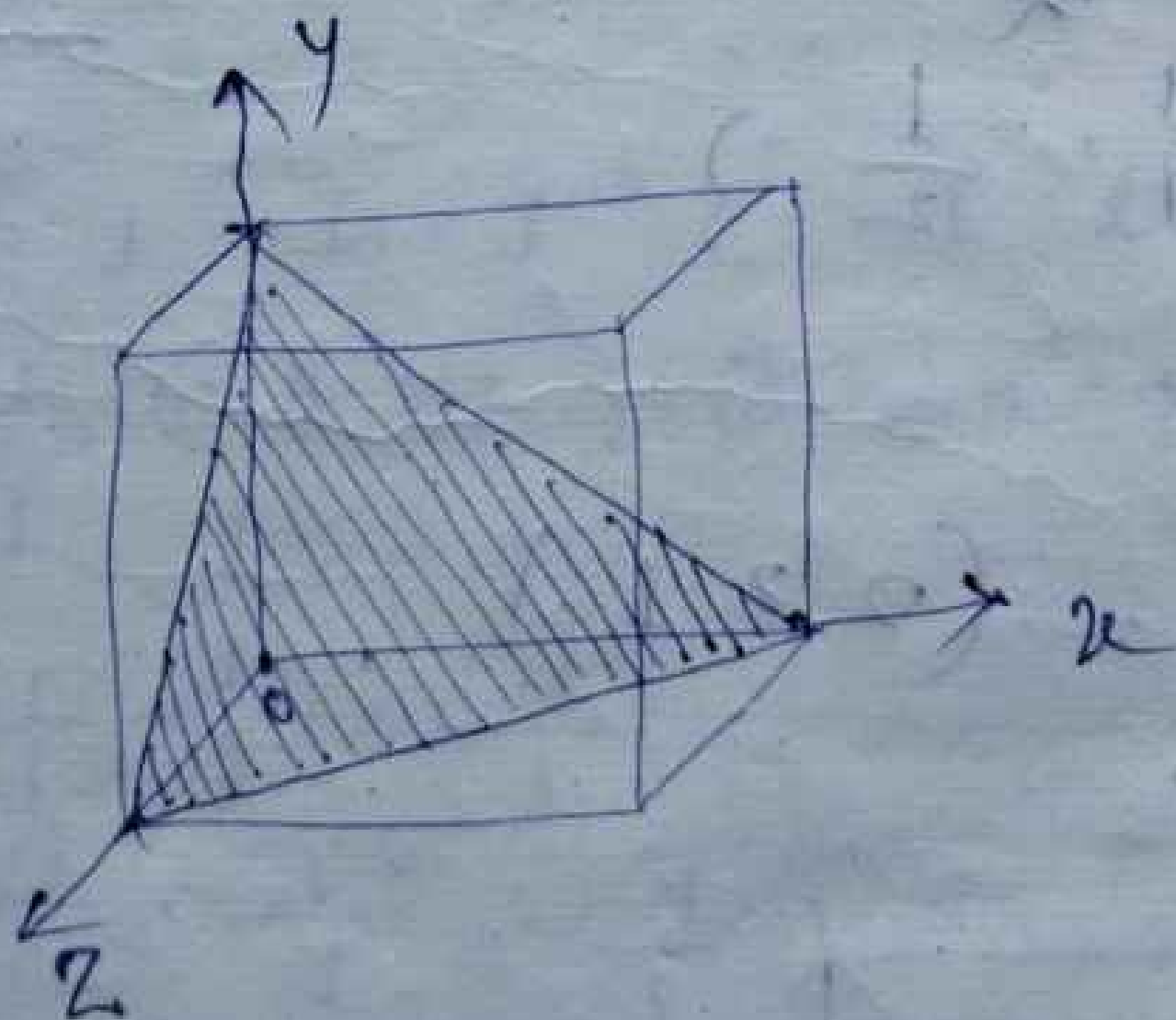
$$(IV) = 2, \infty, 1$$

$\therefore$ The miller indices for above lattice parameters is $(2 \infty 1)$.



Q. $a=1$ $b=1$ $c=1$

then miller indices $(hkl) = (111)$.

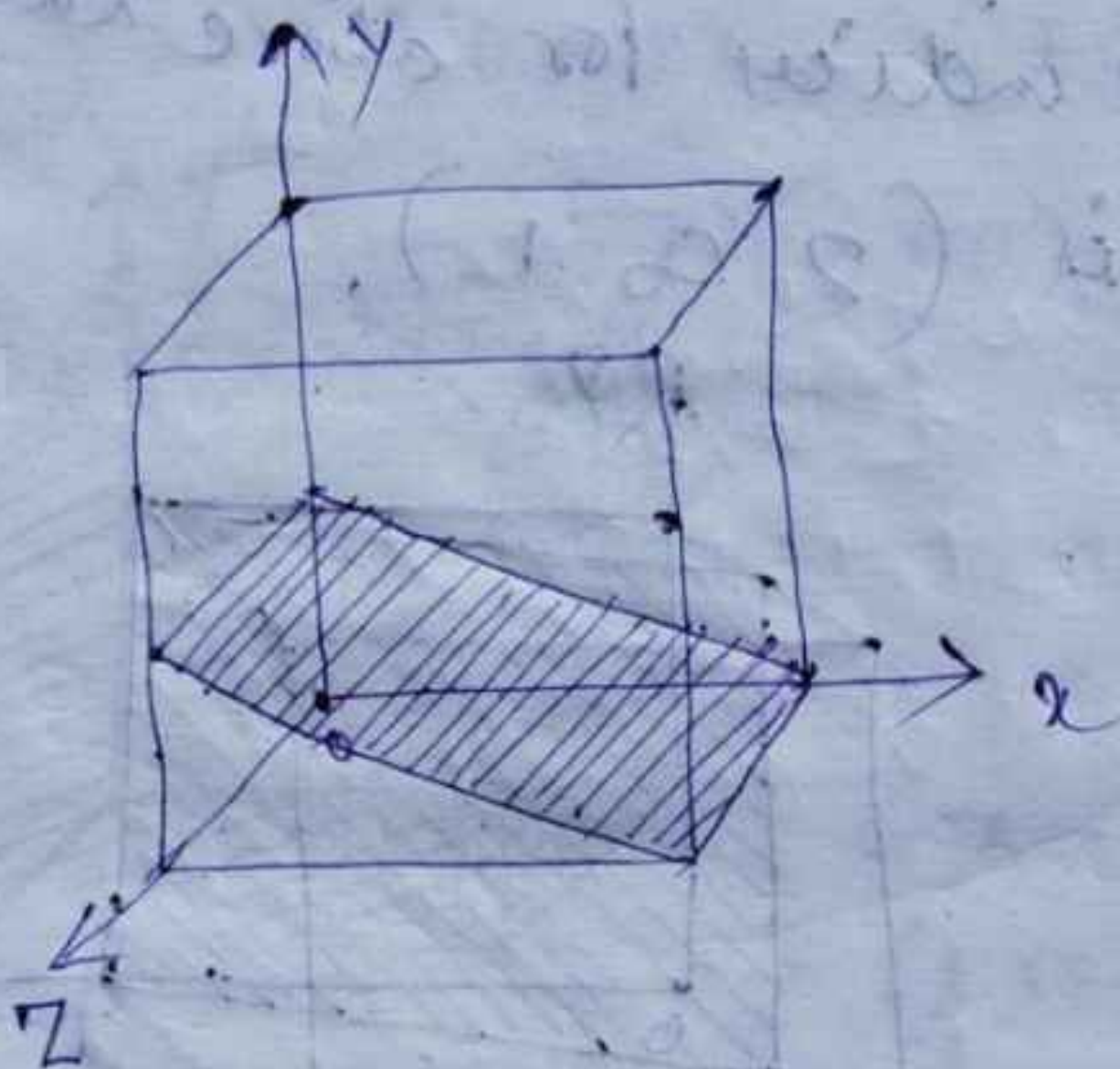


Q. If $a=1$ $b=2$ $c=0$ the miller indices (hkl) for a plane is $(1, 2, 0)$

$$(i) = \frac{1}{1}, \frac{1}{2}, \frac{1}{0}$$

$$(iii) = 2 \times \left(\frac{1}{1}, \frac{1}{2}, \infty \right)$$

$$(iv) = (2, 1, \infty) \text{ as } (hkl)$$



Q. If $a=1$ $b=1$ $c=2$ then the miller indices (hkl) for a plane is,

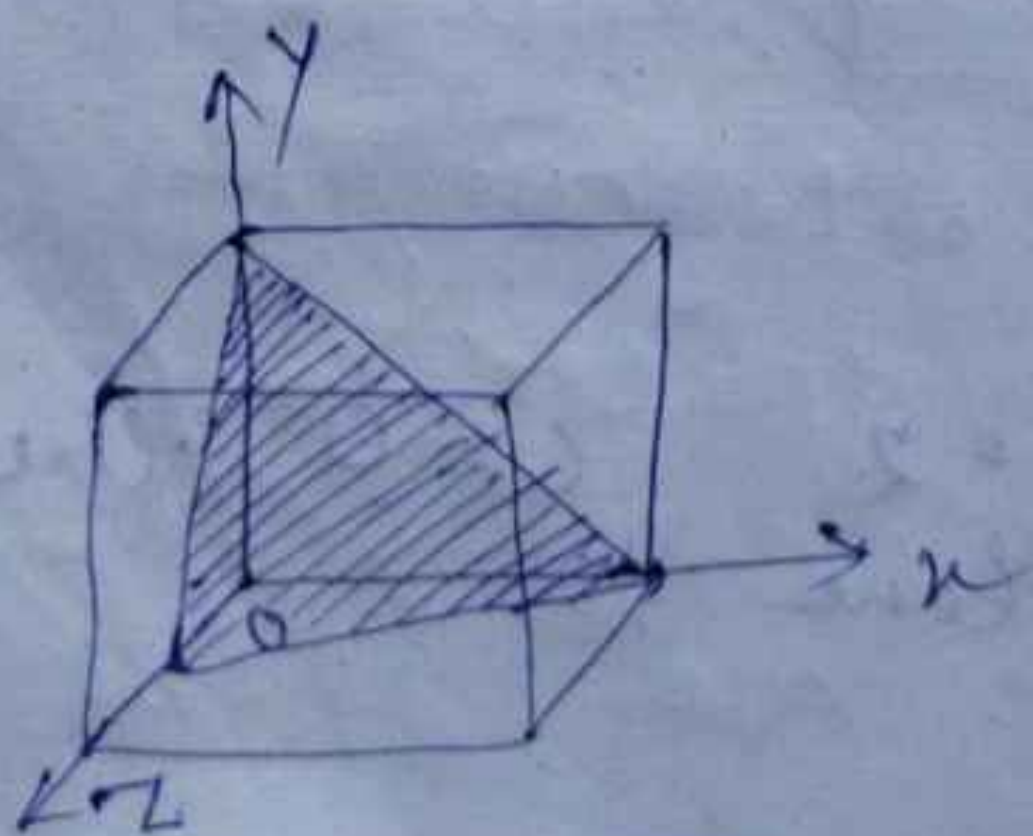
$$(i) = 1, 1, 2$$

$$(ii) = \frac{1}{1}, \frac{1}{1}, \frac{1}{2}$$

$$(iii) = 2 \times \left(\frac{1}{1}, \frac{1}{1}, \frac{1}{2} \right)$$

$$(iv) = 2, 2, 1$$

$$\therefore (hkl) = (2, 2, 1)$$



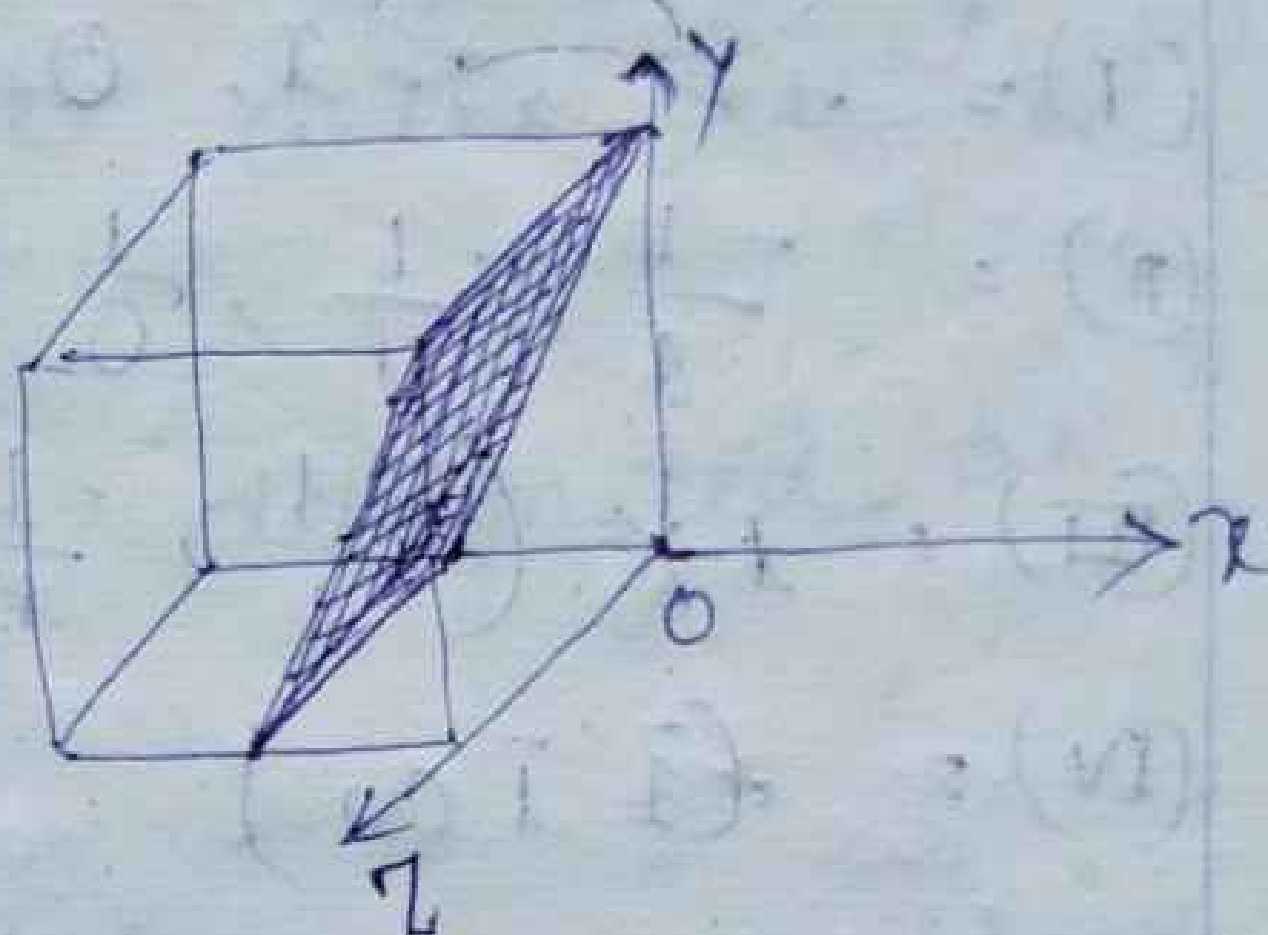
Q. If $a = -2$, $b = 1$, $c = 0$ then the miller indices for a plane is (hkl) ,

(i) $= -2, 1, 0$

(ii) $= \frac{1}{-2}, \frac{1}{1}, \frac{1}{0}$

(iii) $= 2 \times \left(-\frac{1}{2}, \frac{1}{1}, \infty \right)$

(iv) $= (\bar{1} 2 \infty)$



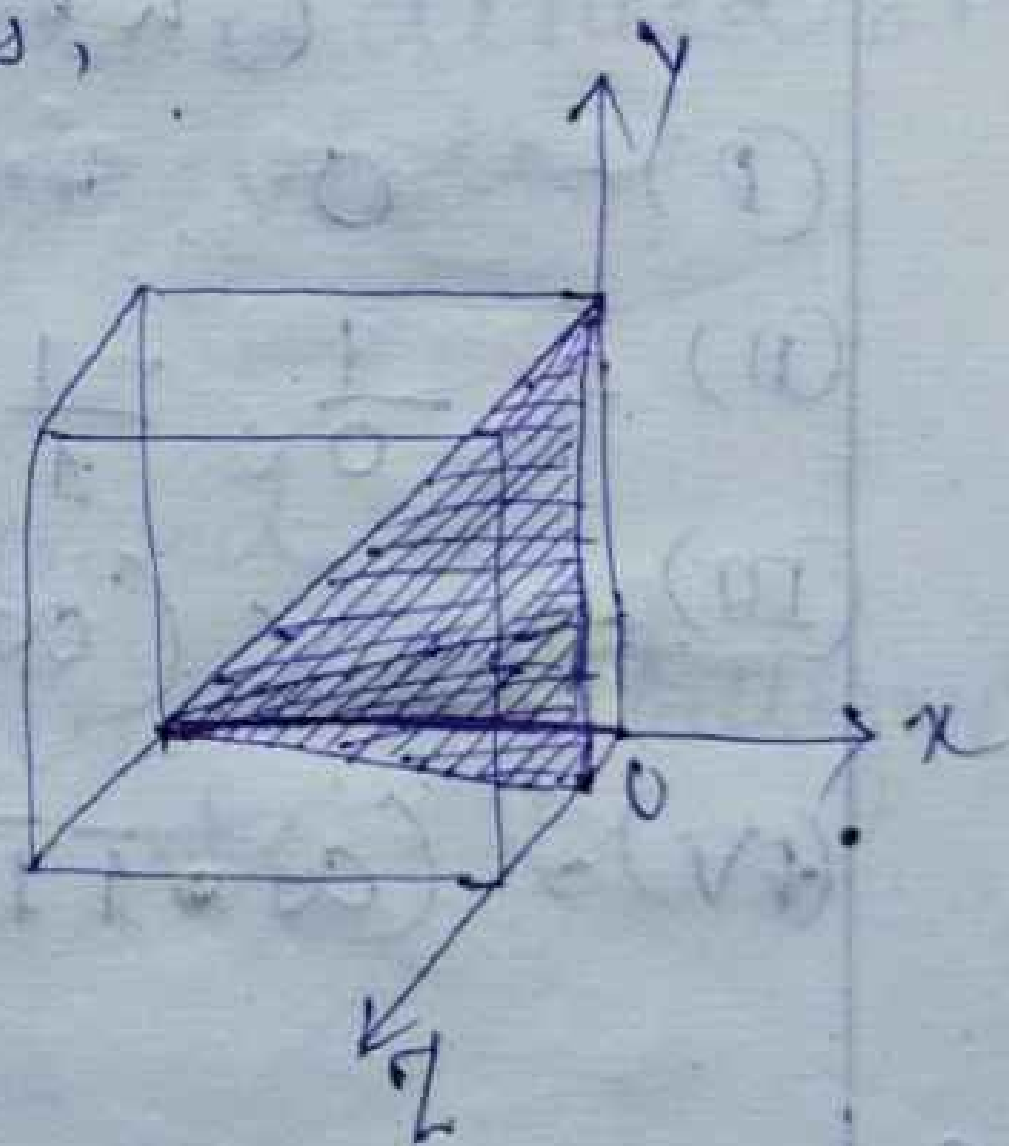
Q. If $a = -1$, $b = 1$, $c = 3$ then the miller indices (hkl) for a plane is,

(i) $= -1, 1, 3$

(ii) $= \frac{-1}{1}, \frac{1}{1}, \frac{1}{3}$

(iii) $= 3 \times \left(\frac{-1}{1}, \frac{1}{1}, \frac{1}{3} \right)$

(iv) $= (\bar{3} 3 1)$



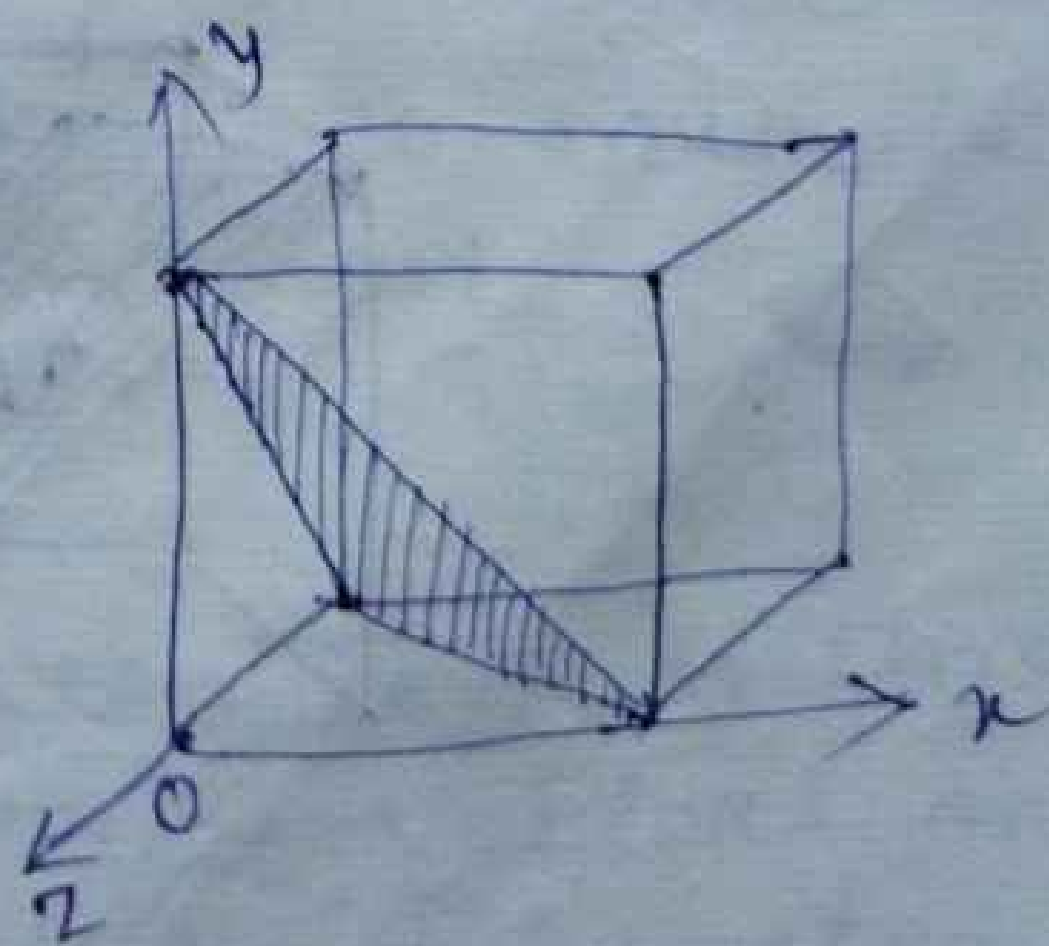
Q. If $a = 1$, $b = 1$, $c = -1$ then the miller indices (hkl) for a plane is,

(i) $= 1, 1, -1$

(ii) $= \frac{1}{1}, \frac{1}{1}, \frac{-1}{1}$

(iii) $= 1 \times \left(\frac{1}{1}, \frac{1}{1}, \frac{-1}{1} \right)$

(iv) $= (1 1 \bar{1})$



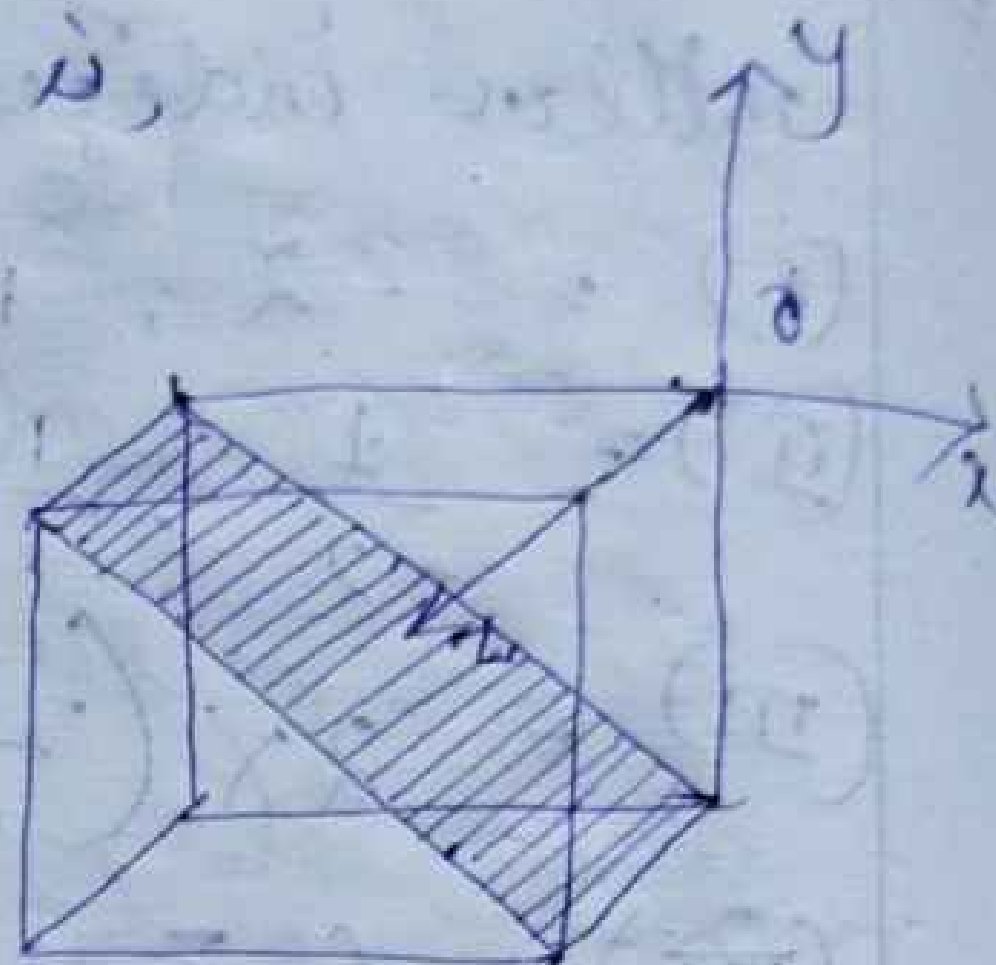
Q. If $a = -1$, $b = -1$, $c = 0$ then the miller indices (hkl) for a plane is,

(I) $= -1, -1, 0$

(II) $= \frac{-1}{1}, \frac{-1}{1}, \frac{1}{0}$

(III) $= 1 \times \left(\frac{-1}{1}, \frac{-1}{1}, \infty \right)$

(IV) $= (\bar{1} \bar{1} \infty)$



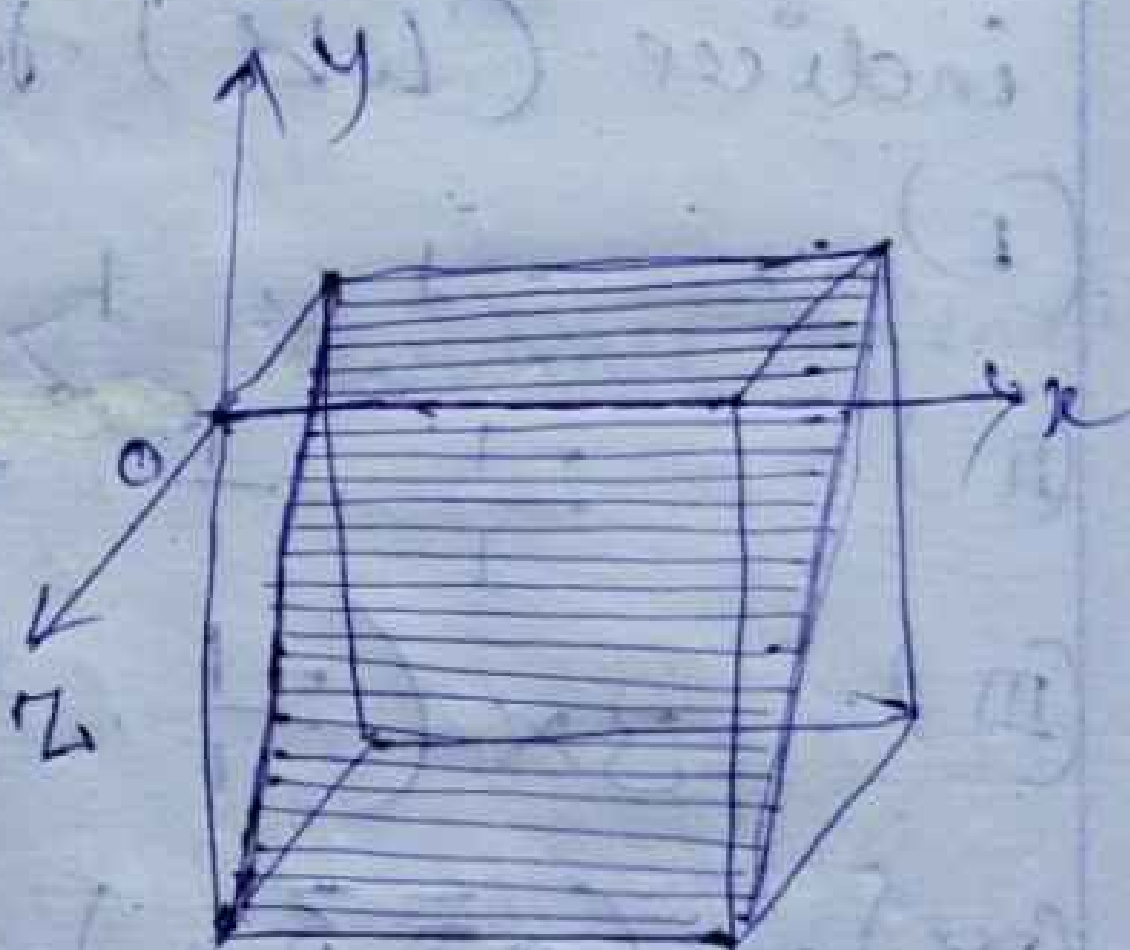
Q. If $a = 0$, $b = -1$, $c = -1$ then the miller indices (hkl) for a plane is,

(I) $= 0, -1, -1$

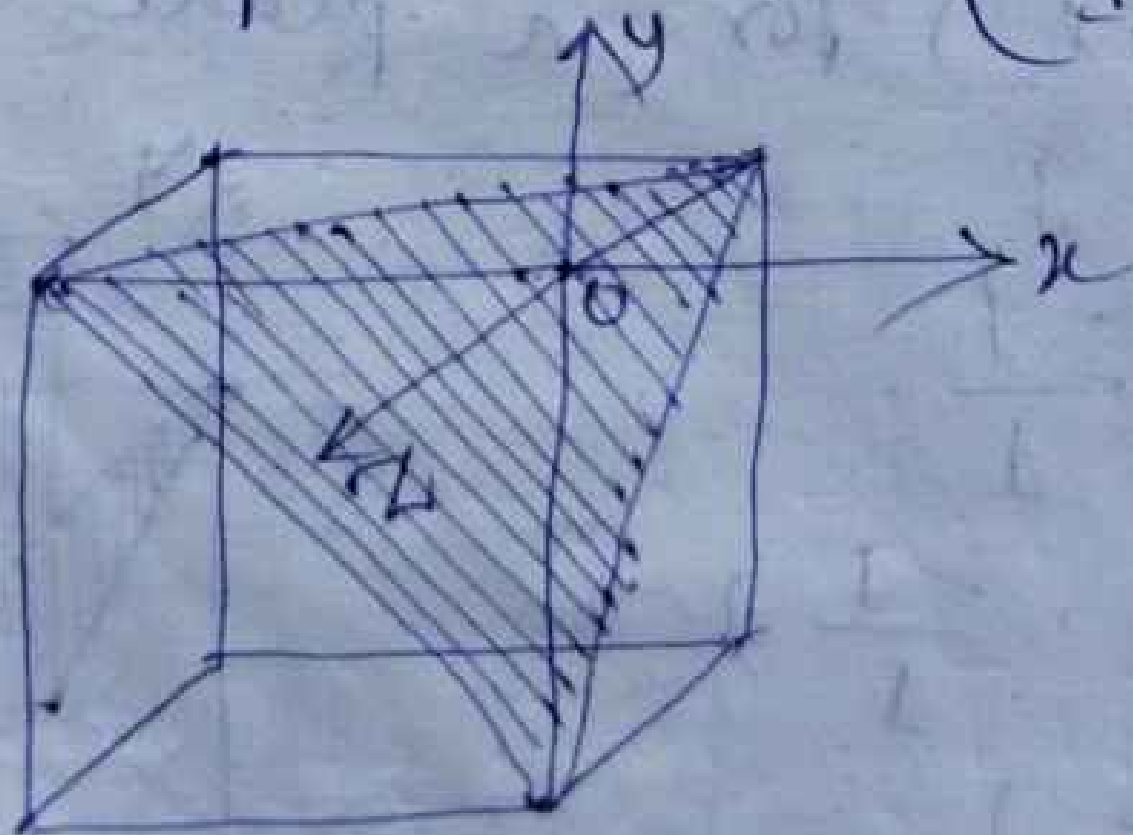
(II) $= \frac{1}{0}, \frac{-1}{1}, \frac{-1}{1}$

(III) $= 1 \times \left(\infty, \frac{-1}{1}, \frac{-1}{1} \right)$

(IV) $= (\infty \bar{1} \bar{1})$



Q. If $a = -1$, $b = -1$, $c = -1$ then the miller indices (hkl) for a plane is, $(\bar{1} \bar{1} \bar{1})$.



• crystallographie direction

→ Miller indices are also used to specify direction with - in the unit cell or crystal.

→ An unknown direction designated as $[uvw]$.

→ Direction in a crystal are specified in a vector notation.

→ A crystallographic direction is defined as a line between two point or vectors through origin.

→ The following steps are followed in determining the miller indices for crystallographic direction.

Step-I

A vector of convenient length is positioned in such a way that it passes simultaneously through the origin of the co-ordinate system and the point of interest.

Step-II

The length of the vector on each of three axes are determined. These vectors are measured in terms of lattice parameter a, b, c .

Step - III

Subsequently these intercepts either multiply and divided by a common factor to reduced them to smallest integer.

Step - IV

The smallest integers are denoted as u, v & w . These are enclosed in square bracket without comma.

Single direction $[uvw]$

Family of direction $\langle uvw \rangle$

Ex:

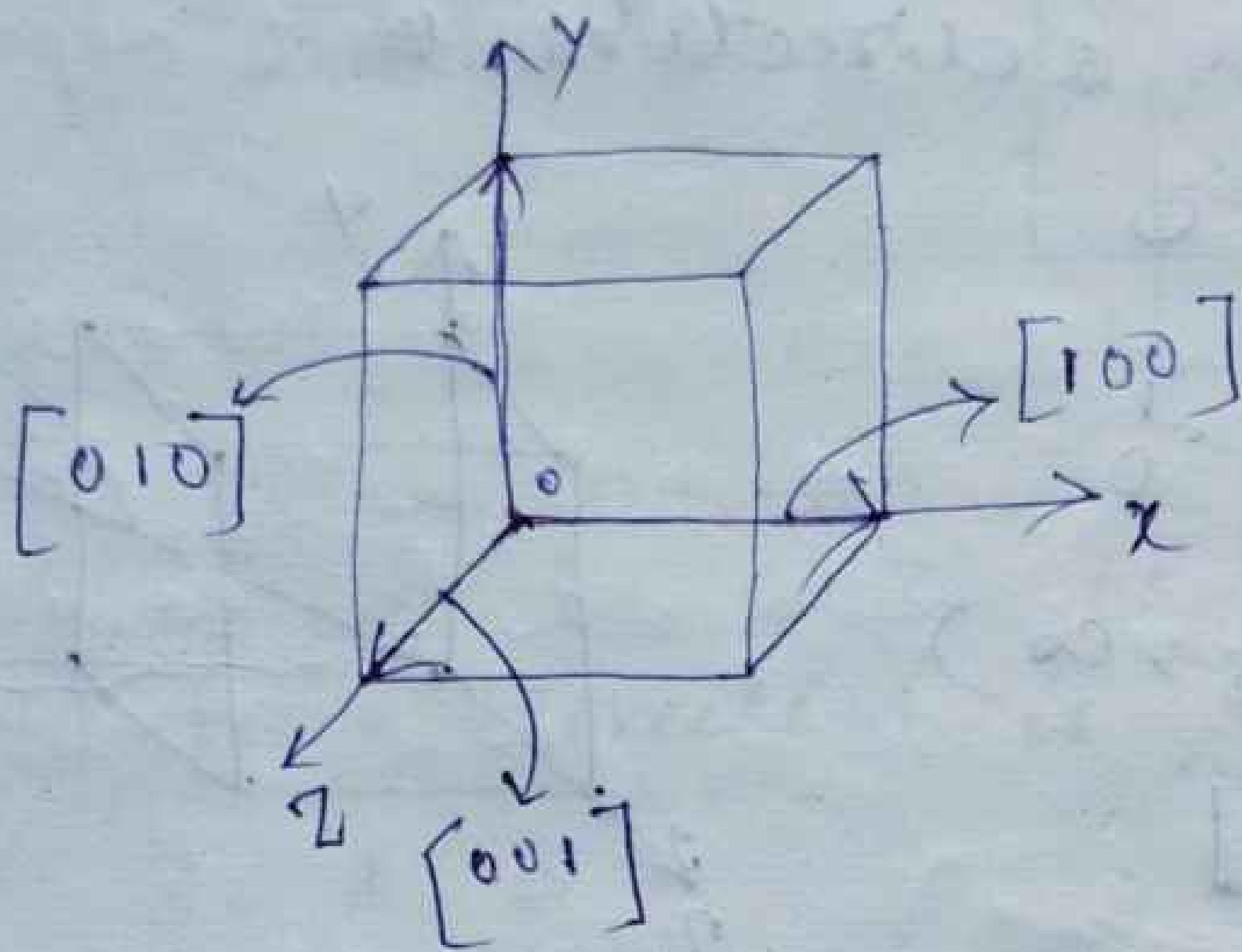
$$\langle 111 \rangle = [111], [\bar{1}11], [1\bar{1}1], [11\bar{1}], [\bar{1}\bar{1}\bar{1}], [1\bar{1}\bar{1}], [\bar{1}1\bar{1}], [\bar{1}\bar{1}1]$$

$$\langle 100 \rangle = [100], [\bar{1}00], [010], [001], [00\bar{1}], [01\bar{0}]$$

$$\langle 110 \rangle = [110], [1\bar{1}0], [011], [01\bar{1}], [10\bar{1}], [\bar{1}10], [\bar{1}\bar{1}0], [\bar{1}0\bar{1}], [\bar{1}1\bar{1}], [0\bar{1}1], [0\bar{1}\bar{1}]$$

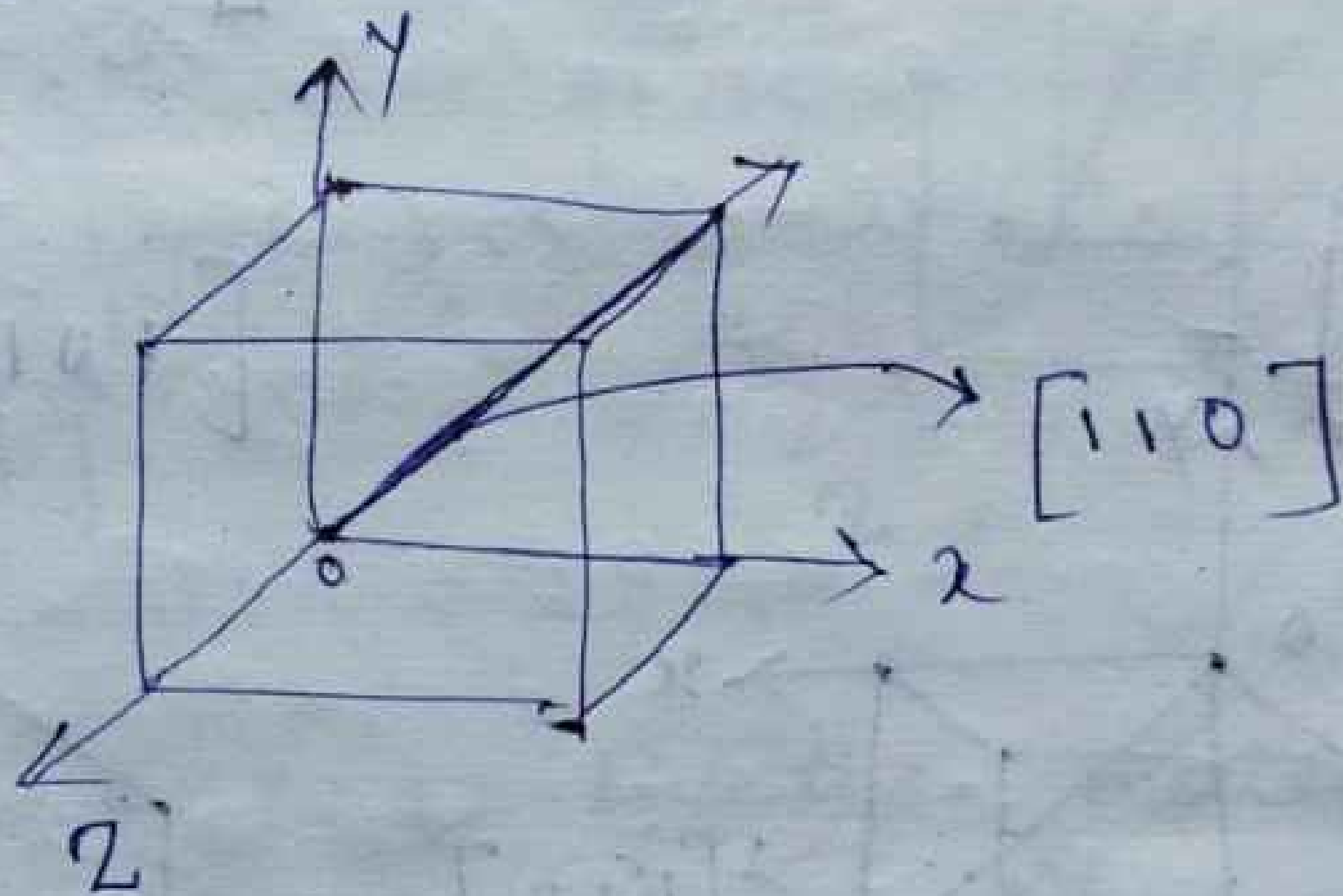
Q.

Draw $[001]$, $[010]$, $[100]$.

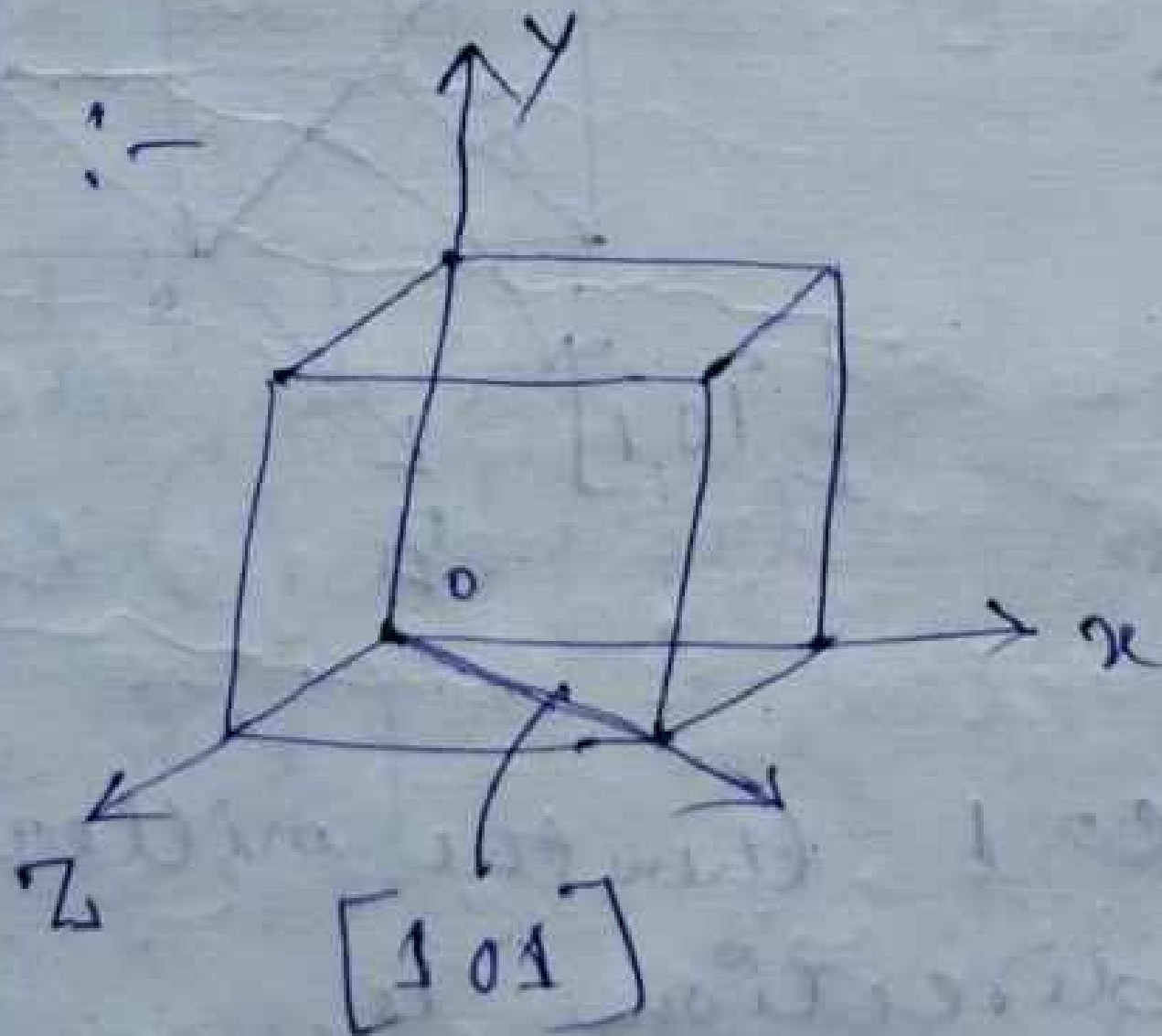


Q.

$[110]$:-



$[101]$:-



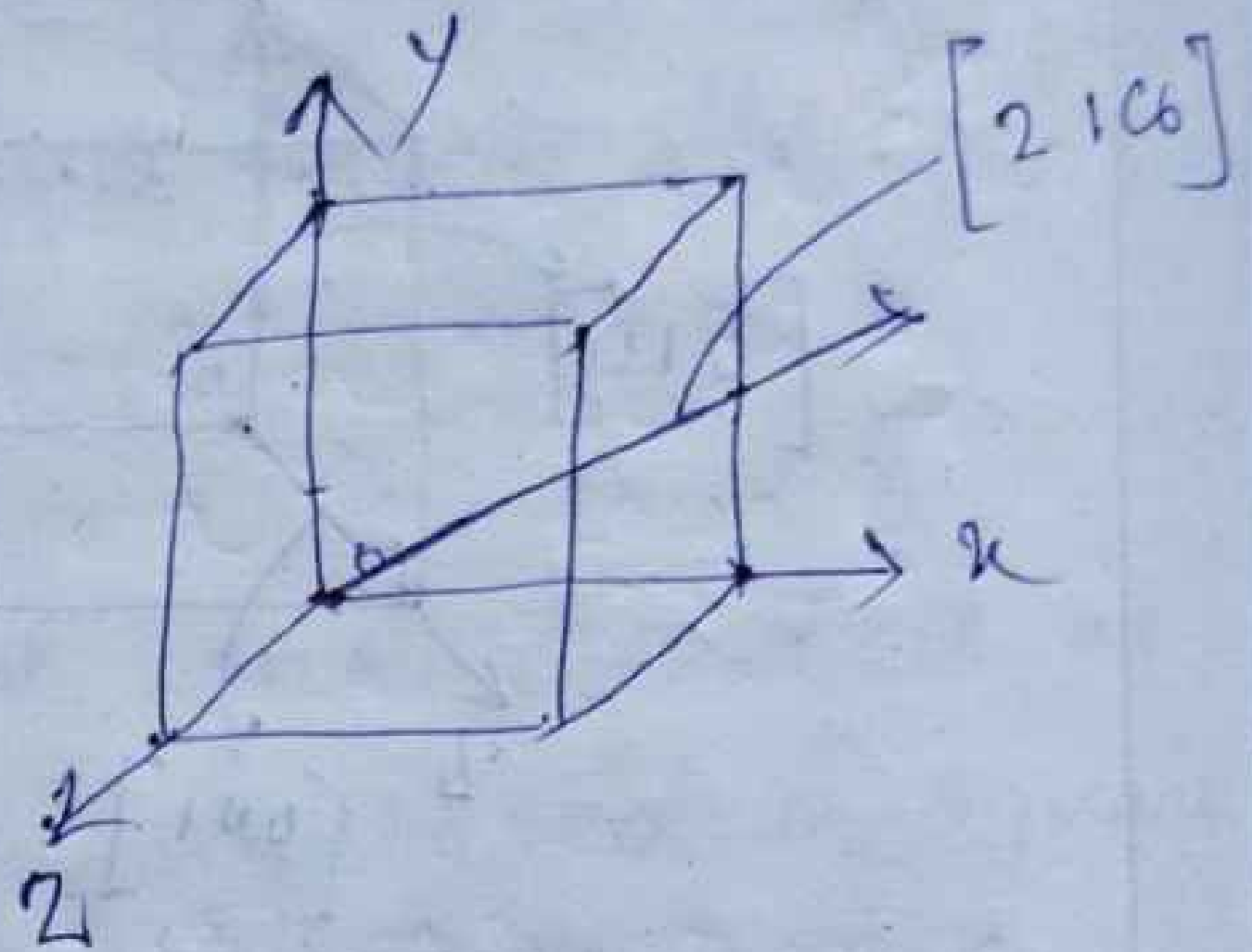
Q. If $a = 1$, $b = 2$, $c = 0$, then the miller indices $[uvw]$ for a direction is,

(I) = $1, 2, 0$

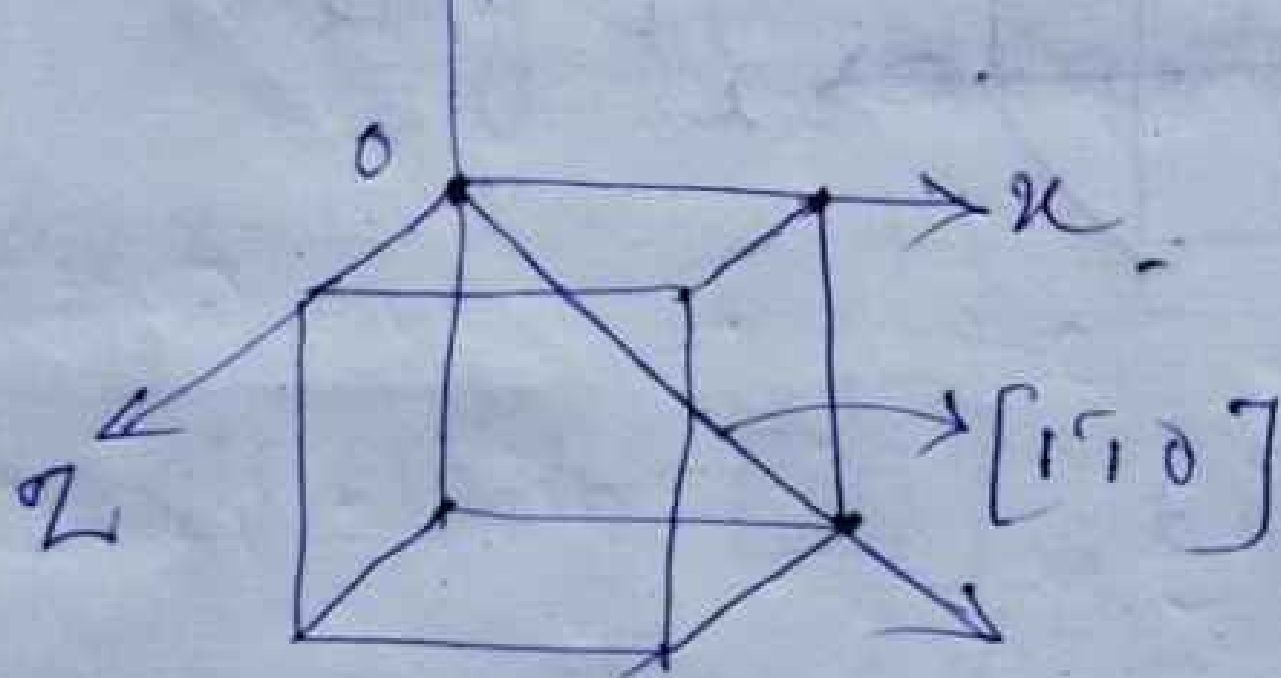
(II) = $\frac{1}{1}, \frac{1}{2}, \frac{1}{0}$

(III) = $2 \times \left(\frac{1}{1}, \frac{1}{2}, \infty\right)$

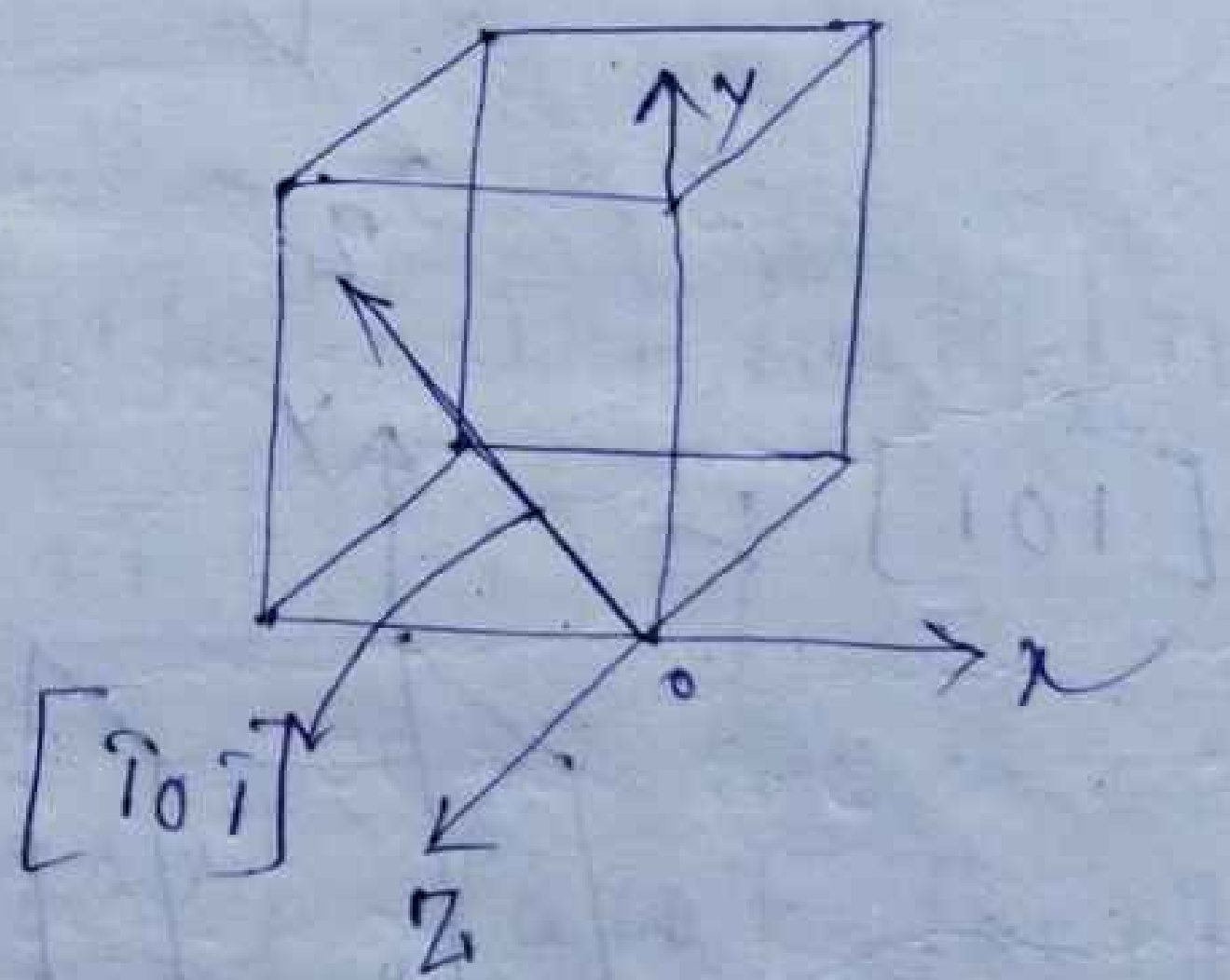
(IV) = $[2 \ 1 \ 0]$



Q. $[1 \bar{1} 0]$



$[\bar{1} 0 \bar{1}]$



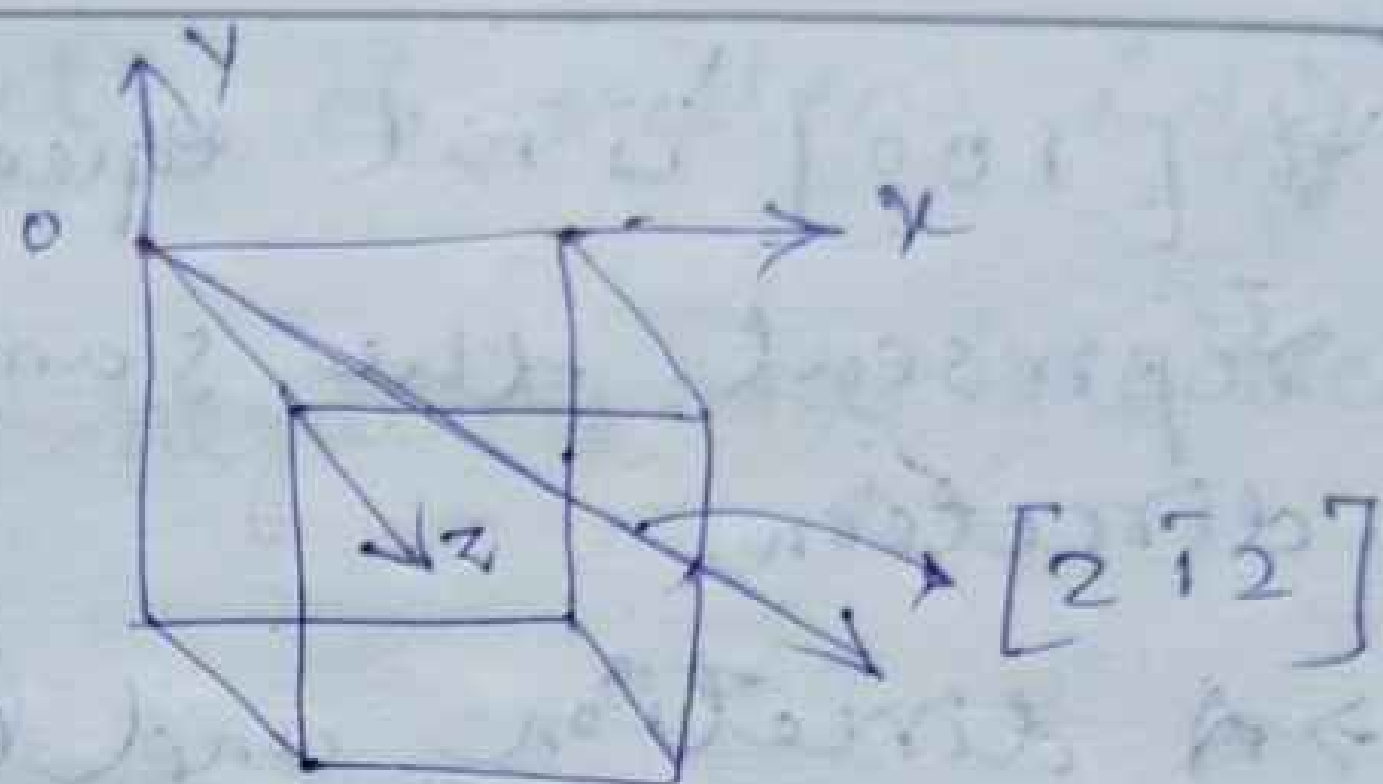
Q. If $a = 1$, $b = -2$, $c = 1$, then the miller indices $[uvw]$ for a direction is,

(I) = $1, -2, 1$

(II) = $\frac{1}{1}, \frac{-1}{2}, \frac{1}{1}$

(III) = $2 \times \left(\frac{1}{1}, \frac{-1}{2}, \frac{1}{1}\right)$

(iv) $[2 \bar{1} 2]$



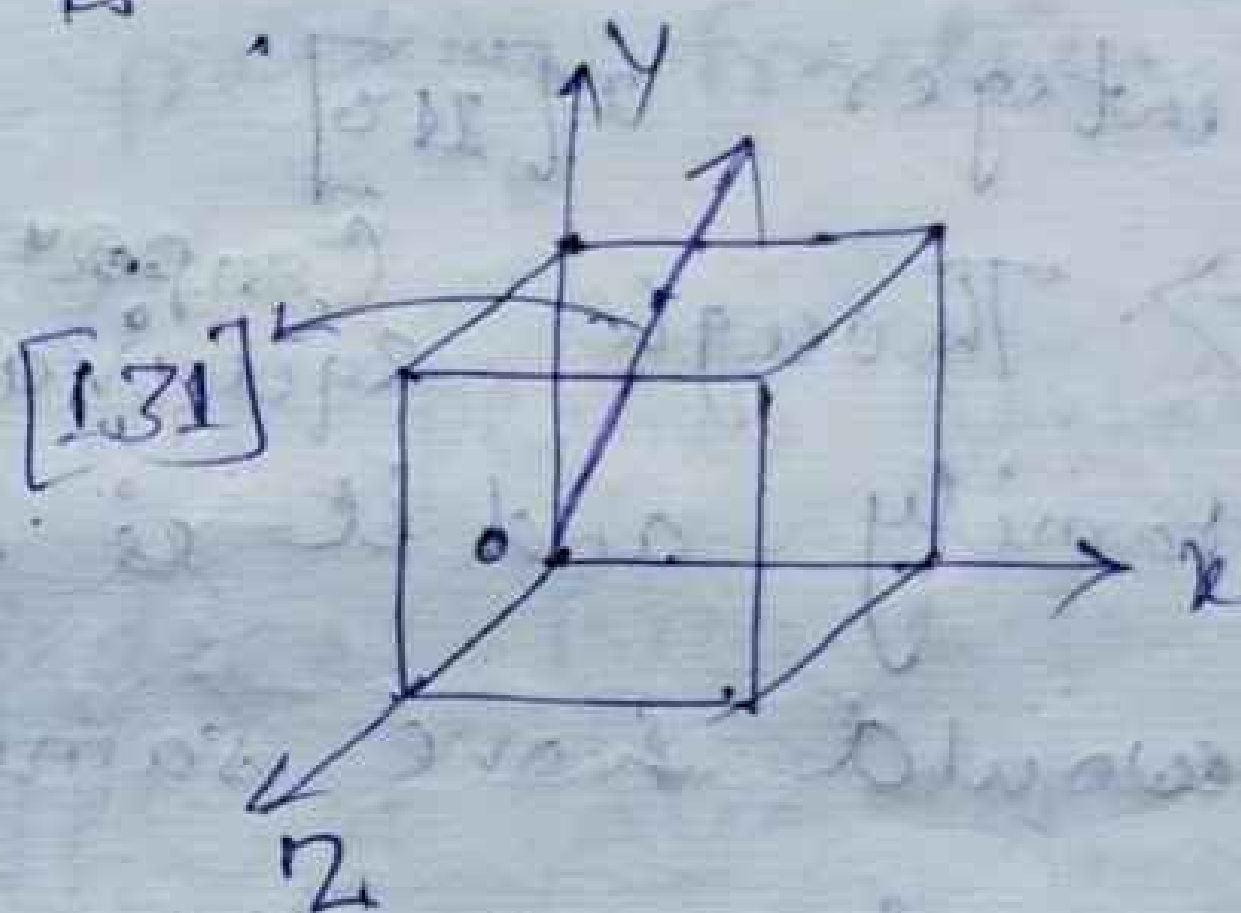
Q. If $a=3$, $b=1$, $c=3$ then the miller indices $[uvw]$ for a direction is

(i) $3, 1, 3$

(ii) $\frac{1}{3}, \frac{1}{1}, \frac{1}{3}$

(iii) $3 \left(\frac{1}{3}, \frac{1}{1}, \frac{1}{3} \right)$

(iv) $[1, 3, 1]$



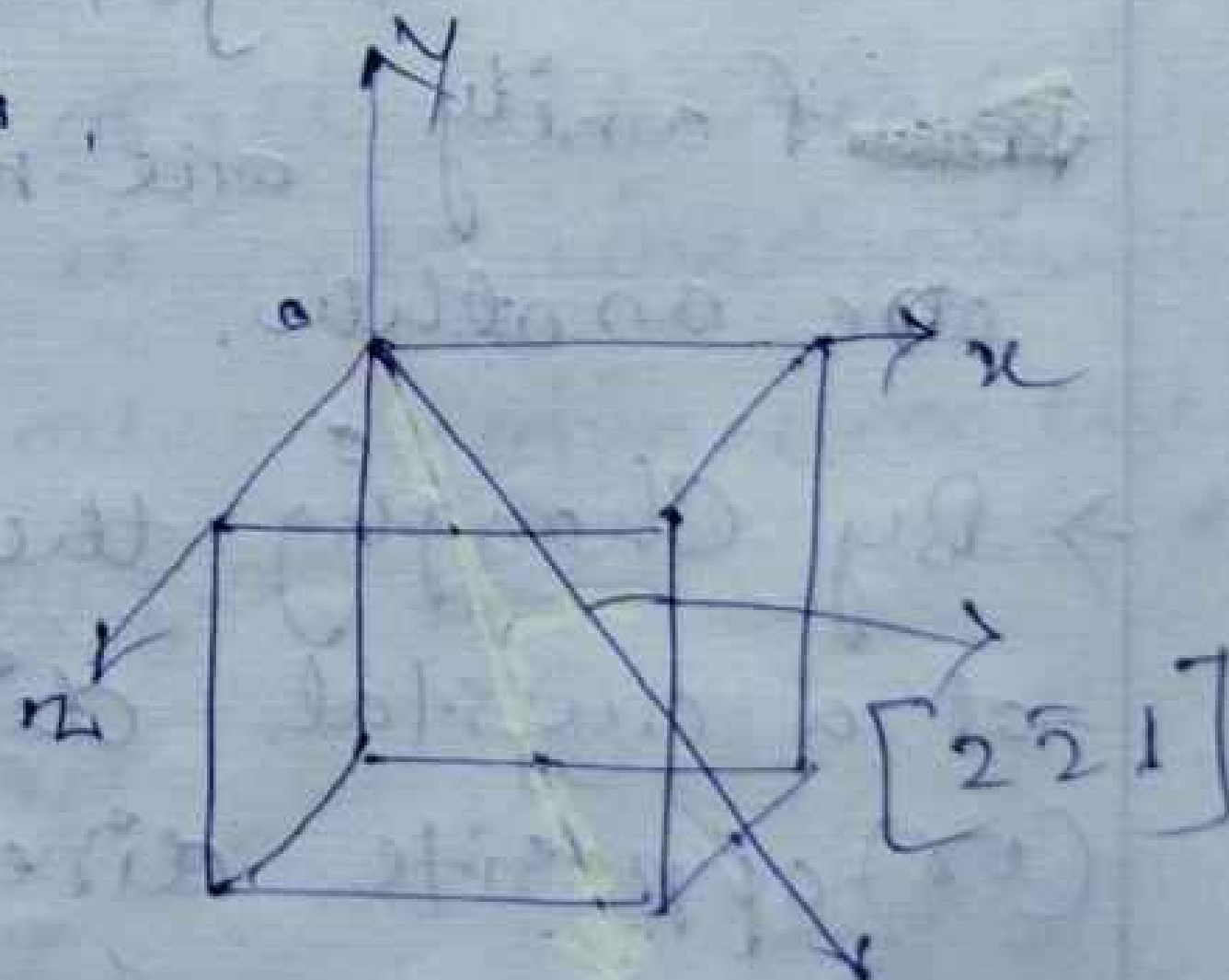
Q. If $a=1$, $b=-1$, $c=2$ then the miller indices $[uvw]$ for a direction is

(i) $1, -1, 2$

(ii) $\frac{1}{1}, \frac{-1}{1}, \frac{1}{2}$

(iii) $2 \times \left(\frac{1}{1}, \frac{-1}{1}, \frac{1}{2} \right)$

(iv) $[2 \bar{2} 1]$



• Some useful aspect about miller indices for direction

→ As direction are where vectors, a direction and its negative are not identical.

→ $[100]$ is not equal to $[\bar{1}00]$ as they represent the same line but opposite in direction.

→ A direction and its multiple are identical. $[110]$ is the same direction as $[220]$.
later has not been reduced to lowest integer $2[110]$

→ Though equivalent direction from a family and it is expected that a material would have same properties.

for example 12 direction of $\langle 110 \rangle$.

→ However crystal directions of a family are not necessarily parallel to one another.

→ By changing the signs of all the indices of a crystal direction, an anti-parallel (or) opposite direction is obtained.

→ In a cubic crystal, a crystal plane and a crystal direction normal to it have the same indices

i.e., $[111] \perp (111)$

- Some useful aspects of miller indices for planes $\{$

→ Planes and their negatives are identical

i.e., $(010) = (0\bar{1}0)$

→ Planes and their multiples are not identical, as their planar densities as well as planar packing fraction are different.

→ In cubic system, all planes having same set of miller indices, form a family, and they have same type of atomic packing. But not all members of a family of planes are parallel to one another.

→ By changing the signs of all the indices of a plane, a plane is obtained which is located at the same distance on the other side of the origin.

i.e., $(111) \& (\bar{1}\bar{1}\bar{1})$.

- Inter planar spacing $\{$

Inter planar spacing between neighbouring plane of miller indices, 'd_{hkl}' is defined as the space between the first such plane and parallel plane passing through the origin.

Generally,

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

where,

d_{hkl} = inter planar spacing.

a = lattice parameter

(hkl) = given plane

Angle between two planes θ

For 1 plane $\rightarrow h_1 k_1 l_1$

2 plane $\rightarrow h_2 k_2 l_2$

$\cos \theta =$

$$\frac{h_1 h_2 + k_1 k_2 + l_1 l_2}{\sqrt{h_1^2 + k_1^2 + l_1^2} \sqrt{h_2^2 + k_2^2 + l_2^2}}$$

• Imperfection in metallic materials

Crystal imperfections are the defects in the regular geometrical arrangement of the atoms in a crystalline solid.

→ A perfect crystal is an idealization, there is no such thing in nature.

→ The defect influence the mechanical, electrical and optical behaviour of the

crystal

→ The imperfection may be classified widely as;

- (1) Point defects (Zero dimensional defect)
- (2) Line defects (One dimensional defect)
- (3) Surface defects (Two dimensional defect)
- (4) Volume defects (Three dimensional defect)

(1) Point defect

A point defect is a very localised disruption in the regularity of a lattice.

→ It is a defect of dimensions just like point. (Zero dimension).

→ The size of the defects could be one atomic or two atomic diameters, which is just like a point.

→ Various types of point defects are:-

(I) Vacancy defect ✓

(II) Impurity defect ✓

a. → Interstitial defect

b. → substitutional defect.

(III) Frenkel defect ✓

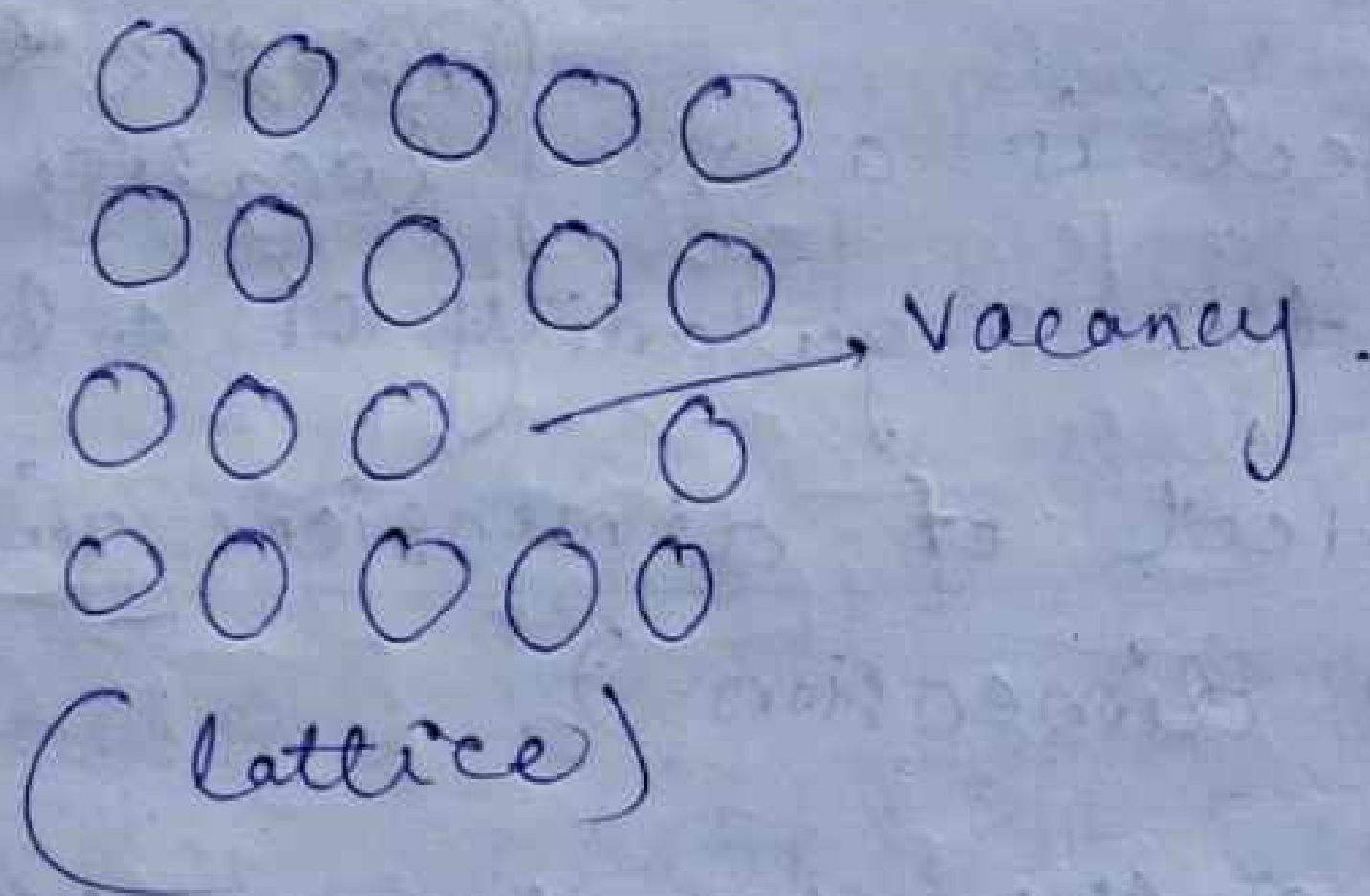
(IV) Schottky defect ✓

(I) Vacancy

→ It is a simplest point defect.

→ When an atom is missing from its lattice site in a crystal structure of a metal, it is called a 'vacancy'.

→ Vacancy is not void, it is a lattice point defect.

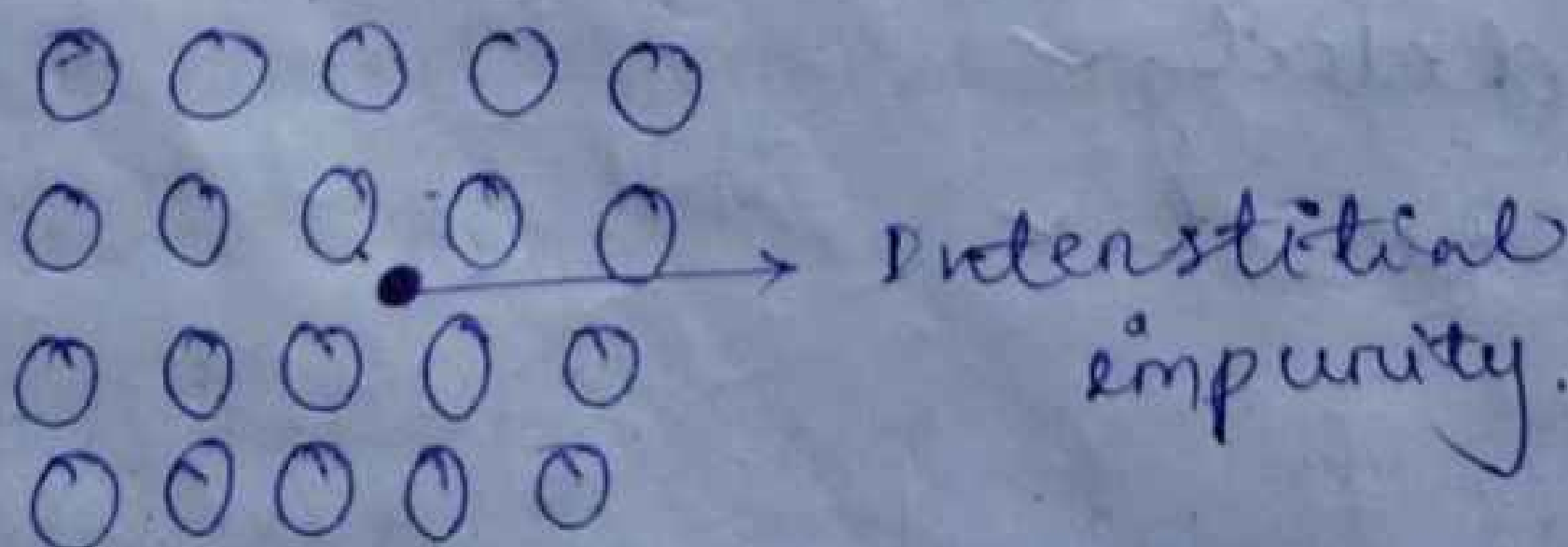


(II) (a) Interstitial impurity (Impurity defect)

If any foreign atom occupies any interstitial void space in the original lattice is termed as an interstitial impurity.

→ Then it is a point defect.

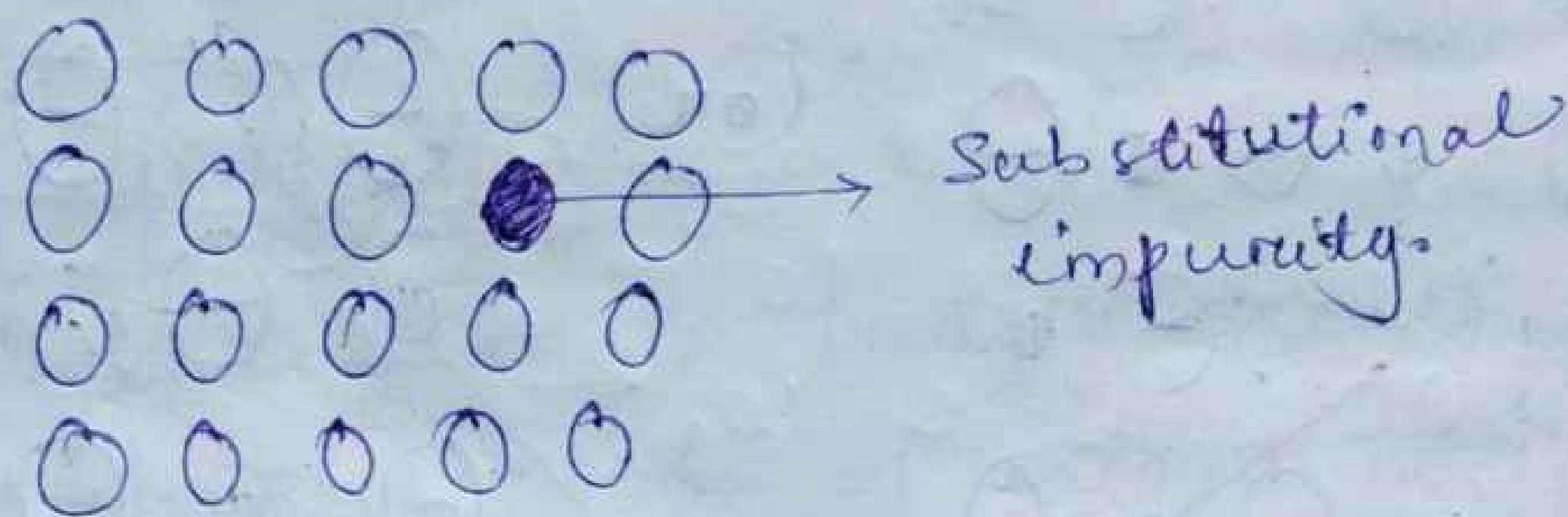
⇒ Impurity atom is smaller in size



(b) Substitutional impurity

If a foreign atom substitute a regular lattice atom from its lattice site, it is known as substitutional impurity.

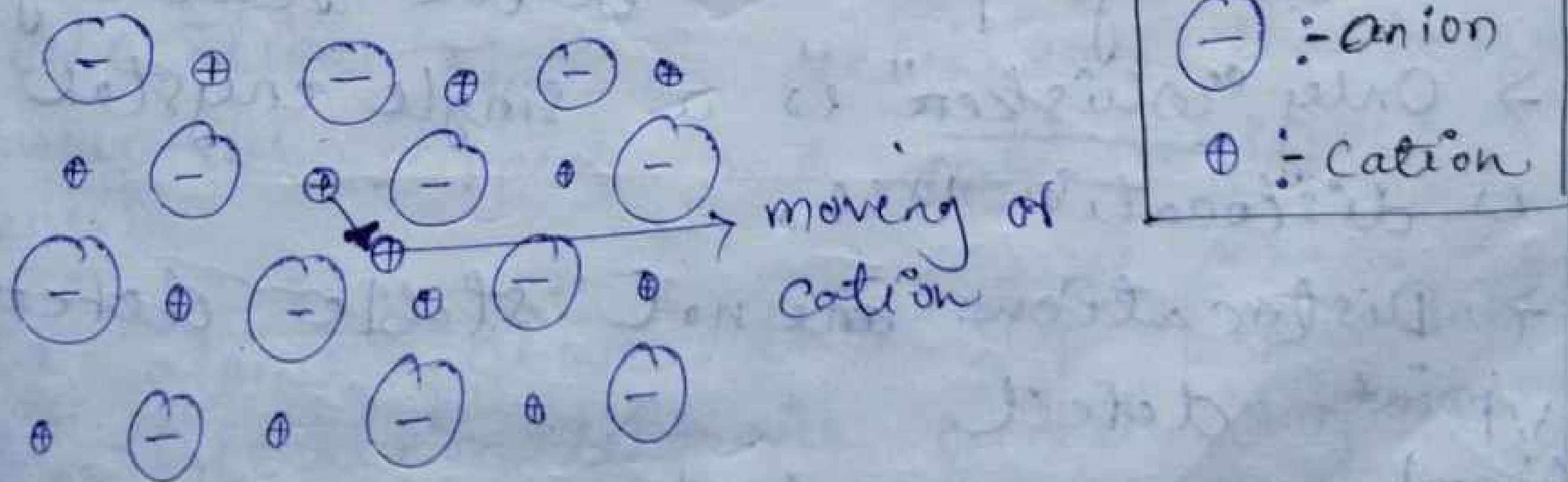
→ Substitutional atom may either larger or smaller than the normal atom in the lattice.



(iv) Frenkel's defect ✓

Frenkel's & Schottky defects are usually occur in ionic crystal rather than metal & alloys. (In place of)

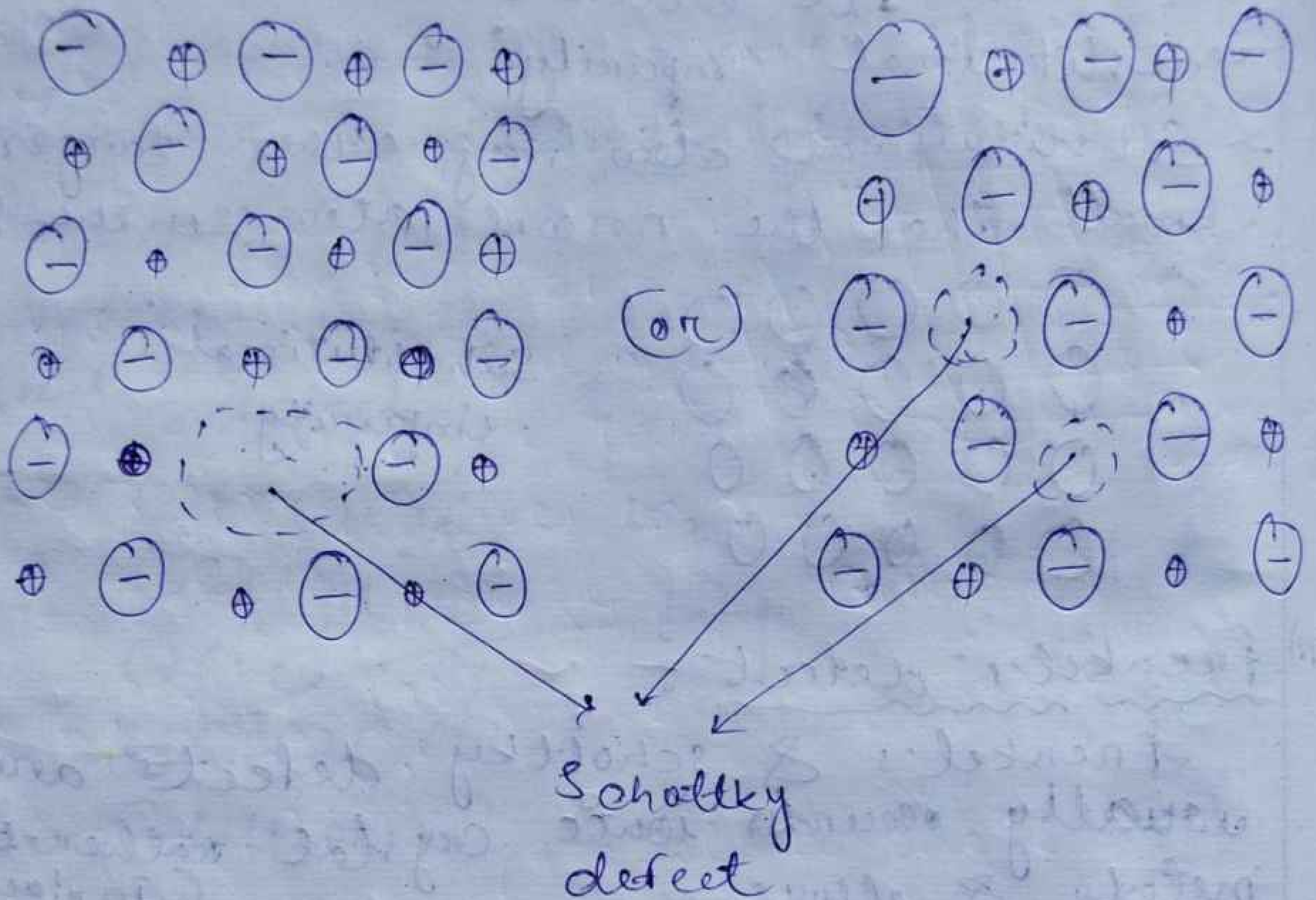
→ Frenkel's defect is formed by a 'cation' leaving its normal position and moving into an interstitial site.



(v) Schottky defect ✓

When a pair of cation and anion is missing from the regular lattice sites of an ionic

crystal, it creates an lattice defect known as 'Schottky's defect'.

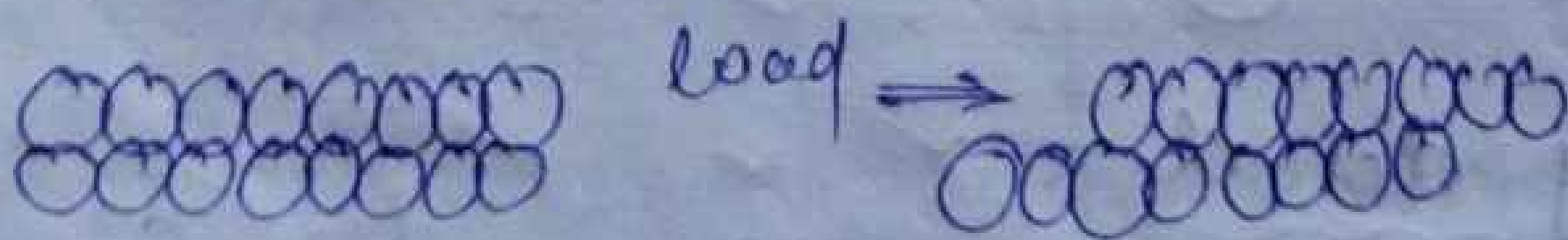


(2) line defect (Dislocation)

Dislocations are the line defects which are always present in the real crystals.

→ Only "whisker" is a single crystal which is dislocation free.

→ Dislocation are not stable defects unlike point defect.



→ Dislocation is a one dimensional (or) a line defect (Just like a line).

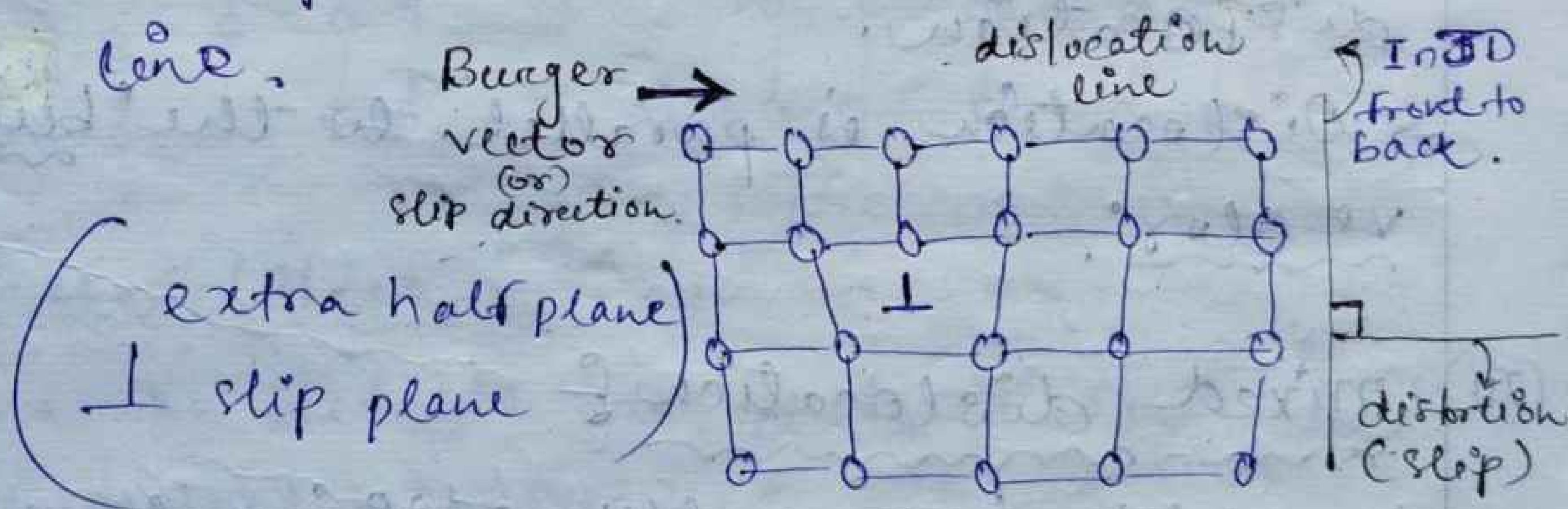
→ Dislocations can be classified into three groups,

- (I) Edge dislocation (I)
- (II) Screw dislocation (II)
- (III) Mixed dislocation (partly screw & partly edge in nature both.)

(I) Edge dislocation

(Perpendicular to burger vector)

→ The displacement of atoms in the planes surrounding the dislocation line is in the direction perpendicular to the dislocation line.



→ Dislocation line is defined as the boundary between the slipped and the unslipped plane.

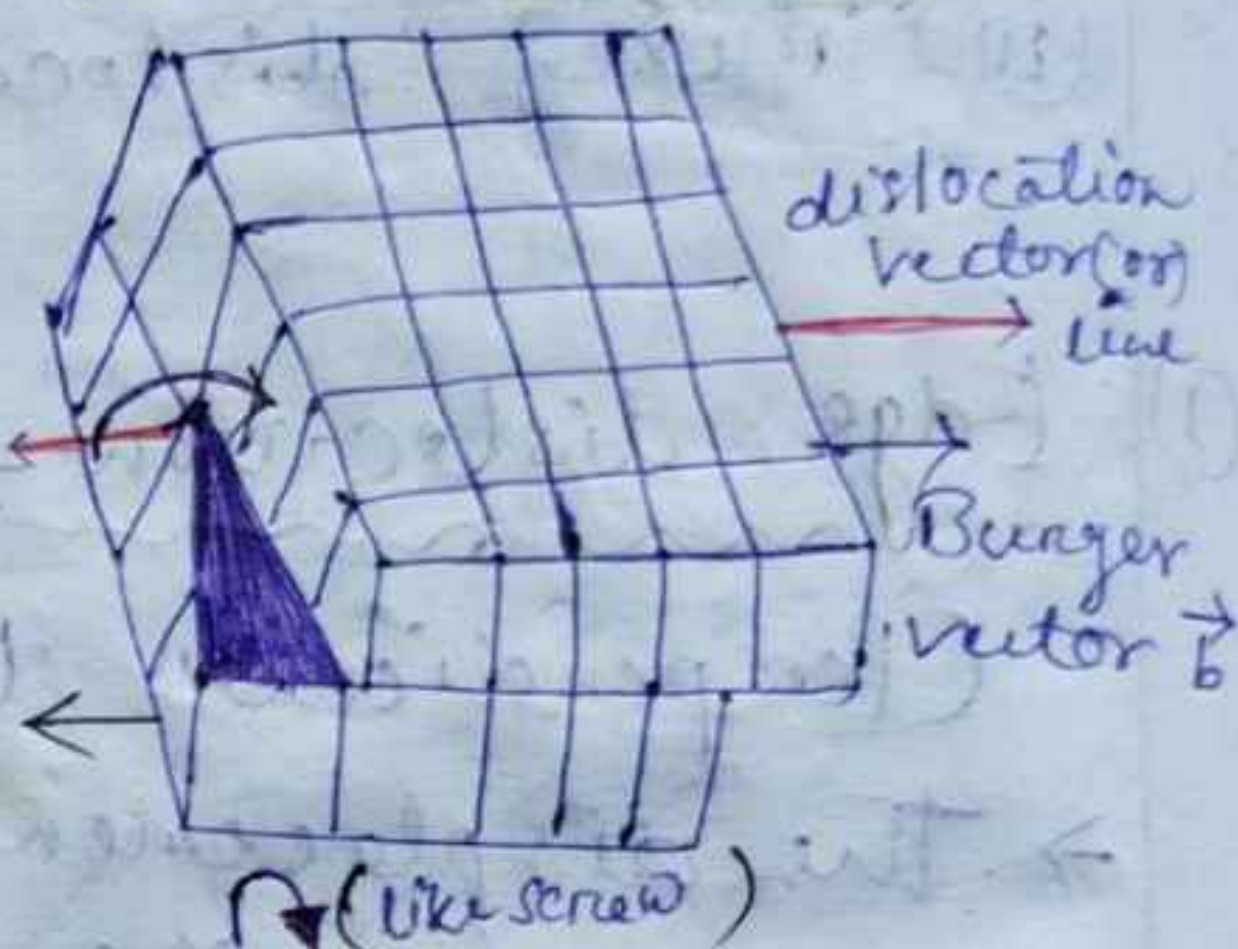
→ The atoms above the slip plane around the dislocation line are under compression and below the slip plane are under tension.

(II) Screw dislocation

(Parallel to burger vector)

→ It is formed by a shear stress that is applied to produce the distortion.

→ The upper region of crystal is shifted one atomic distance to the region relative to the bottom portion



→ shear vector is parallel to the screw dislocation.

→ Dislocation is parallel to the 'Burger vector'.

(III) Mixed dislocation

→ which has partly edge in nature and partly screw in nature.

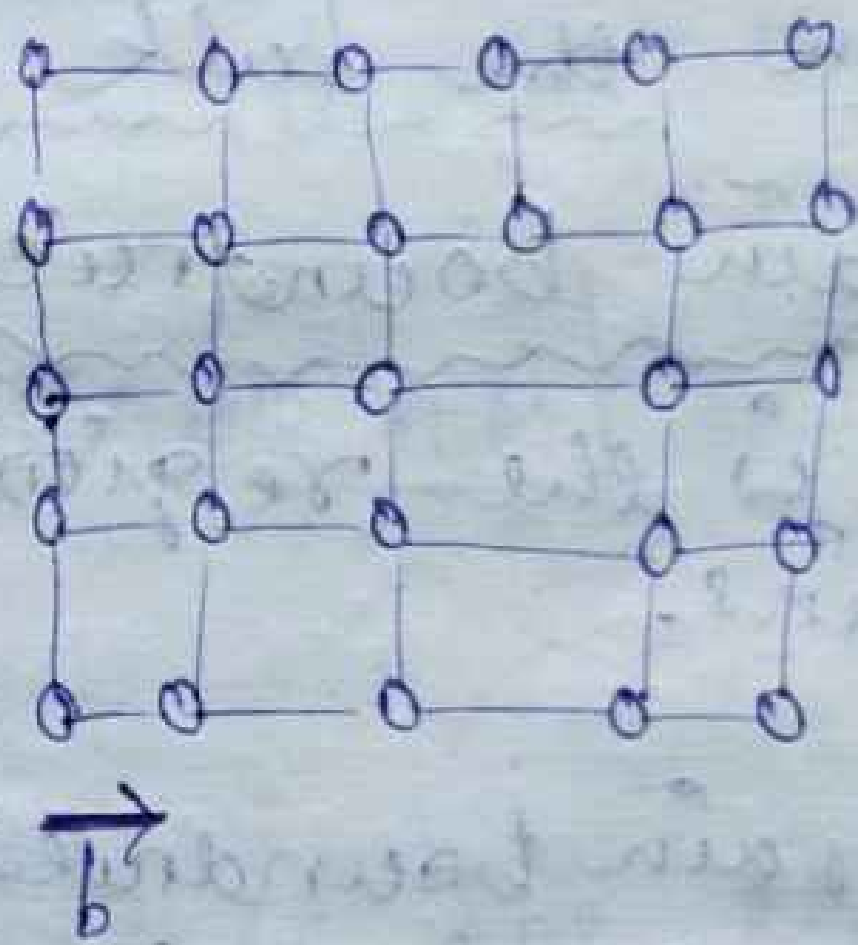
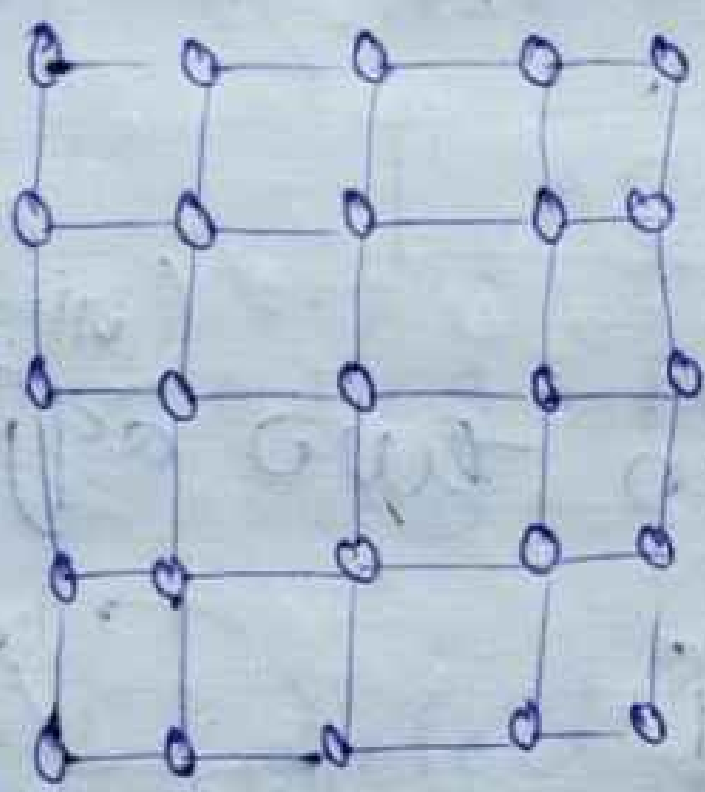
• Burger vector

The motion of a dislocation in a crystal produces a displacement of one plane of atoms over the other in definite distance.

→ The magnitude and the direction of the displacement are defined by a vector called 'Burger vector', which characterizes a dislocation line.

→ The burger vector is determined by carrying out a procedure by tracing out a burger circuit.

→ It is denoted as $\vec{b}$.



(3) Surface defect

→ Surface defects are defects of two dimensional nature.

→ Surface defects are associated with boundaries that are separate regions of the materials and have different crystal structure.

→ Types of surface defect:

(i) Free Surface ✓

(ii) Grain boundary ✓

(iii) Stacking fault ✓

(I) Free surface & (External surface)

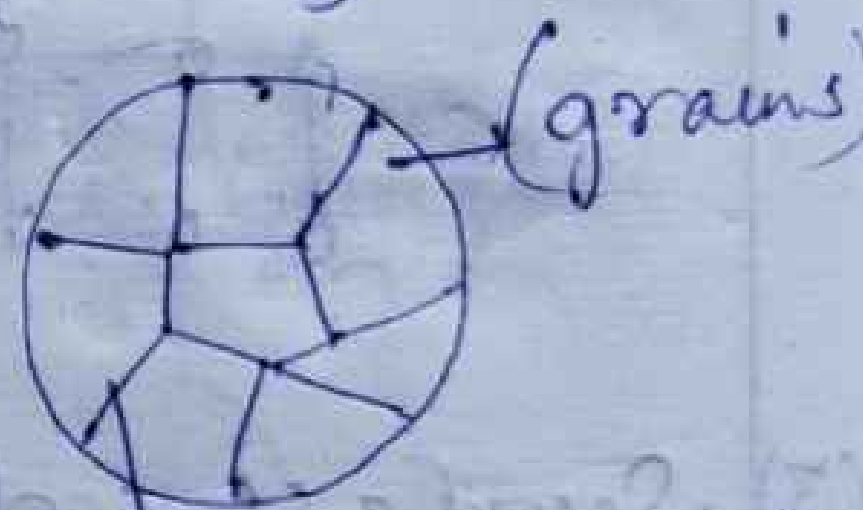
Free surface of materials are surface defects in the sense that, growth of crystal has stopped abruptly/suddenly at the surface that is a "free surface imperfection".

→ Surface atoms have unsatisfied atomic bonds, and higher surface energies, than the bulk atoms.

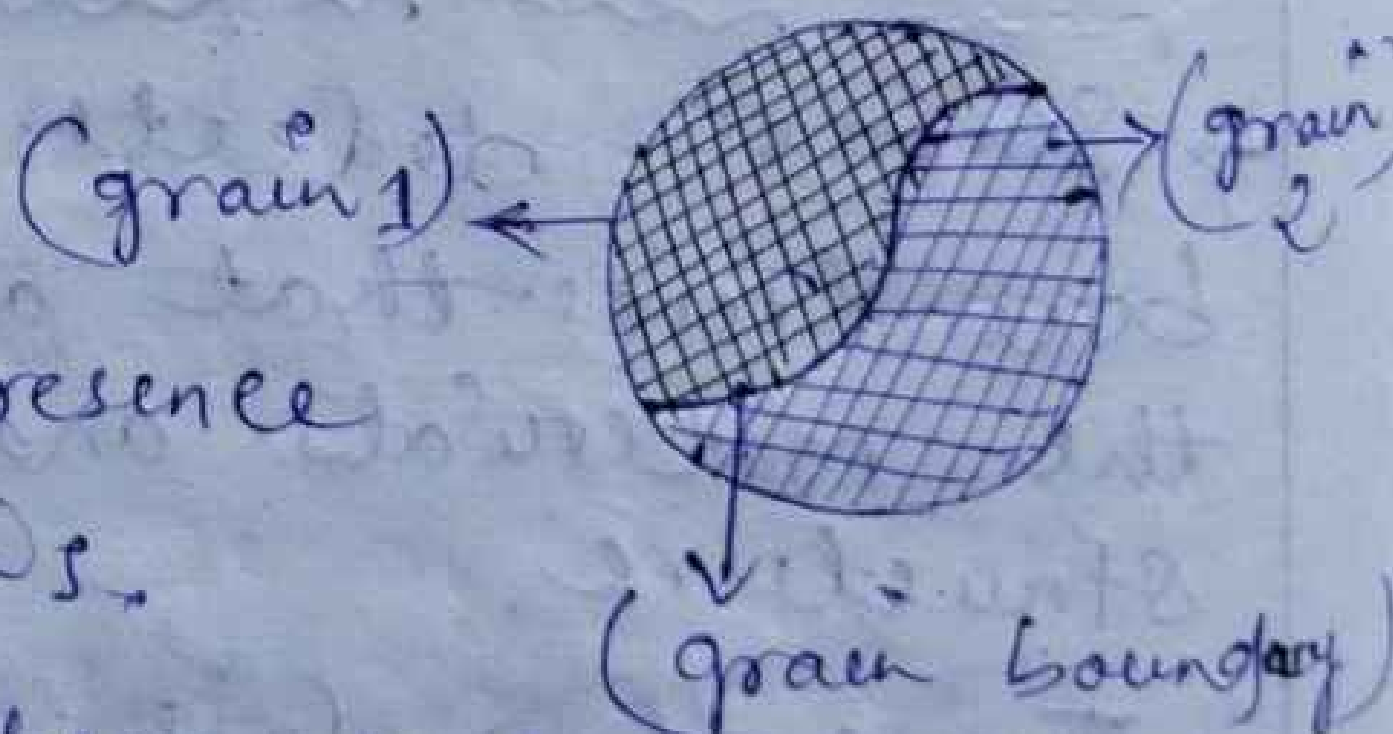
(II) Grain boundaries &

It is the region between two adjacent grains.

→ Grain boundaries separate crystals/grains of different orientation in a polycrystalline material during crystallisation.



→ The shape of the grain is usually influenced by the presence of surrounding grains.



→ In the boundary where the crystal or grains change abruptly, the orientation of difference between neighbouring grain is more than "10-15°" & the boundaries are known as "high angle grain boundaries".