

Chapter no.3 STRUCTURE OF CRYSTALLINE SOLIDS.

Q.

Differentiate between Crystalline & Amorphous Solids.

Crystalline Solids

(i) Crystalline solids have well defined ordered 3D structure

Amorphous Solids.

Amorphous solid have an irregular undefined structure.

(ii) They are isotropic because they have same properties throughout the crystal lattice.

They are anisotropic since their physical properties are different in different directions.

(iii) Example:

Crystalline SiO_2
(Quartz)
(Tetrahedral)

Example:

Amorphous SiO_2
(Glass).

Q. Define Unit Cell:-

Unit Cell is the basic structural unit or building block of the crystal structure and defines the crystal structure by the virtue of its geometry and the position of the atom within.

- Body-centred Unit Cell

Face centred unit cell :-

- It has a particle at each corner
- It has a particle at the centre.

- particle at each corner and face
- no particle at centre

*

If the unit is isolated from the lattice

\Rightarrow all corner particle

combine to give one atom or particle.

\Rightarrow one particle at the centre.

\therefore 2 particles full per unit cell

- if the unit cell is isolated from lattice

- all corners give 1 particle.

- two faces each give one.

all face $\Rightarrow \frac{1}{3}$

\therefore 0.4 particles full per unit cell

(volume of unit cell) -

$$\frac{3\sqrt{2}}{2} R^3$$

side

HFC is a type of (a = 2R)

crystal lattice arrangement in which each atom is

\Rightarrow

$6R^2 c \sqrt{3}$

arranged at the corner of a hexagonal and one

each at the center of the hexagonal face.

* page no. 91 of book is very important.

Q. describe polymorphism and allotropy.

example: Alkaline metals.

equivalent of Ionic compound

Cu

$a = \frac{4R}{\sqrt{3}}$ \rightarrow atomic radius

Au

Ag

Al

length of unit cell.

(V_s) \Rightarrow Volume of FCC unit cell = $16R^3 \sqrt{2}$

Galaxy

$$APF = \frac{\text{volume of atoms}}{\text{total unit cell volume}} = \frac{V_s}{V_c} \Rightarrow$$

Hexagonal Face structured:-

coordination no. $\Rightarrow 12$

APF $\Rightarrow 0.74$

Examples :- Cd, Mg, Ti, Zn etc. height

Vc (Volume of unit cell) -

$$\frac{3\sqrt{2}}{2} R^3$$

side

height

$\sqrt{3} R$

length

$\sqrt{2} R$

Galaxy

some metals and non-metals may have more than one structure (crystal) this phenomena is known as polymorphism. When found in elemental solids, it is termed as allotropy.

The types/changed type of crystal structure depends upon both

i) Ambient temperature

Galaxy

BCC & FCC \Rightarrow cubic crystal systems

HCP \Rightarrow hexagonal system.

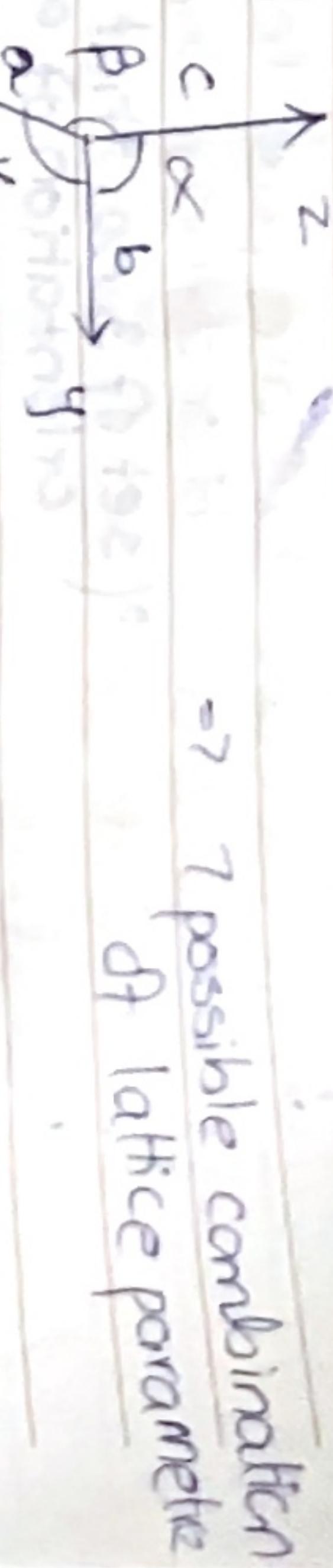
Example:

Require:

Carbon: (i) graphite (ambient condition)
(ii) Diamond. (high ext. pressure)

- Lattice Parameters.

Iron: (i) pure iron BCC (normal condition)
pure iron FCC (912°C)

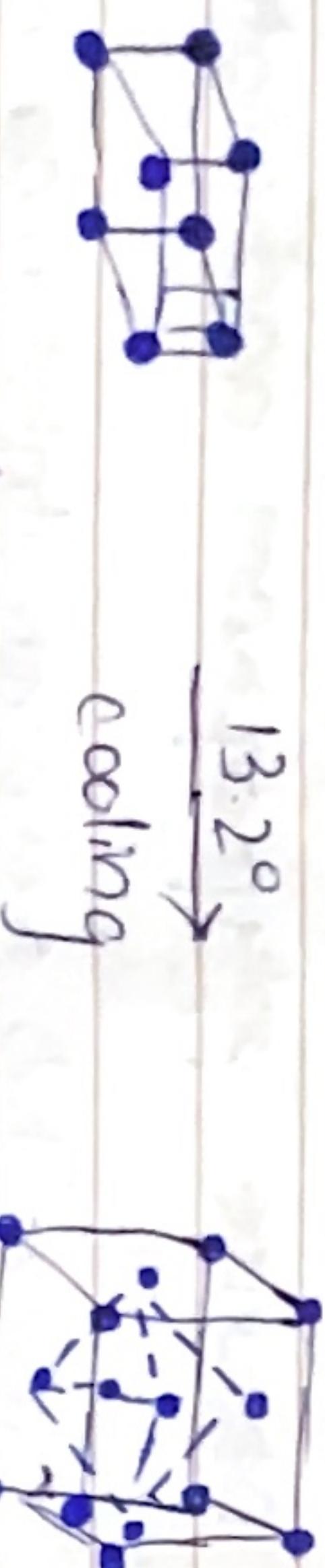


- * change in density or other physical properties also assist this transformation.

Q. Schematically describe the allotrophic transformation of tin. (RSO Russia)

(tin disease).

The allotrophic transformation of tin occurs at 13.2°C cooling where it changes from β tin (white) into α tin (gray).



Crystallographic directions:-

Defined as a line between two points or a vector. steps to determine the three directional indices

1. construct x, y, z plane / coordinate system & set origin at one corner.

2. Two points may be required for tail (e.g. x_1, y_1, z_1) and head (x_2, y_2, z_2).
3. subtract $(x_2 - x_1, y_2 - y_1, z_2 - z_1)$
4. These are then normalized in terms of their respective a, b, c i.e. $(\frac{x_2 - x_1}{a}, \frac{y_2 - y_1}{b}, \frac{z_2 - z_1}{c})$

5. If necessary these three no.s are multiplied and divided by a number to reduce to smallest integer value.
6. Lastly they are enclosed in square brackets without commas.

$\nabla T \propto$ faster rx.

$\nabla T \propto 7^\circ\text{C}$ of this change)

$\Delta V (7.50\text{ g/cm}^3 \text{ to } 5.77\text{ g/cm}^3)$

Galaxy

* Analyze fig. 3.10 from slides.

* Ex 3.12 & 3.11

1 Getting plane points.

Any two planes that are parallel to each other are equivalent & and have the same Miller indices.

(set of 3 no. that describe orientation of a set of planes)

If a plane passes through the selected origin either another parallel plane must be constructed or a new origin must be established at the corner of another unit cell.

(ii) At this point the plane intersect or parallels each of the three axes, the coordinates of intersection are determined (through) referenced to the origin (with each axes).

These x, y, z intercepts will be designate A, B, C.

(iii) The reciprocal of these intercepts in take. A plane that parallel an axis is considered to have infinite intercepts and therefore a zero index.

(iv) The reciprocal are x with respect a, b, c.

(v) They are reduced to smallest integer values.

(vi) The values are then enclosed in the round brackets without comma.

plane (a,b,c) give reciprocal; decrease by x in size.

Reciprocal these steps when drawing \rightarrow reciprocal; draw Galaxy increase by x in size.

* direction equal in magnitude are called equivalent.

Q. Why turbine blades are made up of single crystals.

Efficient strong Ni single crystal turbine blade burn less fuel at higher temp because the blades are grown in $[110]$ closely packed direction FCC Ni

* As they are single crystal the mechanical & thermal stress doesn't accumulate at the grain boundary & decreases the chances of breakage.



* While drawing planes, return to the origin for the piezoelectric material;

* plotting of next point.

\rightarrow Voltage & stress \downarrow 1st make mirror images.

\rightarrow object -

Q. Why are crystallographic point, direction & planes important?

They are important

(i) To locate position of atoms in a structure

(ii) To analyze alloying ability (if vacant spaces are present)

(iii) To analyze critical points (at high temp & pressure) Galaxy

single crystal, monocrystalline
polycrystalline \rightarrow anisotropic
due to multiple grains

* corner atom shares $1/8^{\text{th}}$
one of three angles $= 112.0^{\circ}$
and the other two are 90°

$\alpha = 90^{\circ}$
 $\beta = 90^{\circ}$
 $\gamma = 90^{\circ}$

Q. Define grain boundaries. grain boundaries

- * Grain boundaries is a microscopic interface or transition zone between adjacent crystalline grains within a polycrystalline material.

* They are high energy regions, therefore melting and boiling always first affect these grain boundaries.

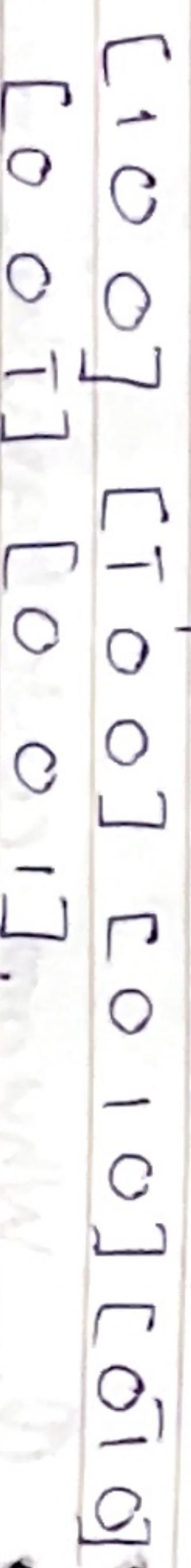
* They act as barrier / hindrance to the motion of charge carriers.

The Family of planes & direction

DIRECTION: The family of directions is represented as

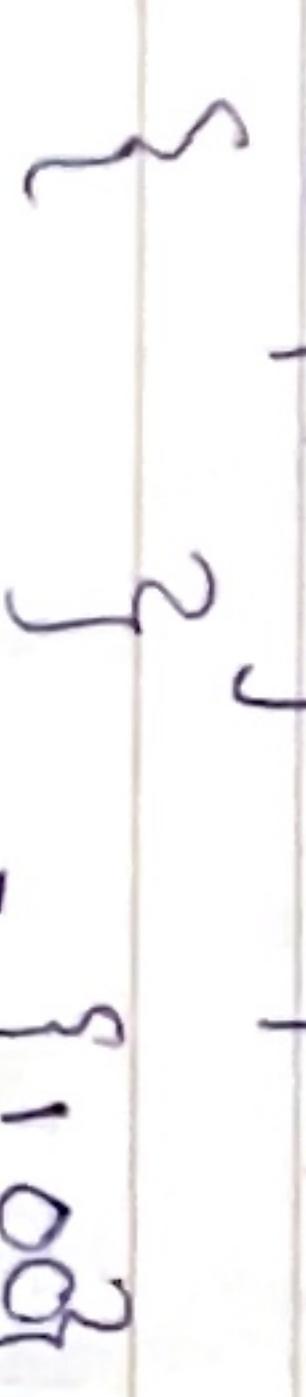
$<$ $>$

Example:- $<100>$, it includes



* Iron has BCC \rightleftharpoons Cu has FCC.

PLANES: The family of planes is represented as



Example : It includes.



* define (logically) critical plane

The type of plane in which when pressure is applied to a cube, it is likely to break first.

VACANT SPACES IN STRUCTURES.

Impurities settle at the vacant spaces in the structures of the atom.

In BCC; vacant spaces are at the edges. 32%.

In FCC; very small vacant spaces at 25%. edges & centre however very small C. less sedimentation.

In simple cube; the vacant spaces are inside the structure. 18%.

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FCC & HCP has APF 0.74.

LAYERING & STACKING:-

AB \Rightarrow stacking of layer on top of vacant space of 1st layer.

ABC \Rightarrow stacking of layer on top of vacant space left even after AB layering.

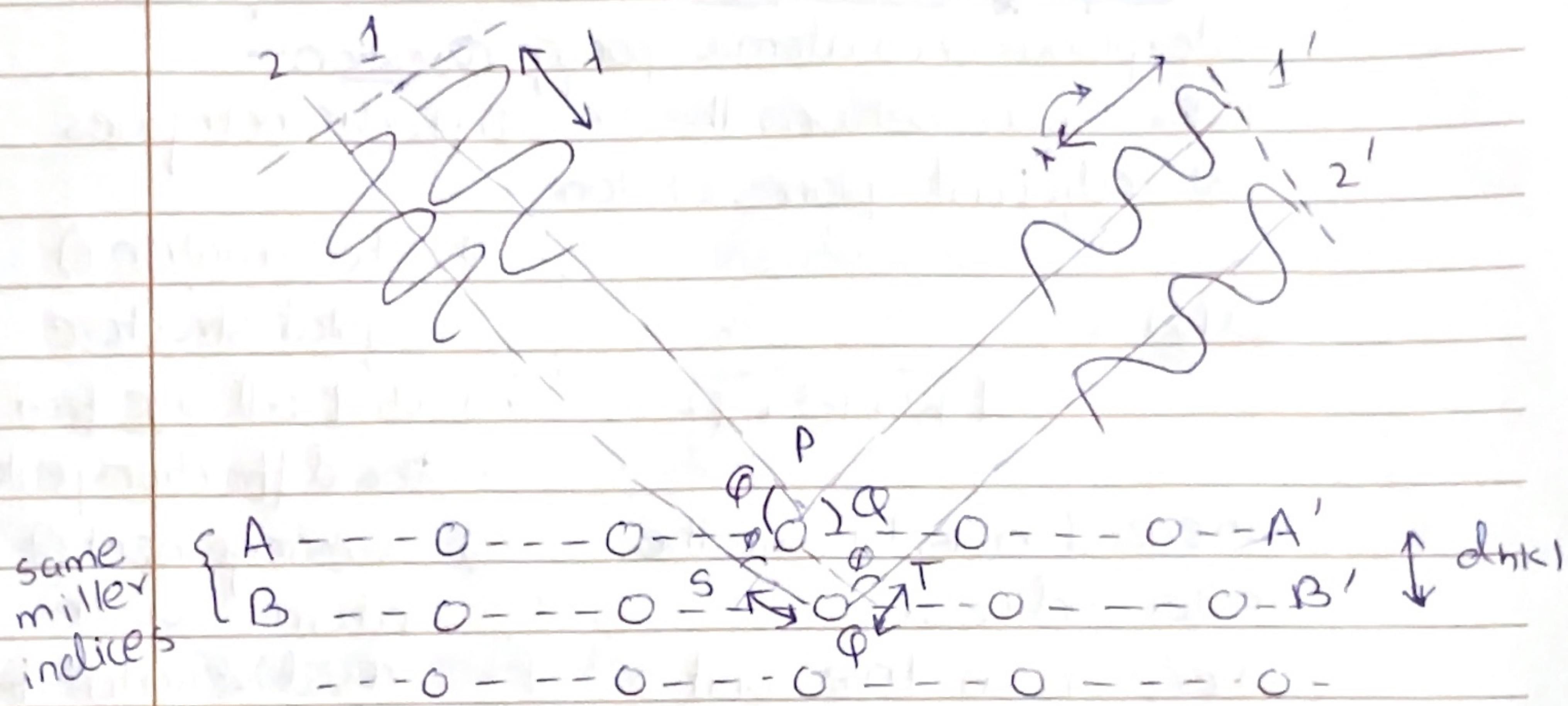
ABA is another combination.

ABA B A B \Rightarrow hexagonal closed packing generating HCP

AB C ABC \Rightarrow generating FCC.

Chapter no. 3Bragg's law & Diffraction through X-rays:-

X-ray are a form of electro-magnetic radiations that have high energies and shorter wavelengths. (λ order on the atomic packing)



Two monochromatic, coherent and parallel X-rays of wavelength λ scatter by atoms P and Q

the condition for diffraction is;

$$\textcircled{n}\lambda = \overline{SQ} + \overline{QT}$$

path length difference

also $n\lambda = d_{hkl} \sin \theta + d_{hkl} \sin \theta$

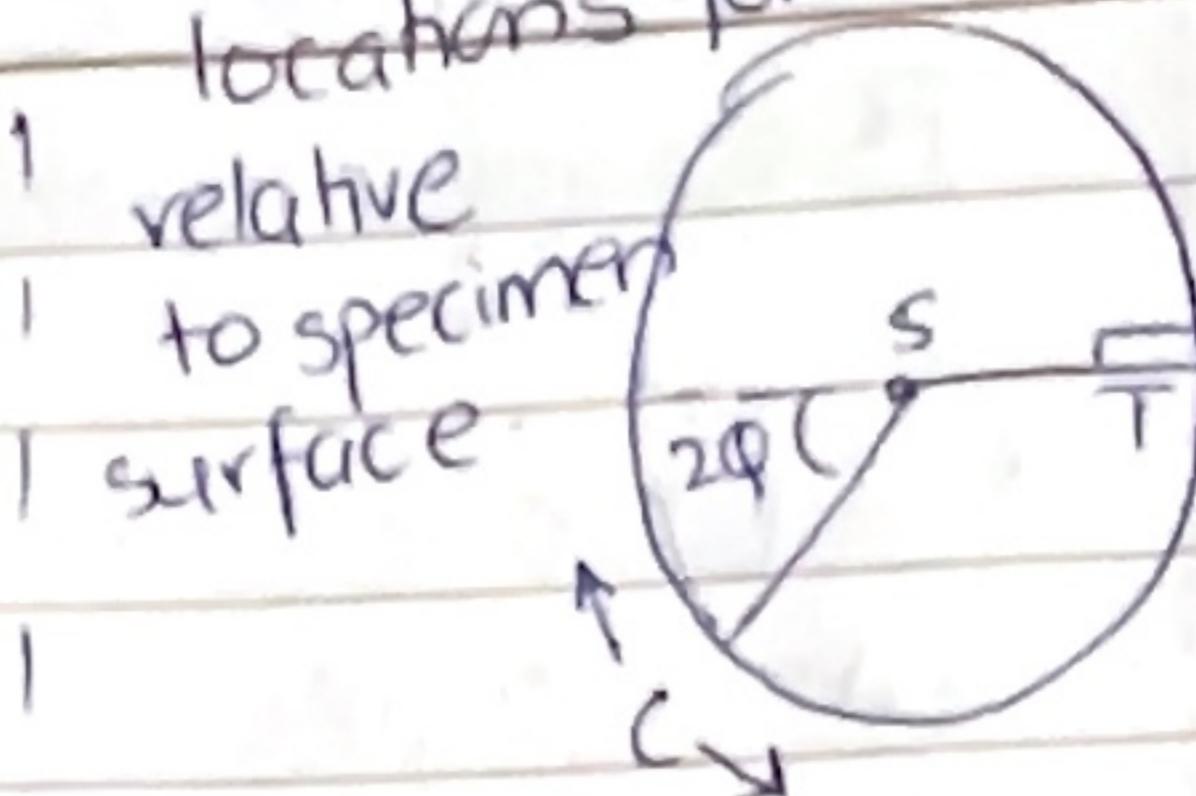
$\textcircled{*} \quad n\lambda = 2d_{hkl} \sin \theta \Rightarrow \text{Bragg's Law}$ Galaxy

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Q here is the angular locations for both T & C

Bragg's law is a relationship between

- (i) wavelength of X-rays
- (ii) interplanar atomic spacings
- (iii) angle of diffracted beam



Interplanar distance

Interplanar or (iii) atomic spacing is the space between the two adjacent planes of atom.

S is the origin
T is the x-ray source
C is the detector.

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

where (h, k, l) are the miller indices.

where a is the unit cell edge length.

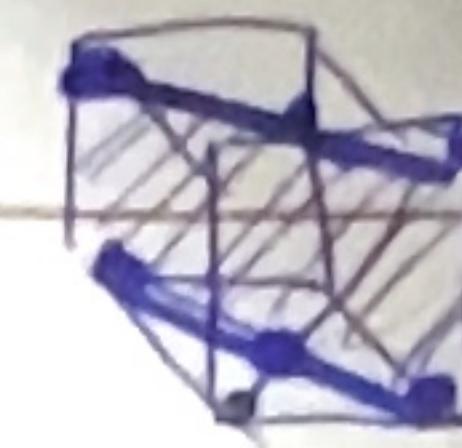
Question:-
Diffraction uses

- ① determination of crystal structure.
- ② Unit cell size from the diffraction peaks.
- ③ arrangement of atoms with relative intensities of these peaks.

The condition is not specific for crystals in real conditions. It is specified for diffraction for unit cells having atoms positioned at cell corners.

area of planar = $(4R) \left(\frac{2R}{\sqrt{2}} \right)$

↓ ↓
horizontal vertical



ABC
DEF

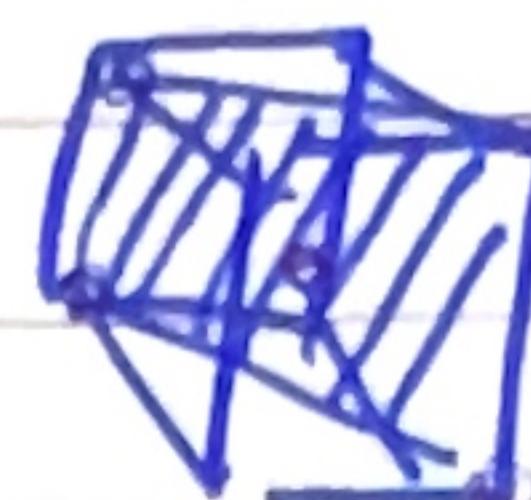
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c.

sharing of atoms in a cube occurs at:-

- (i) corner of the cube
- (ii) Inside a cube.
- (iii) on a face of the cube
- (iv) On the edges of //

area of planar region in BCC



$PD_{110} = 2 \text{ atoms}$

LINEAR DENSITY \times $(\text{nm}^{-1} \text{ or } \text{m}^{-1})$

$[16\sqrt{2} R^2/3]$

$LD = \frac{\text{number of atoms centred on direction vector}}{\text{length of the direction vector}}$

→ LD of equivalent directions are identical

PLANAR DENSITY :- $(\text{nm}^{-2} \text{ or } \text{m}^{-2})$.

$PD = \frac{\text{no. of atoms centred along a plane}}{\text{area of the plane.}}$

* LD & PD are important to study for slip mechanism i.e. by which metals plastically deform.