

Free Study Material from All Lab Experiments



**Solid-State Physics Notes
for NET/GATE Physical Sciences
Classification of Solids #**

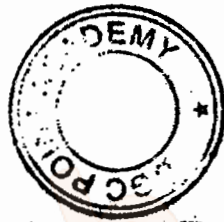
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Solid State Physics

Books

- Kittel
- Ashcroft & Mermin
- Puri & Babber
- Wahab



Matter

There are 4 states of matter

- i) solid
- ii) liquid
- iii) gas
- iv) Plasma



We need to study the Properties of Solids :-

Electrical properties :- To differentiate b/w Insulator, conductor & semiconductor.

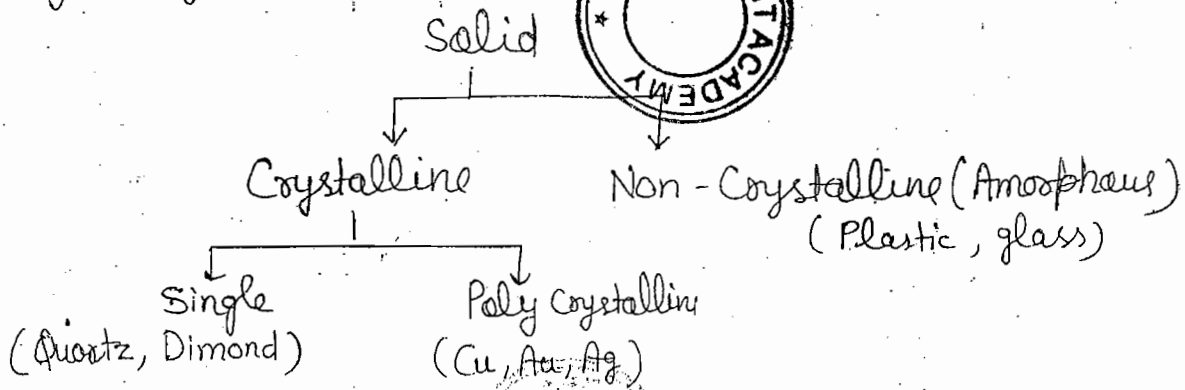
Magnetic properties :- Magnets are ferromagnetic materials. To know about para, dia, ferro, we need this prop.

Thermal properties :- To know which solid is thermal insulator or thermal conductor.

Mechanical properties :- To know which solid is mechanically strong.

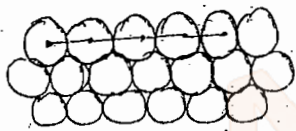
Optical / optoelectronic properties :- Which material is require to make solar cell is decided by optical prop.

Types of Solids :-



Crystalline solids are characterised by regular or periodic arrangement of atoms or molecules.

Every solid is made up of atoms or molecules.



Atoms are repeating themselves after a certain distance.

Non Crystalline solids are characterised by random arrangement of atoms or molecules.

Arrangement of atoms will decide their properties.

Plastic is Non-crystalline.

Copper is crystalline.

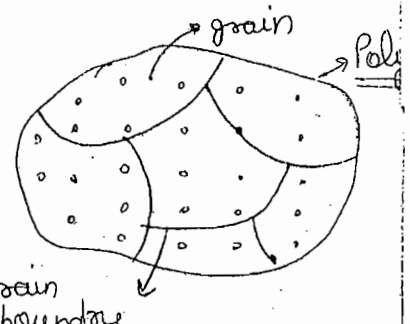
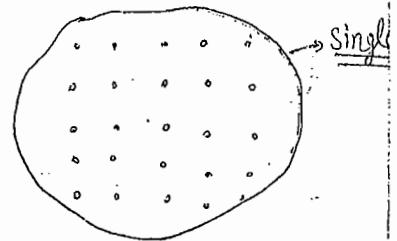
Diamond & Copper both are crystalline but diamond is a single crystal & copper is poly-crystalline.

Single: Throughout the crystal, we have same type of arrangement then the crystal will be single crystal.

Polycrystalline crystalline :-

Polycrystalline is the arrangement of aggregate of large no. of single crystals.

The small single crystals are known as Grain & boundaries separating these crystals are Grain Boundary.

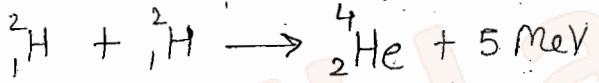


If we consider graphite & quartz then their properties are different bcoz their properties depends upon their bonding

In nature, Most of the solids are in the form of crystalline solids bcoz crystalline solid is more stable as compared to amorphous solid as energy released during the formation of crystalline material is more than amorphous solid.

→ As more energy released in the formation of a crystal, crystal will be more stable.

eg. Helium nucleus is formed by 2 deuterium nuclei & energy released. → 5 MeV. - To break He into $1H^2 + 1H^2$ we need to supply 5 MeV energy.

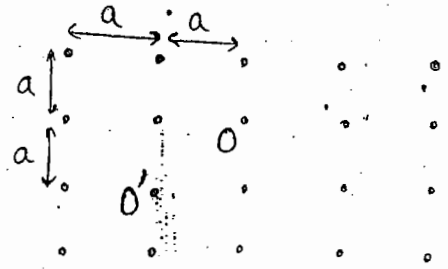


https://alllabexperiments.com

Study the Crystal Structure

Lattice :- Lattice is periodic arrangement of imaginary points in the space.

This is a periodic arrangement of ~~atoms~~ points. This is a Mathematical concept.



This Lattice will be a Branais

Lattice or Space Lattice if each lattice point has identical surroundings.

e.g. Lattice point O & O' has same surrounding.

Basis :- Basis is an atom or group of atoms. By attaching the basis to each lattice point, we'll get Crystal Structure.

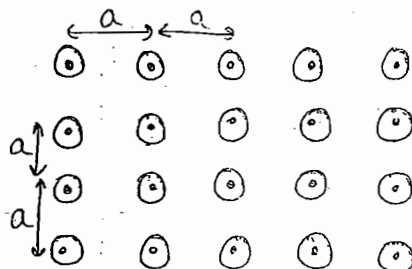
Lattice + Basis = Crystal It is also called Motif.

Basis of 1 atom is called Monatomic Crystal

" " more than 1 atom is called Polyatomic crystal.

If we are attaching atoms on each lattice point so this will become physical.

As lattice points are periodic so atoms will be periodic so this arrangement will become Crystalline Solid.



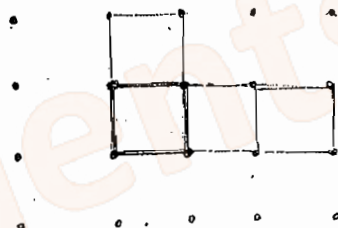
Unit Cell :- Ideal crystal is infinite in dimension, real crystal can not be infinite.

Nothing can be ideal so it must have finite dimension.

Unit cell is the smallest unit of the crystal or lattice which on continuous repetition can generate whole lattice.

This is the representative of lattice or crystal structure.

If we want to construct the crystal structure then we have to arrange the unit cells side by side.



→ Grain can contain large no. of unit cells.

Unit cells are of 2 types,

- i) Primitive
- ii) Non-primitive

{ dim. of unit cell tells
→ at what distance lattice point will repeat itself }

Primitive :- Lattice points are belonging only to the corners of the unit cells.

OR

Effective no. of lattice points per unit cell is one.

Non-primitive :- Lattice points are belonging to the corners as well as to the other position of the unit cell.

OR

Effective no. of lattice points are more than one.

- 1 atom basis → Each lattice point will contain 1 atom
- 2 " " → " " " 2 "

2 " " → " " " 2 "

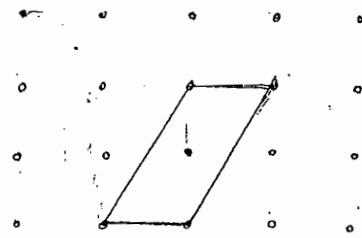
→ (Sides of unit cell → lattice constant or lattice parameter) (3)

A primitive cell can have more than 1 atom but have only 1 lattice point.

1 lattice point is shared by 4 unit cells for primitive cell.

$$\frac{1}{4} \times 4 = 1$$

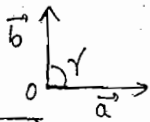
For Non-primitive → Angle/360°

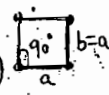


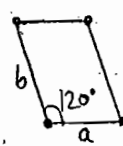


Non-primitive unit cell



Types of lattice in 2-dim. To define a lattice \vec{a} , \vec{b} & γ .

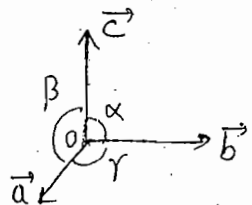


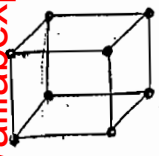
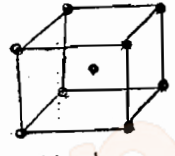
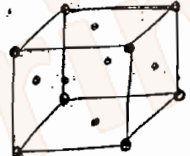
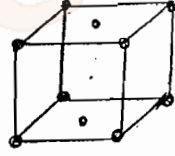
Crystal Structure	Lattice	Condition
1. Square	1. Square (primitive) 	$a = b, \gamma = 90^\circ$
2. Rectangular	2. Rectangular Primitive  3. Rectangular Centred 	$a \neq b, \gamma \neq 90^\circ$
3. Hexagonal	4. Hexagonal primitive 	$a = b, \gamma = 120^\circ$
4. Oblique	5. Oblique primitive	$a \neq b, \gamma \neq 90^\circ$

In 2 dim, there are 5 types of lattice (Bravais) & 4 types of crystal structure.

Here square, rectangle & Hexagonal are the special cases of Oblique.

Types of lattice in 3 dim. :-
(simple means primitive)



Crystal Structure	Lattice	Conditions
1. Cubic	1. Simple 2. Body Centred (bcc) 3. Face Centred (fcc)	$a=b=c,$ $\alpha=\beta=\gamma=90^\circ$
2. Tetragonal	4. Simple 5. body centred (bct)	$a=b \neq c,$ $\alpha=\beta=\gamma=90^\circ$
3. Orthorhombic	6. Simple 7. body centred 8. face " 9. Base/end centred	$a \neq b \neq c$ $\alpha=\beta=\gamma=90^\circ$
 (Simple)  (body)  (face)  (bace)		
4. Trigonal	10. Simple	$a=b=c, \alpha=\beta=\gamma \neq 90^\circ$
5. Hexagonal	11. Simple	$a=b \neq c, \alpha=\beta=90^\circ$ $\gamma=120^\circ$
6. Monoclinic	12. Simple 13. Base centred	$a \neq b \neq c, \alpha=\beta=90^\circ \neq \gamma$
7. Triclinic	14. Simple	$a \neq b \neq c, \alpha \neq \beta \neq \gamma$

Hence, in 3-Dim, We have 14 crystal structure & 14 space lattices.

Notations :-

- Cubic P → primitive (simple)
- I → body centred
- F → face "
- C → end "

Interplanar Spacing :-

It is denoted as d_{hkl} , $hkl \Rightarrow$ Miller Indices

d is the interplanar spacing i.e. spacing b/w two successive planes.

atoms to form
Layer of crystals called Plane.

Miller Indices → tells the orientation of planes in the crystal.
 d will be different for diff. orientation.

$$d_{hkl} = \frac{1}{\sqrt{\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}}$$



This formula is valid only for Cubic, tetragonal & orthorhombic.

for Cubic crystal,

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

Miller Indices :- To find the orientation of planes in the crystal, miller indices used. They are written as (hkl) .

Note :- In small bracket without commas. $(100) \rightarrow$ Miller indices
But $[1,0,0] \rightarrow$ Position co-ordinate,
Miller Indices is the Identity of planes.

$[hkl] \Rightarrow$ direction indices

$\{hkl\} \Rightarrow$ crystallographic plane without commas.

- $(hkl) \rightarrow$ Miller Indices
- $[hkl] \rightarrow$ direction Indices
- $\{hkl\} \rightarrow$ family of planes
- $\langle hkl \rangle \rightarrow$ family of direction Indices

How to Sketch the M.I.?

$$h : k : l = \frac{a}{OA} : \frac{b}{OB} : \frac{c}{OC}$$

$a \rightarrow$ lattice parameter along x dirⁿ,

$b \rightarrow$ " " " y "

$c \rightarrow$ " " " z "

$OA \rightarrow$ Intercept on a -axis

$OB \rightarrow$ " " b "

$OC \rightarrow$ " " c "

$hkl \rightarrow$ Miller Indices.

Suppose we have a Cubic crystal

If we want to sketch (100) plane

$$h=1, k=0, l=0$$

for (100) plane OB & OC should

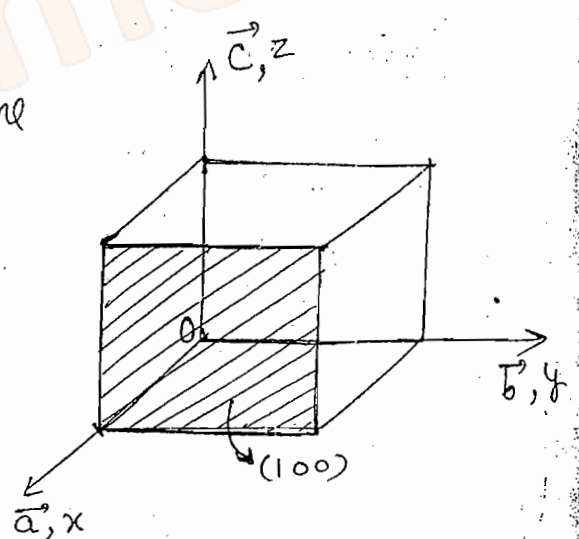
be ∞ . Infinite means

Intercept parallel to that axis.

$$OA \rightarrow a$$

$$OB \rightarrow \infty$$

$$OC \rightarrow \infty$$

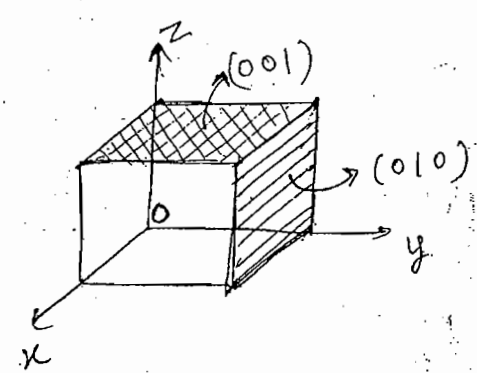


$$(010), \quad h=0, k=1, l=0$$

$$OA \rightarrow \infty, \quad OB \rightarrow a, \quad OC \rightarrow \infty$$

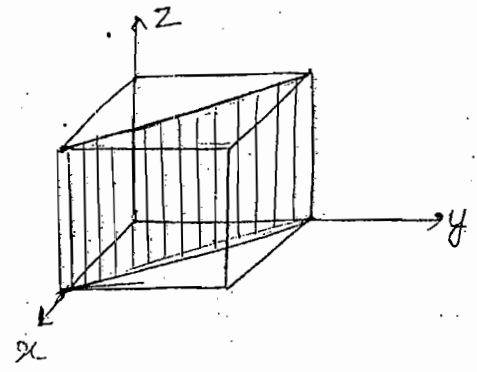
$$(001), \quad h=0, k=0, l=1$$

$$OA \rightarrow \infty, \quad OB \rightarrow \infty, \quad OC \rightarrow a$$



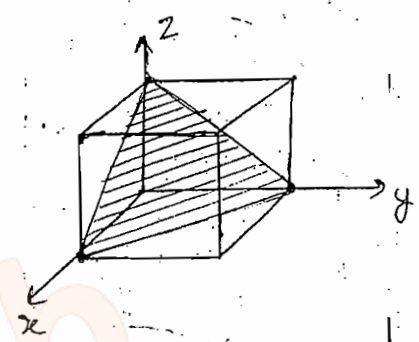
(110)

$h=1, k=1, l=0$
 $OA \rightarrow a, OB \rightarrow a, OC \rightarrow \infty$



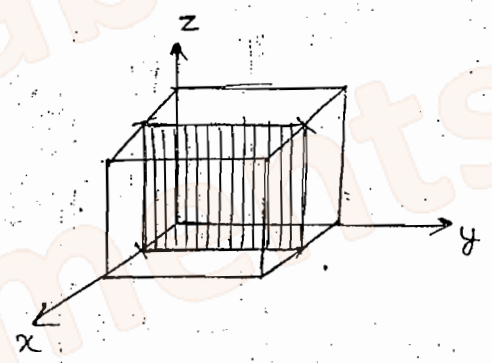
(111)

$h=1, k=1, l=1$
 $OA \rightarrow a, OB \rightarrow a, OC \rightarrow a$



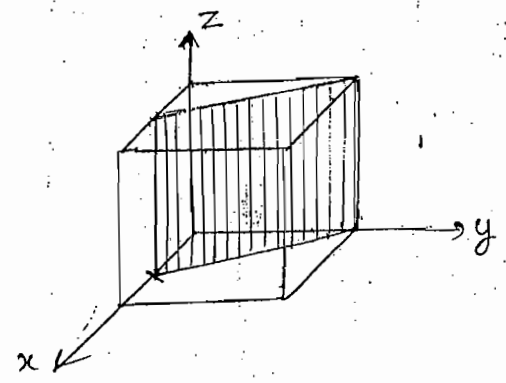
(200)

$h=2, k=0, l=0$
 $OA \rightarrow a/2, OB \rightarrow \infty, OC \rightarrow \infty$
 $OA:OB:OC = \frac{a}{h} : \frac{b}{k} : \frac{c}{l}$
 $OA:OB:OC = \frac{a}{2} : \infty : \infty$



(210)

$h=2, k=1, l=0$
 $OA:OB:OC = \frac{a}{h} : \frac{b}{k} : \frac{c}{l}$
 $= \frac{a}{2} : b : \infty$



Note :- Parallel ~~Plates~~ planes have same miller - indices

Negative Sketch :-

If h is -1 then it is repⁿ as $\bar{1}$
 i.e. eg. $(\bar{1}00)$

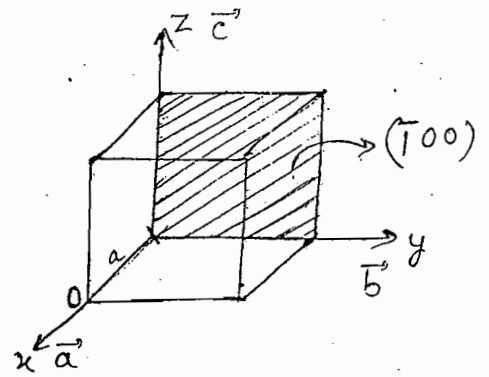
($\bar{1}00$)

$h = -1, k = 0, l = 0$

OA = -a i.e. intercept on -ve axis.

To draw this shift the origin.

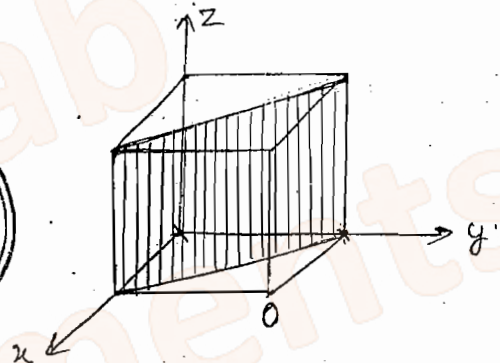
d_{hkl} will be same for (100) & ($\bar{1}00$) planes.



$$d_{hkl} = \frac{a}{\sqrt{(1)^2 + (0)^2 + (0)^2}} = \frac{a}{\sqrt{(-1)^2 + (0)^2 + (0)^2}} = a$$

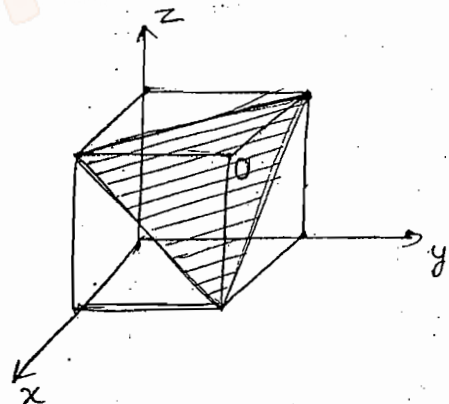
($\bar{1}\bar{1}0$)

$h = -1, k = -1, l = 0$

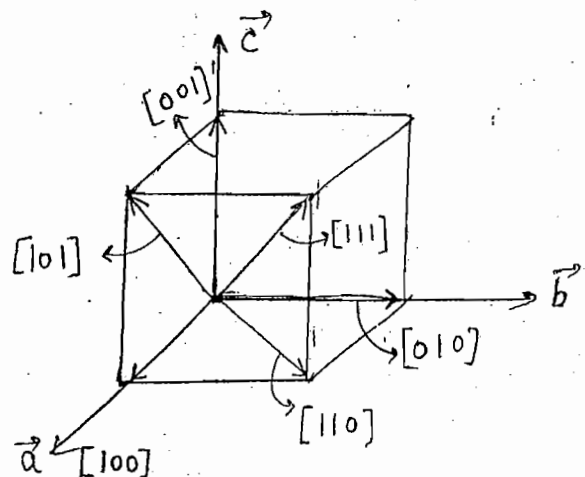


($\bar{1}\bar{1}\bar{1}$)

$h = -1, k = -1, l = -1$



Direction Indices :-



<https://alllabexperiments.com>

Family of planes :-

{100} means family of planes (100) (100)
(010) (010)
(001) (001)

Family of direction Indices

<100> means family of [100] [100]
[010] [010]
[001] [001]

Ques. 1:- Find the Miller indices of a plane that makes intercepts on \vec{a} , \vec{b} & \vec{c} axis equal to 3\AA , 4\AA & 3\AA in a tetragonal crystal with $\frac{c}{a} = 1.5$.

$$OA : OB : OC = 3\text{\AA} : 4\text{\AA} : 3\text{\AA}$$
$$\frac{c}{a} = 1.5$$

for tetragonal, $a = b \neq c$

$$\therefore b = a, c = 1.5a$$

$$h : k : l = \frac{a}{OA} : \frac{b}{OB} : \frac{c}{OC}$$
$$= \frac{a}{3\text{\AA}} : \frac{a}{4\text{\AA}} : \frac{1.5a}{3\text{\AA}} = \frac{1}{3} : \frac{1}{4} : \frac{1}{2}$$
$$= 4 : 3 : 6$$

$$(hkl) \equiv (436) \quad \underline{Ae}$$



Q.2:- Determine M.I. of the plane that makes intercepts of 2\AA , 3\AA , 4\AA on the co-ordinate axis of orthorhombic crystal with $a : b : c = 4 : 3 : 2$.

for orthorhombic, $a \neq b \neq c$

$$OA:OB:OC = 2:3:4 \quad (A)$$

$$h:k:l = \frac{a}{OA} : \frac{b}{OB} : \frac{c}{OC}$$

$$= \frac{4}{2} : \frac{3}{3} : \frac{2}{4}$$

$$= 2:1:\frac{1}{2} = 4:2:1$$

$$(hkl) \equiv (421) \quad \text{Ans}$$

Q.3:- A plane makes intercepts of 1 & 2 Å on \vec{a} & \vec{b} axis respectively but parallel to \vec{c} axis. find M.I. if $a:b:c = 3:2:1$.

$$OA:OB:OC = 1\text{Å} : 2\text{Å} : \infty$$

$$h:k:l = \frac{a}{OA} : \frac{b}{OB} : \frac{c}{OC}$$

$$= \frac{3}{1\text{Å}} : \frac{2}{2\text{Å}} : \frac{1}{\infty}$$

$$= 3:1:0$$

$$(hkl) \equiv (310) \quad \text{Ans}$$



https://alllabexperiments.com

Relation between Lattice Parameters & Mass density of a Cubic Crystal:-

Lattice parameter \rightarrow sides of the unit cell.
This is valid only for cubic crystal.

$$a = \left(\frac{n M_A}{N_A \rho_m} \right)^{1/3}$$

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

$M_A \rightarrow$ atomic mass / atomic weight

$N_A \rightarrow$ Avogadro No.

$\rho_m \rightarrow$ Mass density / specific gravity / Relative density

$a \rightarrow$ Lattice parameter of a cubic crystal.

If M_A is given in amu. (e.g. $Cl \rightarrow 35 \text{ amu}$) so to change it in gm or kgm, multiply by ~~kgm~~ Avogadro no.

Unit $\rightarrow \text{kg/m}^3 - \text{gm/cm}^3$

\downarrow \downarrow Avogadro no. used
 $N_A = 6.023 \times 10^{26}$ $N = 6.023 \times 10^{23}$
 \downarrow \downarrow
 Unit of a \rightarrow m cm

\rightarrow Volume of the unit cell, $a^3 = \left(\frac{n M_A}{N_A \rho_m} \right)$ Imp

No. of atoms/unit volume, $\frac{n}{a^3} = \frac{N_A \rho_m}{M_A}$

This is called, No. density / Atomic density / Atomic concentration

\Rightarrow R.H.S. is valid for all the crystals.
L.H.S. is valid only for cubic crystal

Mass density / Relative density / specific gravity is Unitless.

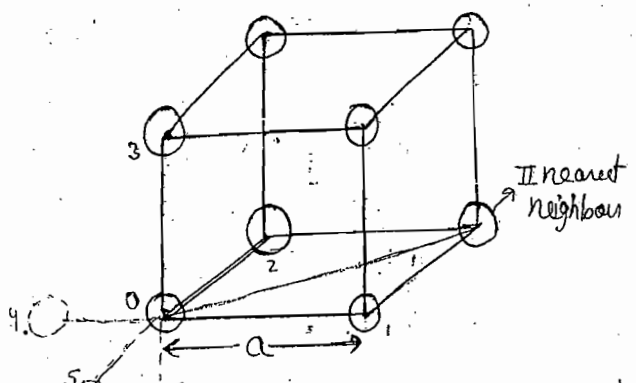
$\rho_m \rightarrow$ Mass density of particular type of crystal w.r. to water.

e.g. $Cu \rightarrow 8.96$ then $\frac{8.96 \text{ gm/cm}^3}{1 \text{ gm/cm}^3} = 8.96$ (unit-less)



Crystal Structures :-

(i) Simple Cubic (primitive Cubic) :- There is only 1 atom is placed at each ~~corner~~ lattice point.



bond length :- nearest neighbour distance (inter nuclear distance)

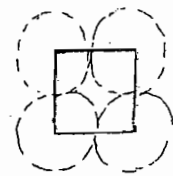
∞

In s.c., all the atoms are of same type so radius is same.

Co-ordination No. \rightarrow No. of atoms with which one atom form bond.

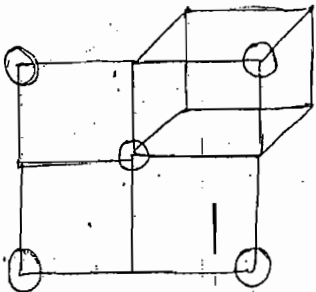
(4) Nearest Neighbour distance

$$2r = a$$



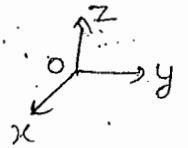
5) 2nd or next nearest Neighbour distance $\Rightarrow \sqrt{2}a$

6) No. of 2nd nearest neighbour = 12



This is y-z plane having 4 2nd near neighbour
 11ly x-z " " 4
 x-y " " 4

(Body diagonal of a cube $\rightarrow \sqrt{3}a$)



7) Volume of unit cell = a^3

8) " " primitive unit cell = a^3
 of S.C.

\Rightarrow If Co-ordination no. < 12 or A.P.F No. $< 74\%$, then it is loosely packed crystal.

2) calculation of A.P.F. :-

$$A.P.F. = \frac{\text{Volume of the atoms in unit cell}}{\text{Volume of the unit cell}}$$

A.P.F. \rightarrow show how much fraction of unit cell is filled with atoms

$$APF = \frac{1 \times \frac{4}{3} \pi r^3}{a^3} \quad (a=2r)$$

$$= \frac{\frac{4}{3} \pi r^3}{8 r^3} = \frac{\pi}{6} = 0.52 = 52\%$$

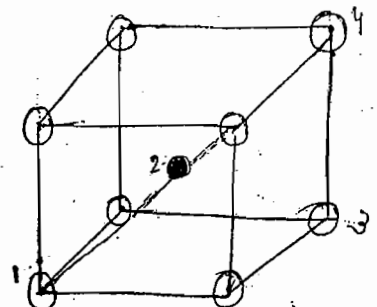
i.e. 52% part of crystal is occupied by atoms & 48% part is empty.

Body Centred Cubic (bcc) :-

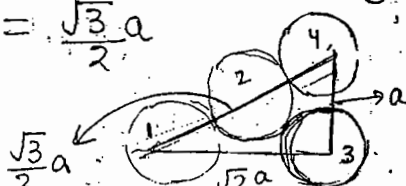
Atoms at corner & 1 atom at body centred position.

3) No. of nearest neighbour = 8
 (Taking \bullet as reference)

4) Nearest Neighbour distance \Rightarrow
 $2r = \frac{\sqrt{3}a}{2}$

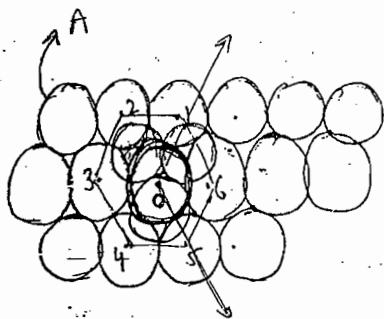


for centre atom \rightarrow nearest neighbour are all the 8 atoms



Property	SC	bcc	fcc	hcp	dc	ZnS
(i) type of unit cell	primitive	Non-Primitive	Non-primitive	Non-primitive	Non-primitive	
(ii) No. of atom/unit cell	$\frac{1}{8} \times 8 = 1$	$\frac{1}{8} \times 8 + 1 = 2$	4	6	8	
(iii) No. of nearest neighbour (co-ordination no.)	6	8	12	12	4	
(iv) Nearest Neighbour distance	a	$\frac{\sqrt{3}}{2}a$	$\frac{a}{\sqrt{2}}$	a	$\frac{\sqrt{3}a}{4}$	$\frac{a}{\sqrt{2}}$
(v) 2nd nearest Neighbour distance	$\sqrt{2}a$	a	a	c	$\frac{a}{\sqrt{2}}$	
(vi) No. of 1st Nearest N.	12	6	6	2	12	
(vii) Volume of unit cell	a^3	a^3	a^3	$\frac{3\sqrt{3}}{2}a^2c$	a^3	
(viii) Vol. of primitive unit cell	a^3	$a^3/2$	$a^3/4$	$\frac{\sqrt{3}}{2}a^2c$	$a^3/4$	
(ix) No. of atom/unit cell	$1/a^3$	$2/a^3$	$4/a^3$	$\frac{4}{\sqrt{3}} \frac{a^2c}{a^3}$	$8/a^3$	
(x) Atomic Radius	$a/2$	$\frac{\sqrt{3}}{4}a$	$\frac{a}{2\sqrt{2}}$	$\frac{a}{2}$	$\frac{\sqrt{3}}{8}a$	
(xi) type of packing	loose packed	loose	close packed	closed	loose	
(xii) Atomic Packing factor (fraction)	52% or 0.52 or $\frac{\pi}{6}$	68% or $\frac{\sqrt{3}\pi}{8}$	74% or $\frac{\pi}{3\sqrt{2}}$	74% or $\frac{\pi}{3\sqrt{2}}$	34% or $\frac{\sqrt{3}\pi}{16}$	$\neq 34\%$
(xiii) Example	Polonium	Na, K, Li	Cu, Ag, Au, Al	Mg, Zn, Cd	Diamond, Si, Ge, Sn	CrAs, Cds, InSb

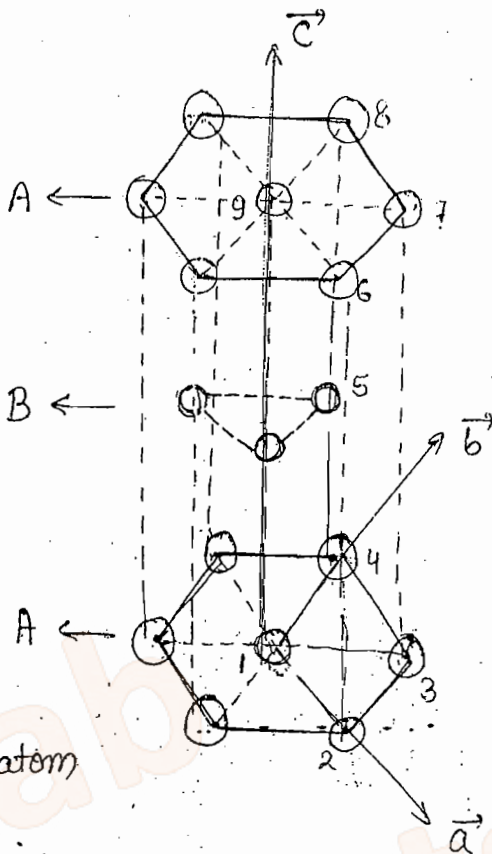
in 1D, e^- concentration is $1/a$ for bcc, fcc, sc-etc.



Centre atom o is touching 6 atoms. If we fall ~~on~~ ball on layer then it will stay on voids.

It is not possible to put atom on each void.

So we have to put atom on alternate void, we get layer B, now void will be at the centre of atom of layer A.



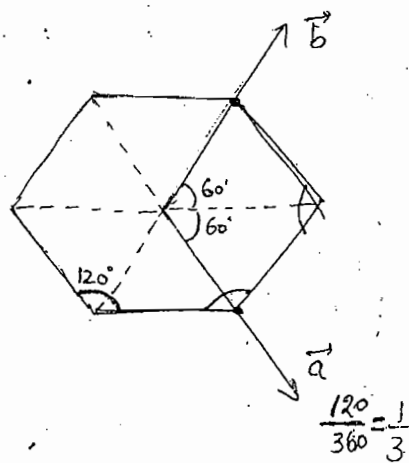
So Hexagonal close structure is ABAB... type in plane, each atom must have 6 atom surrounding. atoms of B layer touches the centre atom of layer A.

CC → FCC is ABC ABC ABC ... type of structure

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

c is called height of unit cell.

$\alpha \rightarrow$ \angle b/w \vec{b} & \vec{c}



1) Non primitive

2) No. of atoms per unit cell $\left\{ \frac{1}{3} \text{ part of } \frac{1}{2} \right\} = \frac{1}{6}$

Corner atoms of layer A = $\frac{1}{6} \times 12 = 2$

Centre atoms is not shared by the atoms above = $\frac{1}{2} \times 2$

3 atoms of layer B will contribute full = $3 \times 1 = 3$

So **total atom per unit cell = 6**

The atoms placed at the void will never coincide at the centre of others so their contribution will be complete.

3) Co-ordination No. \rightarrow If centre atom is reference atom then
 $= 12$

4) Nearest Neighbour distance $2r = a$ but $a \neq c$
 $a \rightarrow$ lattice parameter

5) 2nd nearest neighbour distance $= c$ (height of unit cell)

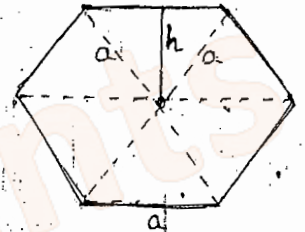
for An Ideal hcp hcp is $\boxed{\frac{c}{a} = \frac{\sqrt{8}}{\sqrt{3}} = 1.633}$

6) No. of II nearest neighbours $= 2$

7) Volume of unit cell $=$ (Area of base part) \times height

The base plane is made up of 6 equilateral triangle.

$$\begin{aligned} \Delta &= \frac{1}{2} \text{Base} \times \text{height} \\ &= \frac{1}{2} a \times \frac{\sqrt{3}a}{2} \\ &= \frac{\sqrt{3}a^2}{4} \end{aligned}$$



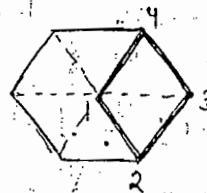
There are 6 triangles do

$$\begin{aligned} \text{Area of 6 equilateral } \Delta &= 6 \times \frac{\sqrt{3}a^2}{4} \\ &= \frac{3\sqrt{3}a^2}{2} \end{aligned}$$

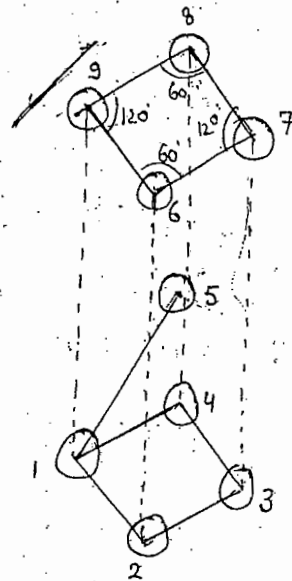
$$h^2 = a^2 - \frac{a^2}{4} = \frac{3a^2}{4}$$

$$\text{Volume of unit cell} = \frac{3\sqrt{3}a^2}{2} \times c = \frac{3\sqrt{3}a^2c}{2}$$

8) volume of primitive unit cell \rightarrow will be $\frac{1}{3}$ of conventional unit cell.



9) Here no. of atoms in a primitive unit cell $= 2$



\therefore Here we have 2 atom basis.

$$\begin{aligned} \left\{ \begin{array}{l} \text{No. of atoms/unit cell} \\ \text{primitive} \end{array} \right. &= \left(\frac{1}{3} \times \frac{1}{2} \right) \times 4 + \left(\frac{1}{2} \times \frac{1}{6} \right) \times 4 \\ &= \frac{1}{6} \times 4 + \frac{1}{12} \times 4 = 1 \end{aligned}$$

Note:- No. of nearest neighbours can never be greater than 12.

$$10) \text{ No. of atoms / unit cell} = \frac{3\sqrt{3}a^2c}{2} \rightarrow \frac{6}{\frac{3\sqrt{3}a^2c}{2}}$$

$$= 8 \cdot \frac{4}{\sqrt{3}a^2c}$$

11) Atomic radius $r = \frac{a}{2}$

12) Type of packing closed

13) Ex - Mg, Zn, Cd etc.

→ Mostly metals have fcc or hcp structure.

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

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

$$= \frac{\pi}{3\sqrt{2}} = 0.74 = 74\%$$

$(a = 2r)$



i.e. Packing fraction of hcp & fcc is same.

Dimond Cubic (dc) :-

This is not a bravias lattice.

It is made by ^{combi.} 2 or more bravias lattices.

Dimond Cubic can be considered as interpenetration of two fcc lattices - 1 is at the position $(0, 0, 0)$ & other is at the position $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$

Dimond has dimond cubic structure.

dimond is made up by atoms of Carbon.

— Place 1 fcc, atom at $(0, 0, 0)$

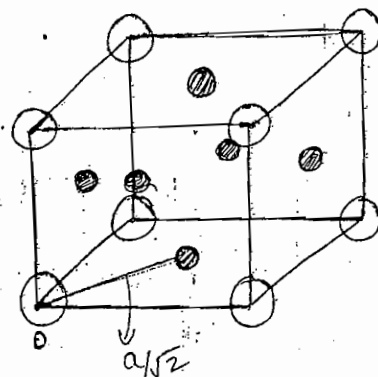
1) Non-primitive

2) No. of atom/unit cell =

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

3) Coordination No. :- 4.

Each C-atom is coordinated to 4 C-atoms.



lesser the coordination no., structure will be loosely pack

4) Nearest neighbour distance = $\frac{\sqrt{3}}{4} a$ i.e. $2r = \frac{\sqrt{3}}{4} a$ { Body diagonals of (000) atom I in $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ & II }

5) Ind " " " = $a/\sqrt{2}$

6) Ind No. of Ind N-N. = 12.

(if 0 is ref. atom then its N.N. atom will be its face centred atom)

7) Vol. of unit cell = a^3

8) Vol. of primitive unit cell = $a^3/4$

diamond cubic is fcc with 2 atom basis.

No. of atoms in primitive unit cell of dc = 2

9) No. of atoms/unit vol = $\frac{8}{a^3}$ (8 atoms in a^3 volume)

10) Atomic Radius $r = \frac{\sqrt{3}}{8} a$



11) Type of packing → loose

Diamond is Insulator → Each C atom is co-ordinated by 4 nearby

C-atom so it'll make 4 covalent bonds. Because No free e^- per C-atom is free. [C → outer shell has 4 e^-] so it is insulator

But it is Electrically Insulator. coz 4 e^- are tightly bound. It is good heat conductor. Structure of S/c & insulator of same only diff. in band gap.

Ex - Si, Ge, diamond, Sn etc.

band gap → 5 to 6 eV

$$\text{APF} = 0.34 \text{ or } 34\% \text{ or } \frac{\sqrt{3}\pi}{16}$$

$$a = \frac{8}{\sqrt{3}} r$$

$$\text{APF} = \frac{8 \times \frac{4}{3} \pi r^3}{a^3} = \frac{8 \times 4 \pi r^3}{3 \left(\frac{8}{\sqrt{3}}\right)^3 r^3}$$

$$= \frac{8 \times 4 \times \pi \times \cancel{8} \times \sqrt{3}}{\cancel{8} \times \cancel{8} \times \cancel{8} \times \cancel{8}} = \frac{\sqrt{3}\pi}{16} = 0.34 = 34\%$$



Zinc Blende Structure (ZnS) :-

This is similar to diamond cubic structure except two interpenetrating lattices have different atoms. If 1st lattice or unit cell is made from Zn atoms then 2nd unit cell is made from sulphide atoms.

If Zn occupies the fcc position then

S " " Tetrahedral " or vice versa.

ZnS is not a atomic structure. It is a molecular structure.

In this case nearest neighbour distance = $r_{zn} + r_s$

In a unit cell \rightarrow 4 Zn atom & 4 S atom

$$\text{APF} = \frac{4 \times \left(\frac{4}{3} \pi r_{zn}^3 + \frac{4}{3} \pi r_s^3 \right)}{a^3}$$

$$a = \frac{4}{\sqrt{3}} (r_{zn} + r_s)$$

$$= \frac{4 \times \frac{4}{3} \pi r_{zn}^3 + 4 \times \frac{4}{3} \pi r_s^3}{\left(\frac{4}{\sqrt{3}}\right)^3 (r_{zn} + r_s)^3}$$

$$= \frac{r_s^3 \left(1 + \frac{r_{zn}^3}{r_s^3} \right)}{r_s^3 \left(1 + \frac{r_{zn}}{r_s} \right)^3}$$

To calculate APF, we should know the ratio $\frac{r_{zn}}{r_s}$

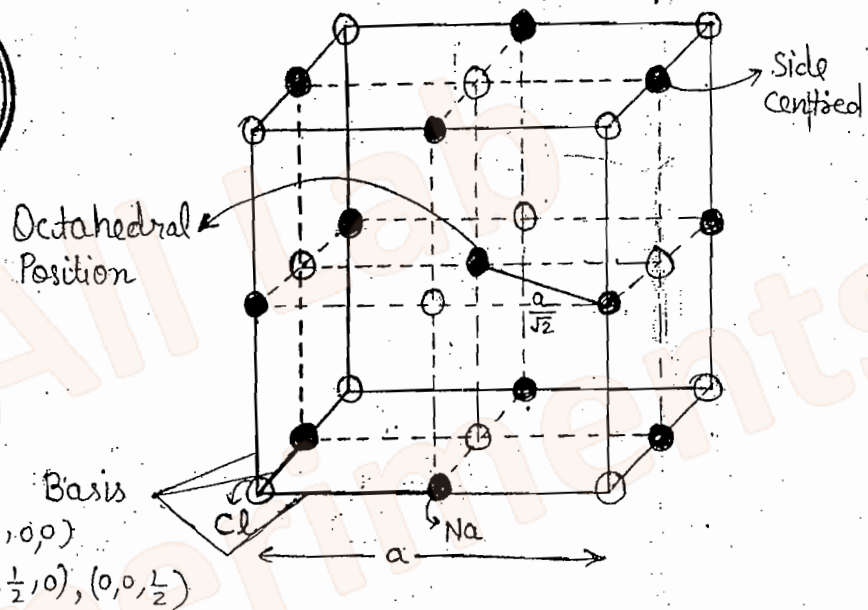
So APF of ZnS \neq 34% exactly.

Ex - GaAs, CdS, InSb etc.

https://allabexperiments.com

Sodium Chloride (NaCl) / Rock Salt :-

This is made up by 2 fcc crystals so NaCl can be considered as two interpenetrating fcc's. One lattice occupying the Na atoms & other occupying the Cl atom such that if one has the origin at $(0,0,0)$ then other has origin at $(\frac{a}{2}, 0, 0)$ or $(0, \frac{a}{2}, 0)$ or $(0, 0, \frac{a}{2})$



If Na atoms occupy the octahedral position, Cl occupies the fcc position.

- 1) Non-primitive
- 2) No. of atoms/unit cell

Total contribution of Cl $\rightarrow 8 \times \frac{1}{8} + 3 = 4$

" " Na $\rightarrow \frac{1}{4} \times 12 + 1 = 3 + 1 = 4$

\downarrow side centred \downarrow centre

$4 \text{ Cl} + 4 \text{ Na}$

This is a molecular crystal structure.

- 3) Co-ordination no. (nearest neighbour)

Nearest neighbour of Na \rightarrow Cl
 \therefore Co-ordination no. = 6

4) Nearest neighbour distance

$$r_{Na} + r_{Cl} = \frac{a}{2}$$

5) IInd nearest neighbour

for centre atom, all black atoms are II n.n.

for Na → II n.n are Na atoms.

& " Cl → " " Cl "

So II nearest neighbour = 12

6) II " " distance = $\frac{a}{\sqrt{2}}$

7) Volume of unit cell = a^3

Volume of primitive unit cell = $\frac{a^3}{4}$

No. of atoms in primitive unit cell :-

at 1 lattice, there is 1 Na & 1 Cl atom placed.

NaCl is fcc with 2 atom basis, 1 is Na atom + 1 Cl

Molecular density = $\frac{4}{a^3}$

Type of packing = loose ($6 < 12$)

13) APF → can't be calculated exactly.

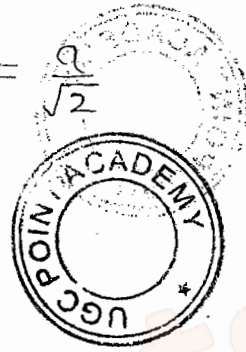
Ex- KCl, KBr, AgBr etc.

All the alkali halides & silver halides have NaCl structure.
(NaCl, KCl, NaBr, KBr, NaI, KI)

Caesium chloride (CsCl) :-

LiCl, RbCl, CsCl crystallises in CsCl structure.

CsCl crystal can be considered as 2 interpenetrating simple cubic lattices. One has the atoms of Cs & other has the atoms of Cl. The origin of one lattice is at (0, 0, 0) & other has origin at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$.



- 1) Non-primitive
- 2) No. of atoms/unit cell

$$\text{Cs} \rightarrow \frac{1}{8} \times 8 = 1$$

$$\text{Cl} \rightarrow 1$$

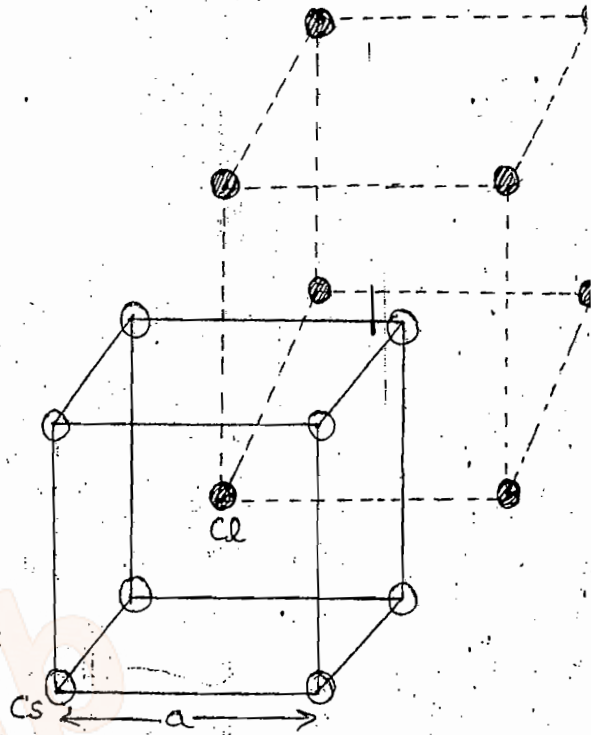
i.e. $1 \text{ Cs} + 1 \text{ Cl} = 1 \text{ CsCl molecule}$

- 3) Co-ordination no.
or nearest neighbour = 8

- 4) I Nearest Neighbour distance = a

- 5) II Nearest Neighbour distance =

$$r_{\text{Cs}} + r_{\text{Cl}} = \frac{\sqrt{3}a}{2}$$



(This is not bcc becoz in bcc centre atom is same but here it is different)

- 6) II nearest neighbour = 6

- 7) Volume of unit cell = a^3

- 8) Vol. of primitive unit cell = a^3

∅ Basis is 2 atom basis $\rightarrow 1 \text{ Cs} \& 1 \text{ Cl}$

- 9) Molecular density = $\frac{1}{a^3}$ ($a^3 \rightarrow 1$)

- 10) Packing \rightarrow loose

- 11) Ex - CsCl, RbCl, CsBr, LiHg

- 12) APF \rightarrow can not find until $r_{\text{Cs}}/r_{\text{Cl}}$ ratio is not known



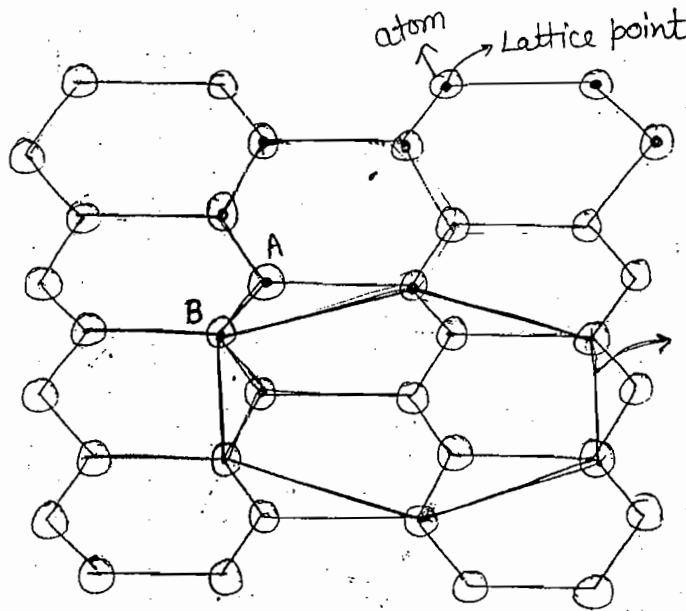
Graphene :-

Graphite structure is made up of graphene layers.

Graphene has Honey comb structure. Carbon atoms are arranged in the honeycomb structure.

In 2-D - One C-atom is shared by 3 nearby C-atoms. This is the Graphite structure in 2-dim.

In 3-D - One C-atom is shared by 6 nearby C-atoms.



Graphite structure is layered structure but graphene is a single layer structure (single layer of carbon atom). Graphite is Conductor \rightarrow per C-atom, $1 e^-$ is free.

If consider, lattice point on each atom position then it will not form a basis becoz surroundings of A & B are different.

Only A-A atoms or B-B atoms can form basis as they have same surrounding.

So Either connect nearby A-A atoms or B-B atoms.

This hexagon (red) is the unit cell of graphene.

1) This unit cell is non-primitive

2) No. of atoms/unit cell

corners atoms $\rightarrow \frac{1}{3} \times 6 = 2$
 inside $\rightarrow 1 \times 4 = 4$

Total no. of atoms/unit cell = 6

side of unit cell \rightarrow lattice parameter / lattice vector, (a)

All the sides will be same.

Lattice parameter $\rightarrow a$

<https://alllabexperiments.com>

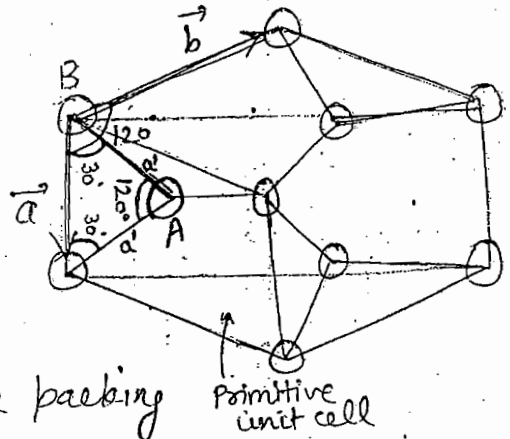
$$|\vec{a}| = |\vec{b}| \neq a, \gamma = 120^\circ$$

3) Nearest Neighbour distance

$$2r = a' = \frac{a}{\sqrt{3}}$$

4) No. of nearest neighbour
= 3

In 2-D, there will be close packing if No. of N.N. are 6 but here 3 so packing will be loose.



5) 2nd nearest N. distance = a

6) No. of 2nd N.N. = 6

$$7) \text{ Area of } \Delta = \frac{1}{2} \times \sqrt{3}a \times \frac{a}{2} = \frac{\sqrt{3}a^2}{4}$$

$$\text{Area of } 2 \Delta = \frac{\sqrt{3}a^2}{2}$$

$$\text{Total Area of unit cell} = \sqrt{3}a^2 + \frac{\sqrt{3}a^2}{2} = \sqrt{3}\left(1 + \frac{1}{2}\right)a^2 = \frac{3\sqrt{3}a^2}{2}$$

8) Area of primitive unit cell = $\frac{1}{3} \times \text{area of unit cell}$

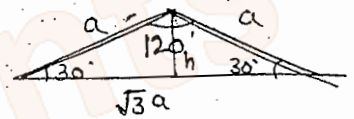
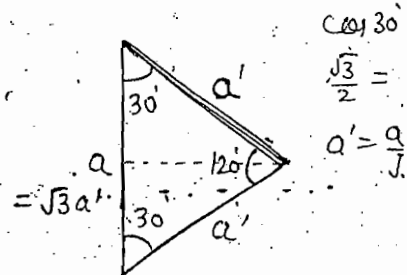
$$= \frac{1}{3} \left(\frac{3\sqrt{3}}{2} \right) a^2$$

$$= \frac{\sqrt{3}a^2}{2}$$

9) No. of atom/primitive unit cell = 1 + 1 = 2

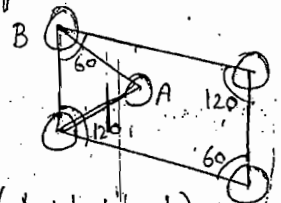
So 2 atoms of graphite inside the primitive cell. So 2 atom basis. (ie. at one lattice point, one atom of A type & one of B type)

In conventional unit cell \rightarrow basis can't be defined



$$h^2 = a^2 - \frac{3}{4}a^2 = \frac{1}{4}a^2$$

$$h = a/2$$



$$\left(\frac{1}{6} + \frac{1}{3} + \frac{1}{3} + \frac{1}{6}\right) = 1$$

1 \rightarrow due to corner
1 \rightarrow centre

10) No. of atom/unit area = $\frac{3\sqrt{3}a^2}{2} \rightarrow 6$
 $1 \rightarrow \frac{6 \times 2}{3\sqrt{3}a^2} = \frac{4}{\sqrt{3}a^2}$

11) Atomic Radius $r = \frac{a}{2\sqrt{3}}$

12) Type of packing \rightarrow loose

13) Ex \rightarrow Graphene

14) APF = $\frac{\text{area of the atoms in unit cell}}{\text{area of unit cell}}$

= $\frac{6 \times \pi r^2}{\frac{3\sqrt{3}a^2}{2}}$ { consider atoms as disc }
 { $a = 2\sqrt{3}r$ } so area = πr^2

= $\frac{2 \times \pi r^2}{3\sqrt{3} \times 4 \times r^2} = \frac{\pi}{3\sqrt{3}} = 60.4\%$

APF $\approx 60\%$



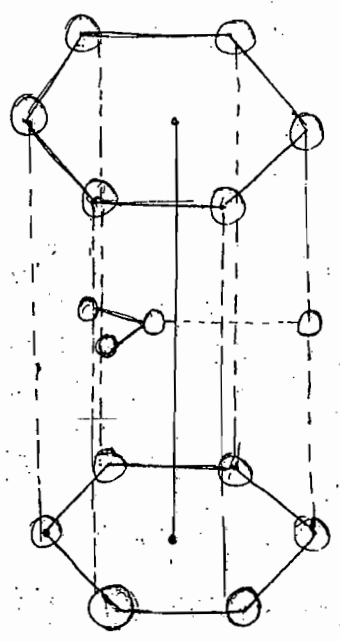
Graphite :- Graphite is a form of Carbon & crystallises in simple hexagonal structure. It contains 4 atoms per primitive unit cell.

No. of atom/unit cell = $\frac{1}{6} \times 12 + \frac{1}{3} \times 3$
 $= 3 + 1 = 4$

height of the unit cell = 4.8 times
 the nearest neighbour distance

Nearest N. distance $\Rightarrow 2r = a$
 $a \rightarrow$ lattice parameter

No. of Nearest N. = 3



https://alllabexperiments.com

1 C-atom can make covalent bond with 3 nearby atoms.
 C-atom of 1 layer can't make bond with C-atom of 2nd layer. That's why graphite sheets slides on each other.
 So Graphite is soft ~~becz~~ layer don't have bonding.

Semiconductors are not conducting at $T=0\text{K}$
 Metals are conducting at $T=0\text{K}$
 Graphite is a semi-metal.

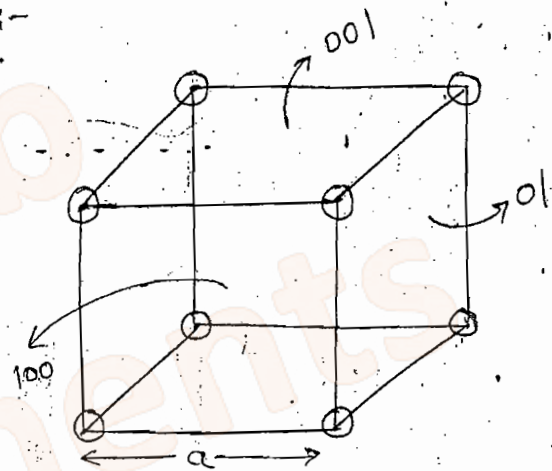
Planes in different Crystals :-

1. Simple Cubic :-

Plane analysis in S.C.

First consider (100) plane

In Planes (010), (001), (100), the properties are same.



No. of atoms on (100) type plane

$$= \frac{1}{4} \times 4 = 1$$

$$\text{Area of plane} = a^2$$

Planner density = no. of atoms per unit area

$$= \frac{1}{a^2} \quad (a^2 \rightarrow 1)$$

for a plane, consider atoms as disc (2d)

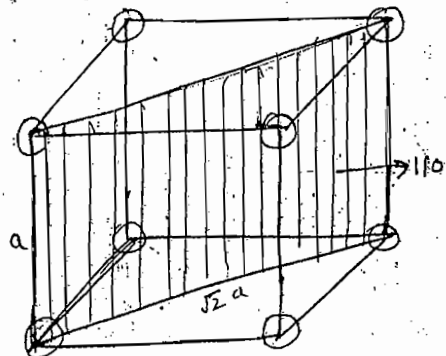
(110) Plane :-

$$\text{No. of atoms} = \frac{1}{2} \times 4 = 2$$

$$\text{Area} = \sqrt{2} a^2$$

$$\text{Planner density} = \frac{1}{\sqrt{2} a^2}$$

Shape \Rightarrow Rectangle



(111) plane :-

No. of atoms = $\frac{1}{8} \times 3 = \frac{1}{2}$

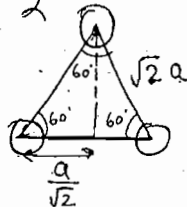
Area = $\frac{1}{2} \times \text{Base} \times \text{height}$

= $\frac{1}{2} (\sqrt{2}a) \sqrt{\frac{3}{2}} a$

= $\frac{\sqrt{3}}{2} a^2$

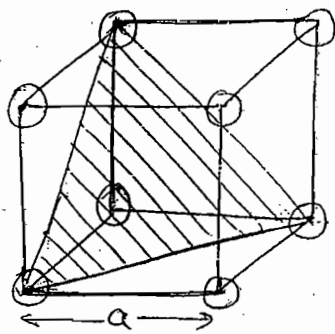
Planer density = $\frac{1}{\sqrt{3} a^2}$

Shape \Rightarrow Triangle



$h^2 = 2a^2 - \frac{a^2}{2}$

$h^2 = \frac{3a^2}{2} \Rightarrow h = \sqrt{\frac{3}{2}} a$



$\frac{60}{360} = \frac{1}{6}$



https://allallexperiments.com

Which plane in S.C. is closed pack plane?

Ans :- Plane having largest Planer density will be closed pack.

(100)

Which direction is closest pack in S.C.?

for 1 Dim \rightarrow atom is considered as a line.
 2 Dim " " " disc.
 3 dim " " " sphere.

Plane having largest line density will be closest pack.

among $[100]_{1/a}$, $[110]_{1/\sqrt{2}a}$, $[111]_{1/\sqrt{3}a}$, $[1\bar{1}0]$

$[100]$ is the closest pack dirⁿ.

(In distance a there are 2 atom ($\frac{1}{2} + \frac{1}{2} = 1$)) (i.e. line density = $\frac{1}{a}$)

B.C.C

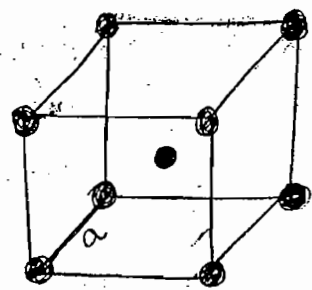
(100) plane :-

No. of atoms = 1
 (no new atom on faces)

Area = a^2

Planer density = $\frac{1}{a^2}$

line " = $\frac{1}{a}$

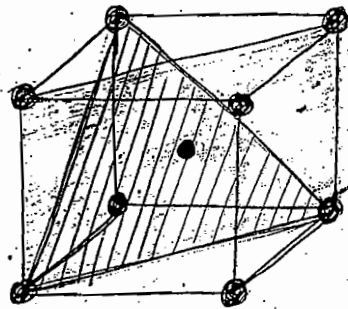


(110) :-

No. of atoms = 2

Area = $\sqrt{2}a^2$

Planner density = $\frac{\sqrt{2}}{a^2}$
line = $\frac{1}{\sqrt{2}a}$



(111) :-

No. of atoms = $\frac{1}{2}$

(body centred atom will not contribute to (111) plane)

Area = $\frac{\sqrt{3}}{2}a^2$

Planner density = $\frac{1}{\sqrt{3}a^2}$, line density = $\frac{2}{\sqrt{3}a}$



* for B.C.C. Closest pack plane is (110)
" " " " direction is [111]

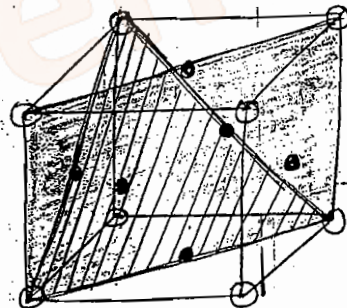


2. F.C.C. :-

(100) plane :-

No. of atoms = $\frac{1}{4} \times 4 + 1$ (corners) (face)
= 2

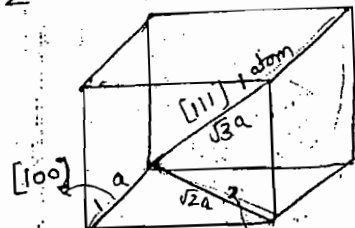
Planner density = $\frac{2}{a^2}$
line = $\frac{1}{a}$



(110) :-

No. of atoms = $\frac{1}{4} \times 4 + \frac{1}{2} \times 2 = 2$

Planner density = $\frac{\sqrt{2}}{a^2}$
line = $\frac{1}{\sqrt{2}a}$



(111) :-

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

Planner density = $\frac{4}{\sqrt{3}a^2}$, line density = $\frac{1}{\sqrt{3}a}$

for F.C.C. Closest pack plane (111)
" " " " direction [110]

Reciprocal Lattice :-

Every crystal is associated with 2 type of lattices :-

- i) direct lattice
- ii) Reciprocal lattice



Need of Reciprocal Lattice :-

In direct lattice, lattice points are arranged according to their position.

In Reciprocal lattice, lattice points are arranged according to their wave vector (\vec{k}) or momentum ($\hbar k$).

Hence direct lattice is defined in position space.
Reciprocal " " " " momentum space or Fourier space.

They are inversely related i.e. position & mom.

are conjugate of each other.

→ direct lattice has the unit of length.

→ Reciprocal " " " " $[\text{length}]^{-1}$

Wave vector is no. of waves per unit wave length.

It tells in which dirⁿ wave is propagating i.e.

$$k = \frac{2\pi}{\lambda}$$

✓ Potⁿ Energy in position space.

✓ K.E. in. Mom. space.

Total Energy is Conserved, i.e. K.E. & P.E. are inversely related. $\{K.E. \downarrow \text{ as much } P.E. \uparrow\}$

If e^- is completely free then it will have K.E. only.

Reasons for need of Rec. Lattice :-

• It is difficult to visualize the crystal plane as order of the plane increases.

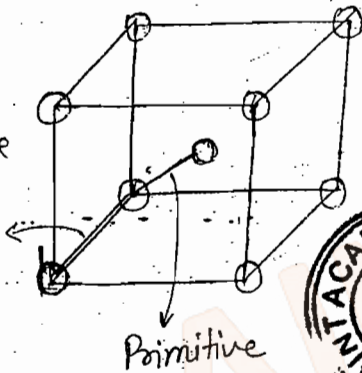
In general

$$\vec{T} = n_1 \vec{a} + n_2 \vec{b} + n_3 \vec{c}$$

It is defining in direct lattice only.

where, a, b, c are Primitive direct lattice vectors.
 bcoz they are joining nearest lattice (points) vectors.
 If they join far lattice points then these vectors will be non-primitive.

B.C.C.



B.C.C. is 1 basis structure.
 Lattice parameter \rightarrow joining 1st and near neighbour.

Here, lattice vector connect non-nearest lattice points. \therefore Non-primitive

Reciprocal lattice, $\vec{A}', \vec{B}', \vec{C}'$ are the primitive Reciprocal lattice vectors.

$$\vec{A}' = \frac{2\pi (\vec{b}' \times \vec{c}')}{\vec{a}' \cdot (\vec{b}' \times \vec{c}')}$$

$$\vec{B}' = \frac{2\pi (\vec{c}' \times \vec{a}')}{\vec{a}' \cdot (\vec{b}' \times \vec{c}')}$$

$$\vec{C}' = \frac{2\pi (\vec{a}' \times \vec{b}')}{\vec{a}' \cdot (\vec{b}' \times \vec{c}')}$$

Reciprocal lattice vector

$$\vec{G}' = h \vec{A}' + k \vec{B}' + l \vec{C}'$$

$$e^{i \vec{G}' \cdot \vec{T}} = 1$$

$$\vec{G}' \cdot \vec{T} = 2\pi n$$

, $n \rightarrow$ some integer

$$n = 0, 1, 2, \dots$$

Reciprocal of S.C. 1-

Primitive lattice vectors,
(as they are joining nearest
lattice vectors)

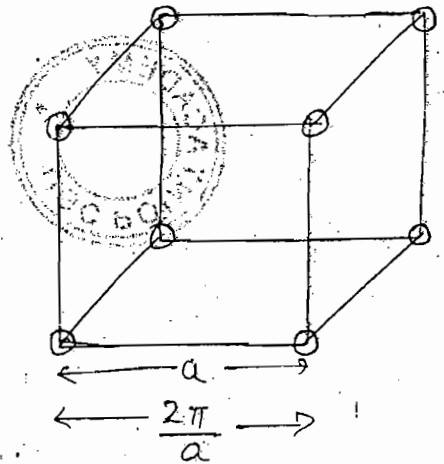
$$\vec{a} = a \hat{i}$$

$$\vec{b} = b \hat{j}$$

$$\vec{c} = c \hat{k}$$



$$\vec{a} \cdot (\vec{b} \times \vec{c}) = a^3$$



for S.C., Volume of primitive unit cell = Volume of
conventional unit cell = a^3

Reciprocal lattice vectors,

$$\vec{A} = \frac{2\pi(\vec{b} \times \vec{c})}{\vec{a} \cdot (\vec{b} \times \vec{c})} = \frac{2\pi a^2}{a^3} \hat{i} \quad (a=b=c)$$

$$= \frac{2\pi}{a} \hat{i}$$

$$\vec{B} = \frac{2\pi}{a} \hat{j}$$

$$\vec{C} = \frac{2\pi}{a} \hat{k}$$

The side of cube in direct lattice $\rightarrow a$
" " " " Reciprocal " $\rightarrow 2\pi/a$

\Rightarrow Reciprocal of S.C. is S.C. with cube side $2\pi/a$. i.e. it
is Self Reciprocal.

\Rightarrow Reciprocal lattice is the first Brillouin Zone.

for S.C., 1 B.Z. is Cube of side $2\pi/a$.

$$\text{Volume of Reciprocal unit cell for S.C.} = \left(\frac{2\pi}{a}\right)^3$$

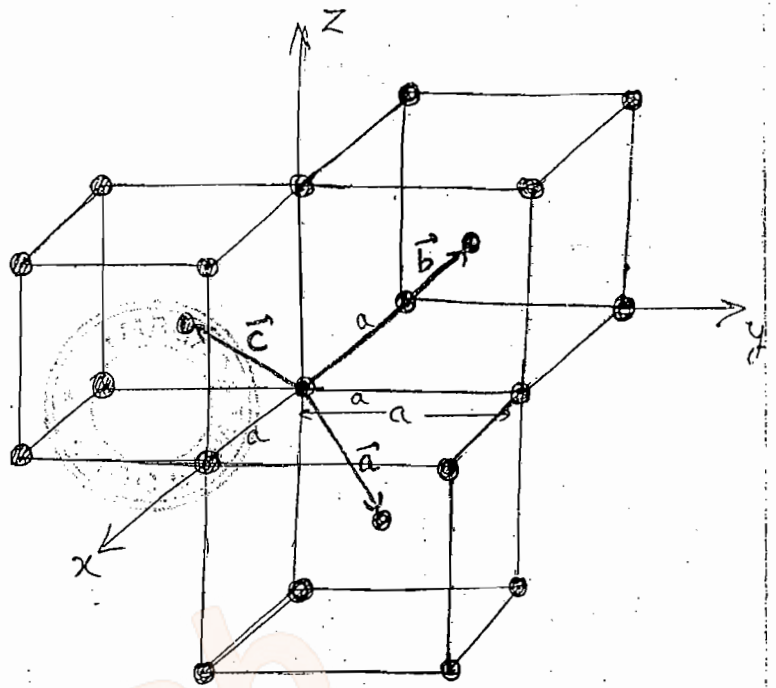
Reciprocal of bcc :-

direct lattice vectors,

$$\vec{a}' = a \hat{i}$$

$$\vec{b}' = b \hat{j}$$

$$\vec{c}' = c \hat{k}$$



Primitive lattice vectors

$$\vec{a} = \frac{a}{2} (\hat{i} + \hat{j} - \hat{k})$$

$$\vec{b} = \frac{a}{2} (-\hat{i} + \hat{j} + \hat{k})$$

$$\vec{c} = \frac{a}{2} (\hat{i} - \hat{j} + \hat{k})$$

$\vec{a} \cdot (\vec{b} \times \vec{c}) \Rightarrow$ Volume of primitive unit cell of bcc.

$$\vec{a} \cdot (\vec{b} \times \vec{c}) = \frac{a^3}{8} \begin{vmatrix} 1 & 1 & -1 \\ -1 & 1 & 1 \\ 1 & -1 & 1 \end{vmatrix} = \frac{a^3}{8} \{ 1(1+1) - 1(-1-1) - 1(1-1) \}$$

$$= \frac{a^3}{8} \times 4 = \frac{a^3}{2}$$

$$\vec{a} \cdot (\vec{b} \times \vec{c}) = \frac{a^3}{2}$$

Reciprocal lattice vectors,

$$\vec{A} = \frac{2\pi (\vec{b} \times \vec{c})}{\vec{a} \cdot (\vec{b} \times \vec{c})} \Rightarrow \vec{A} = \frac{2\pi}{a} (\hat{i} + \hat{j})$$

$$\vec{B} = \frac{2\pi (\vec{c} \times \vec{a})}{\vec{a} \cdot (\vec{b} \times \vec{c})} \Rightarrow \vec{B} = \frac{2\pi}{a} (\hat{j} + \hat{k})$$

$$\vec{C} = \frac{2\pi (\vec{a} \times \vec{b})}{\vec{a} \cdot (\vec{b} \times \vec{c})} \Rightarrow \vec{C} = \frac{2\pi}{a} (\hat{i} + \hat{k})$$

These are the primitive vectors of Reciprocal lattice vectors.

\Rightarrow Reciprocal of bcc is fcc with cube sides $\frac{4\pi}{a}$

Volume of Reciprocal Unit Cell - $\vec{A} \cdot (\vec{B} \times \vec{C})$

$$\vec{A} \cdot (\vec{B} \times \vec{C}) = 2 \left(\frac{2\pi}{a} \right)^3$$

formula $V_R = \frac{(2\pi)^3}{V_d}$



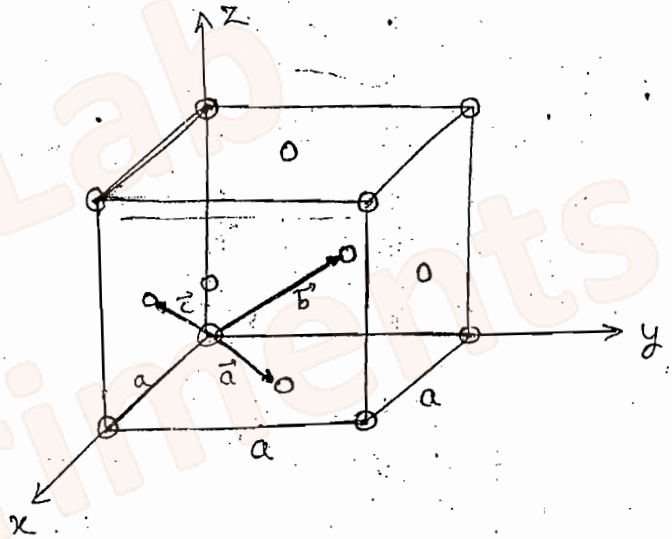
Reciprocal of fcc -

Primitive vectors of fcc,

$$\vec{a} = \frac{a}{2} (\hat{i} + \hat{j})$$

$$\vec{b} = \frac{a}{2} (\hat{j} + \hat{k})$$

$$\vec{c} = \frac{a}{2} (\hat{i} + \hat{k})$$



Volume of direct unit cell,

$$\vec{a} \cdot (\vec{b} \times \vec{c}) = \frac{a^3}{4}$$

$$\vec{A} = \frac{2\pi (\vec{b} \times \vec{c})}{\vec{a} \cdot (\vec{b} \times \vec{c})} \Rightarrow$$

$$\vec{A} = \frac{2\pi}{a} (\hat{i} + \hat{j} - \hat{k})$$

$$\vec{B} = \frac{2\pi}{a} (-\hat{i} + \hat{j} + \hat{k})$$

$$\vec{C} = \frac{2\pi}{a} (\hat{i} - \hat{j} + \hat{k})$$

$$\vec{B} = \frac{2\pi (\vec{c} \times \vec{a})}{\vec{a} \cdot (\vec{b} \times \vec{c})}$$

$$\vec{C} = \frac{2\pi (\vec{a} \times \vec{b})}{\vec{a} \cdot (\vec{b} \times \vec{c})}$$

\Rightarrow Reciprocal of fcc \rightarrow bcc with cube side $\frac{4\pi}{a}$

Volume of Reciprocal unit cell $\Rightarrow V_R = \vec{A} \cdot (\vec{B} \times \vec{C})$

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

Reciprocal of hcp :-

hcp is self reciprocal.



X-Ray diffraction :- (XRD)

X-rays are E.M. waves of very short W.L. $\rightarrow 1 \text{ \AA} \rightarrow 10 \text{ \AA}$

As smaller the W.L., energy will be larger.

$$W.L. \downarrow \Rightarrow E \uparrow$$

So X-rays are very high energy E.M. waves.

Diffraction :- (Bending of X-rays.)

All the longitudinal & transverse waves & sound wave show diffraction. (sound wave \rightarrow not show polarisation)

Bending of X-rays around the corners of an obstacle is called Diffraction.

Condition \rightarrow Size of the aperture or size of the obstacle should be comparable to the W.L. of wave for diffraction to occur.

$$\text{size} \leftrightarrow \lambda$$

In diffraction grating \rightarrow we use n slits.

grating are used for optical light (4000 \AA - 7000 \AA)

i.e. (0.4 μm - 0.7 μm).

- Grating can not diffract X-rays bcoz W.L. of X-ray is very small. & such a fine grating can not be available.
- If we incident some X-ray on crystal then it'll be diffracted from atomic planes. (Crystal is made up by placing atomic planes) (1st plane \rightarrow II \rightarrow so on)
- By One plane $\rightarrow 10^{-3} - 10^{-5}$ th part of X-ray is diffracted. So to diffract X-ray, we need $10^3 - 10^5$ planes.

→ If a detector is placed & path diff. b/w diffracted waves is $\lambda/2$ then detector will detect the Intensity Minima. There will be destructive interference.

→ If path diff. is λ then Constructive Interference & detector will detect Intensity Maxima.

→ If $2d \sin \theta = n\lambda$ condⁿ is satisfied then detector will observe a diffraction peak.

→ For Constructive Interference \Rightarrow Energy \uparrow Intensity \uparrow & Path diff. must be integral multiple of w.l. λ .

Either fix λ & vary θ (use Monochromatic X-ray to fix λ)
or fix θ & vary λ to satisfy the condⁿ

$$2d_{hkl} \sin \theta = n\lambda$$

$$n = 1, 2, 3, \dots$$

So that, d_{hkl} can be calculated & crystal structure can be formed.

This is called Bragg's law.

& n is order of diffraction.



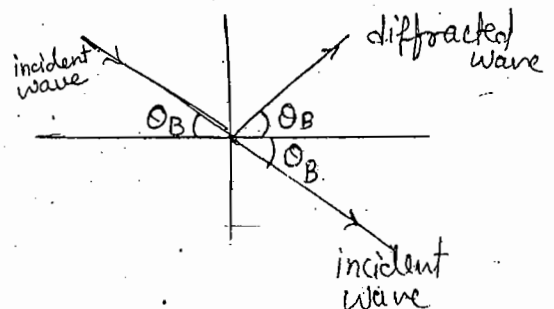
Note :- In Numericals, use 1st order i.e. $n=1$

$$2d \sin \theta = \lambda$$

Diffraction Angle :-

Angle b/w incident wave & diffracted wave.

$$\text{diffraction angle} = 2\theta_B$$
$$\text{Bragg angle} = \theta_B$$



* Bragg's law is consequence of periodicity of lattice

Effect of Stress & Strain on XRD Pattern:-

X-ray diffraction pattern is Intensity v/s diffraction angle.

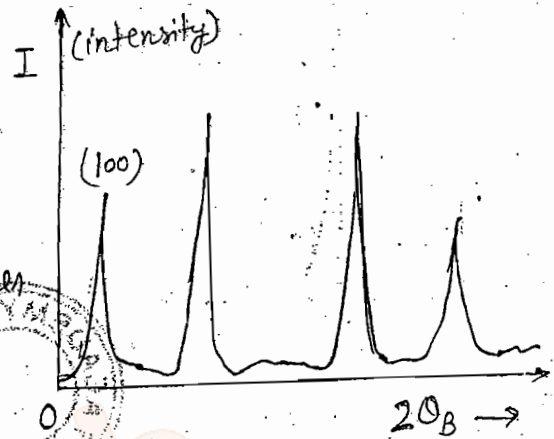
If I is v/s $2\theta_B$ then

$I \uparrow$ & $2\theta_B \downarrow$

$d_{hkl} \downarrow$

θ_B has the limit $\rightarrow 0$ to 90° .

So as diff. angle \uparrow , interplaner spacing $d \downarrow$.



These peaks are the

consequence of Bragg's condⁿ,
 $2d \sin \theta = n\lambda$ when this condⁿ is
 satisfied, we get peaks.

Maximum interplaner spacing is of (100) plane.

$$d_{100} = a$$

\rightarrow If d Max then θ_B should be min. s.t. their product remain constant.

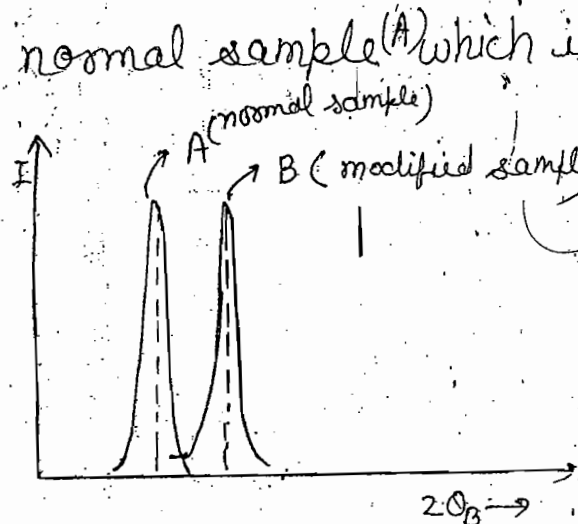
\rightarrow So Here, 1st peak correspond to smallest Bragg angle & largest d_{hkl} .

Indexing of 1st peak \rightarrow (100)

* Suppose we have a peak of normal sample (A) which is unstretched & uncompressed.

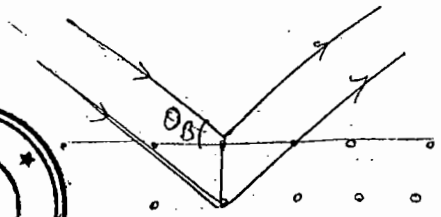
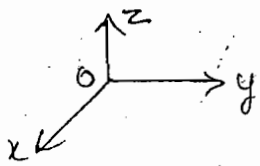
Now if peak is stretched or compress by applying some pressure \rightarrow B

Intensity & shape is same but both peaks have diff. position stretched peak is at different diff. angle.



Which one is correct for above curve ???

- a) Sample β is stretched uniformly in x, y & z dirⁿ
- b) " " compressed " " " " " "
- c) Possibly stretched in z-dirⁿ & compressed in x & y dirⁿ.
(Non-uniform stretch)
- d) " compressed " stretched " " " "



{ $d_{hkl} \uparrow$ & $\theta_B \downarrow$ }

In uniform stress/strain There is No change in the shape of the peak & Intensity.
(or) In Uniform stretching or compression)

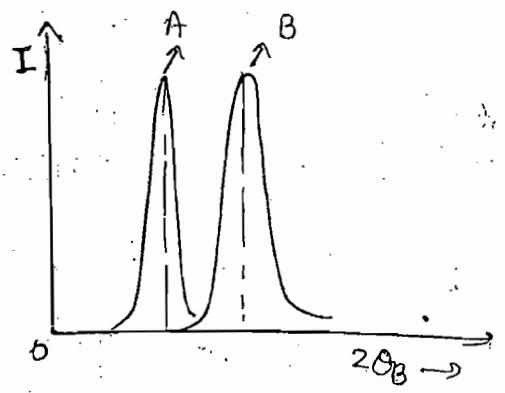
In ~~Non~~ Uniform stress or strain, stretching & compression same in all dirⁿ. In Non-uniform, effects are not same in all dirⁿ.

In this case, there is no change in shape of peak.

uniform & but $\theta \rightarrow$ increase
so $d \rightarrow$ decrease

d is decreasing means Compression, so (b) is correct.

In this case, $d \rightarrow \uparrow$ (shape change)
Modified peak is broad, i.e.
Stress & strain will be
Non-uniform. (iv) is correct

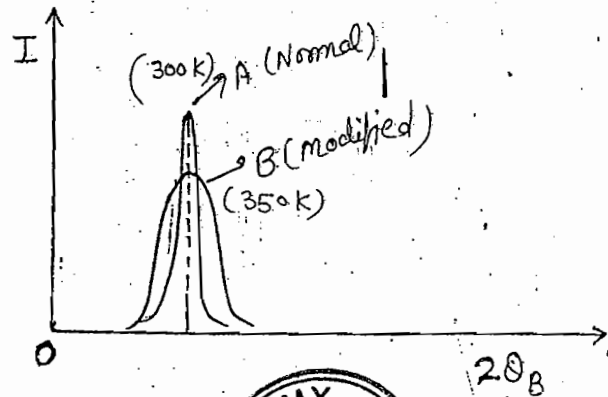


NOTE \rightarrow If peak is shifted towards lower Bragg's angle \Rightarrow stretching.

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Effect of temperature on XRD Pattern:-

Consider normal & modified sample. Maxima of A & B are same i.e. they are lying on same value of $2\theta_B$. There is No stretching & No compression bcoz in stretching & compression θ_B changes.



This is the effect of temperature.

The peak which is broader \Rightarrow having less intensity & should be taken at high temperature.
(position not change)

The atoms of any solid can be considered as harmonic oscillators, bcoz atoms vibrate at their equilibrium position.

$$\begin{aligned} F &\propto x \\ U &\propto x^2 \end{aligned}$$

This S.H.M. is valid only when temp. is not high. bcoz at high temp., vibrations are large & bond will break.

So simple harmonic motion is considered as there is No thermal expansion.

Due to vibration (No thermal expansion), interplanar spacing is not changing, $d \sin \theta \rightarrow$ Not changing then peak is fix. But initially Bragg condⁿ is satisfied for sharp peak & due to vibration, Bragg condⁿ satisfies for a range of diffraction angle.

Effect of temp.

- ① \rightarrow Peak is broadened
- ② \rightarrow Intensity decreases
- ③ \rightarrow Peak position unchanged

- (Diffraction peaks are also called Diffraction lines.)
- On increasing temp, line spacing (distance b/w two peaks) decreases.
 - No. of peaks increases.
 - ↳ Extra peaks in comparison of previous peaks called diffuse lines.

Atomic scattering factor (f) :- It is defined as

$$f = \frac{\text{Amplitude of X-ray scattered by an atom}}{\text{Amplitude of X-ray scattered by an } e^-}$$

Intensity of X-ray peak depending upon 2 factors

- Atomic sca. factor (f)
- geometrical structure factor (S)

$$\text{Intensity} \propto (\text{amplitude})^2$$

- Smallest scattering centre is $\rightarrow e^-$
- X-rays interacting with atoms then amplitude or intensity of diffracted X-ray depends upon how many e^- on each lattice point.

1st depend \rightarrow how many atoms on each lattice points &
then \rightarrow " " e^- s

Amplitude, $F = fS$

$$I \propto F^2 \Rightarrow (\text{amplitude})^2 \Rightarrow I = f^2 S^2$$

e.g. $\begin{matrix} \text{Li} & \& \text{Na} \\ \downarrow & & \downarrow \end{matrix}$

3 e^- on 1 lattice point 11 e^- s

So f will be different for both.



https://alllabexperiments.com

⇒ Intensity depends on f & S also.
 S → how the atoms are arranged.

⇒ If two crystals are of different structure or either have same structure then their intensity is not same.
 If structure is same then f will be diff. [$I \rightarrow S \& f$
 $S \rightarrow$ same but f diff]

⇒ Structure factor :-

$$S = \sum_j e^{2\pi i(u_j h + v_j k + w_j l)}$$

- f is the summation on no. of atoms in unit cell.
- u_j, v_j, w_j are the position co-ordinates of j -th atoms.

Structure factor for S.C. :-

In S.C., there is 1 atom at position $(0,0,0)$

$$S = e^{2\pi i(0h+0k+0l)} = e^0$$

$$S = 1$$

It means, Scattered amp. ⇒ $F = f$

$$(F = fs)$$

& Intensity ⇒ $I = f^2$

Intensity does not depend on h, k, l .
 i.e. " " " on any particular type of plane i.e. same for all planes (all the reflections are allowed) No restriction on h, k, l .

(ii) S for bcc :-

Effective no. of atoms → 2 $\{ (0,0,0) \& (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \}$

$$S = e^{2\pi i(0+0+0)} + e^{2\pi i(\frac{h}{2} + \frac{k}{2} + \frac{l}{2})}$$

$$S = 1 + e^{\pi i(h+k+l)}$$

S is depending on h, k, l i.e. particular type of plane.



So intensity is also depending upon particular type of plane.

1) If $h+k+l = \text{even}$
 $e^{i\pi(h+k+l)} = 1$

So $S = 2 \Rightarrow F = 2f$

2) If $h+k+l = \text{odd}$
 $e^{i\pi(h+k+l)} = -1$

$S = 0 \Rightarrow F = 0$

Intensity $I = f^2 S^2$

$I = 4f^2$ ($h+k+l \rightarrow \text{even}$)
 $I = 0$ ($h+k+l \rightarrow \text{odd}$)



All the reflections to be allowed,
 $(h+k+l)$ should be even

iii) S for fcc

These are 4 atoms at $(0,0,0), (\frac{1}{2}, \frac{1}{2}, 0), (0, \frac{1}{2}, \frac{1}{2}), (\frac{1}{2}, 0, \frac{1}{2})$

$$S = \sum_j e^{2\pi i(u_j h + v_j k + w_j l)}$$

$$S = 1 + e^{\pi i(h+k)} + e^{\pi i(k+l)} + e^{\pi i(h+l)}$$

S depending upon h, k, l ,

(1) If (h, k, l) are all odd or all even

$$S = 1 + 1 + 1 + 1$$

$$S = 4$$

$$F = 4f$$

$$I = F^2 \Rightarrow I = 16f^2$$

Reflections are allowed when (h, k, l) are all even or odd.

(2) if (hkl) is mixed.

Suppose (1,0,0) i.e. $h \rightarrow \text{odd}$ & $k, l \rightarrow \text{Even}$ then $S = 1 + e^{i\pi} + e^{i\pi}$

$$S = |1| + |-1|$$

$$S = 0$$

$$F = 0$$

$$I = 0$$

So for these reflections will be absent.

(IV) Diamond Cubic (dc) :-

Selection Rule

→ All Odd, then all reflections allowed.

→ All Even, then $(h+k+l)$ must be divisible by 4 [only these reflections will be allowed.]

(V) NaCl :- Combination of two fcc.

When NaCl crystallize, $\text{NaCl} \rightarrow \text{Na}^+ + \text{Cl}^-$

10 atoms are placed on lattice site

18

Beoz e's are different so their Scf. factor \rightarrow different.

$$f_{\text{Na}^+} \neq f_{\text{Cl}^-}$$

That's why NaCl follows the reflections of fcc.

* KBr comes in the category of NaCl. i.e. KBr also follow fcc

* KCl does not follow the reflection of fcc beoz $\text{KCl} \rightarrow \text{K}^+ + \text{Cl}^-$

$$f_{\text{K}^+} = f_{\text{Cl}^-}$$

18 18

In this case, X-ray can not differentiate b/w 2 types of atoms (K^+ & Cl^-)

⇒ KCl follows the reflection of simple cubic with lattice parameter

$$\frac{a}{2}$$



Hence Reflections of S.C. $\Rightarrow (100) (110) (111)$
 " " KCl $\Rightarrow (200) (220) (222)$

Order of Reflection :-

$(100), (110), (111), (200), (210), (211), (220), (300), (310), (311), (222), (320), (321)$

This is the decreasing order of d .
 This is of the form $(h^2+k^2+l^2)$



for S.C. \rightarrow All reflection allowed ~~(111)~~ ~~(112)~~ $(100) \rightarrow a = d_{hkl}$
 for bcc $\rightarrow (110), (200), (211), (220), (310), (222), (321)$

1st peak of bcc is $\frac{a}{\sqrt{2}} (110)$ corresponding to Interplane spacing $d_{hkl} = \frac{a}{\sqrt{2}}$

for fcc $\rightarrow (111), (200), (220), (311), (222)$

$(h^2+k^2+l^2) \Rightarrow$

- \rightarrow SC $\Rightarrow 1; 2; 3; 4; 5; 6; 8; \dots$
- \rightarrow bcc $\Rightarrow 2; 4; 6; 8; 10; 12; 14; 16; \dots$
 $1; 2; 3; 4; 5; 6; 7; 8; \dots$
- \rightarrow fcc $\Rightarrow \cancel{1}; \cancel{2}; 3; 4; 8; 11; 12; \dots$

for dc $\rightarrow (111), (220), (311)$

NaCl \rightarrow same as fcc.

KCl $\rightarrow (200), (220), (222)$

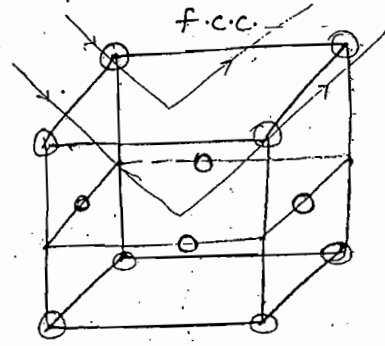
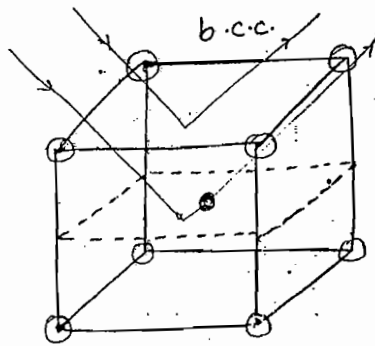
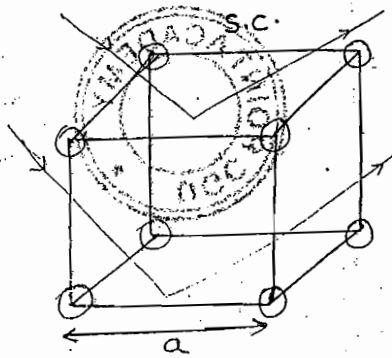
Largest Interplaner spacing for

S.C. $\rightarrow d_{100} = a$
 bcc $\rightarrow d_{110} = \frac{a}{\sqrt{2}}$
 fcc $\rightarrow d_{111} = \frac{a}{\sqrt{3}}$

https://allalabexperiments.com

Ques :- Calculate d_{100} for bcc.

$$d_{100} = \frac{a}{2}$$



In bcc & fcc, all the atoms are not covered by (100) plane so draw extra plane.

Due to 2 extra plane, interplaner spacing = $a/2$.

Due to extra plane: path diff \rightarrow will be half so phase diff will be half & condⁿ of constructive Int. will be changed into destructive.



	d_{100}	d_{110}	d_{111}
SC	a	$\frac{a}{\sqrt{2}}$	$\frac{a}{\sqrt{3}}$
bcc	$\frac{a}{2}$	$\left(\frac{a}{\sqrt{2}}\right)$	$\frac{a}{2\sqrt{3}}$
fcc	$\frac{a}{2}$	$\frac{a}{2\sqrt{2}}$	$\left(\frac{a}{\sqrt{3}}\right)$

I-reflection is for largest d.

• The plane which is not present i.e. ref. not allowed for that plane, \rightarrow multiply by $\frac{1}{2}$.

for SC $\Rightarrow d_{100} : d_{110} : d_{111} = 1 : \frac{1}{\sqrt{2}} : \frac{1}{\sqrt{3}} \Rightarrow \sqrt{6} : \sqrt{3} : \sqrt{2}$

bcc $\Rightarrow d_{100} : d_{110} : d_{111} = \frac{1}{2} : \frac{1}{\sqrt{2}} : \frac{1}{2\sqrt{3}} \Rightarrow \sqrt{6} : 2\sqrt{3} : \sqrt{2}$

fcc $\Rightarrow d_{100} : d_{110} : d_{111} = \frac{1}{2} : \frac{1}{2\sqrt{2}} : \frac{1}{\sqrt{3}} \Rightarrow \sqrt{6} : \sqrt{3} : 2\sqrt{2}$

Bragg's Law in Reciprocal lattice :-

$2d \sin \theta = n \lambda$ is the Bragg's law in direct lattice.

In Reciprocal lattice; we need to replace

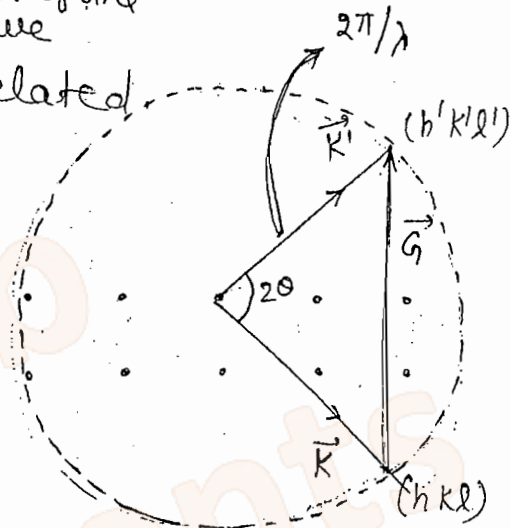
$$d \rightarrow G \quad \& \quad \lambda \rightarrow k$$

\downarrow Reciprocal lattice vectors. \downarrow wave vector of the wave



d & G and λ & k are inversely related.

If \vec{k} be the wave vector of incident x-rays & \vec{k}' be the wave vector of diffracted x-rays, & G is the reciprocal lattice vector.



Magnitude of \vec{k} is

$$|\vec{k}| = \frac{2\pi}{\lambda}$$

So Mag. of \vec{k}' is $|\vec{k}'| = \frac{2\pi}{\lambda}$ i.e. $|\vec{k}| = \frac{2\pi}{\lambda} = |\vec{k}'|$

bcz w.l. of incident & diffracted wave is same so

Mag. of \vec{k} & \vec{k}' are same but their dirⁿ are different

That's why they are different.

Length of wave vectors depend upon λ & length of \vec{k} & \vec{k}' will be same bcz λ is same.

Trace a circle of radius $2\pi/\lambda$ then

\Rightarrow All the points lying on the circle will satisfies the Bragg's Condⁿ (Circumference)

$$\vec{k}' = \vec{k} + \vec{G} \quad \text{--- (1)}$$

$$\Rightarrow \vec{k}' - \vec{k} = \vec{G}$$

\Rightarrow $\Delta \vec{k} = \vec{G}$ \rightarrow This is the form of Bragg's law in reciprocal lattice vector.

i.e. difference of wave vector is equal to Rec. lattice vector of inci. & diffracted wave

\vec{G} gives the difference of two points having Miller indices (hkl) and $(h'k'l')$ from incident to diffracted.

Now, squaring G^2 (1),

$$(k')^2 = k^2 + G^2 + 2\vec{k} \cdot \vec{G}$$

$$2\vec{k} \cdot \vec{G} \neq G^2 = 0$$

This is the Bragg's law in reciprocal lattice

In 2 Dim \rightarrow Circle

In 3 Dim \rightarrow Sphere called Ewald-sphere

tells position of Bragg diffracted plane point

\Rightarrow In X-ray Machines generally $\lambda = 1.54 \text{ \AA}$ W.L, Cu-K α radia is used.

So K α is incident on Cu crystal. It is monochromatic.

~~Brillouin~~ Brillouin

~~Brillouin~~ Zones (BZ):- BZ are the boundaries where Bragg's conditions will be satisfied in reciprocal lattice.

BZ is the locus of all K-values which are Bragg diffracted

Reciprocal lattice unit cell of any crystal is the first BZ.

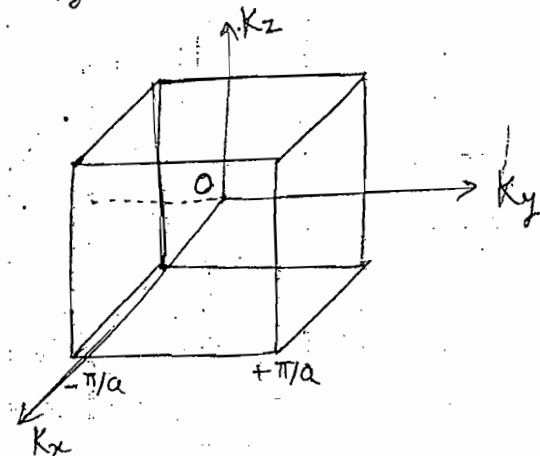
i.e. 1st BZ of simple cubic is S.C.

(In R.L., always take origin at centre)

K_x, K_y, K_z are those K-values which are Bragg diffracted.

In X-dirⁿ at $K_x = \pi/a$ & In -X dirⁿ

at $K_x = -\pi/a$, Bragg condⁿ is satisfied.



Bragg's law in Reciprocal lattice

$$2\vec{k} \cdot \vec{G} + G^2 = 0$$

In 2 Dim, Consider a square of side a .

In direct lattice, lattice vectors are

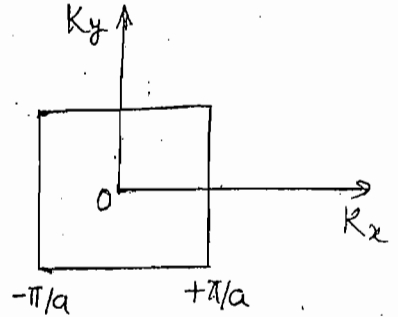
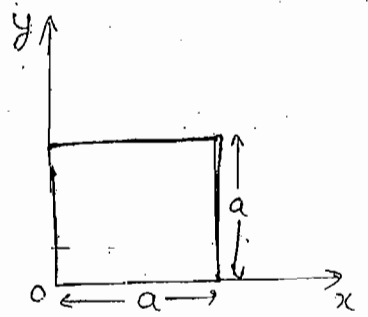
$$\vec{a} = a \hat{i}$$

$$\vec{b} = b \hat{j}$$

In Reciprocal lattice, let $c = c \hat{k}$

$$\vec{A} = \frac{2\pi(\vec{b} \times \vec{c})}{a \cdot (\vec{b} \times \vec{c})} = \frac{2\pi}{a} \hat{i}$$

$$\vec{B} = \frac{2\pi(\vec{c} \times \vec{a})}{a \cdot (\vec{b} \times \vec{c})} = \frac{2\pi}{a} \hat{j}$$



So reciprocal of square is a square of side $2\pi/a$.

Now, from \vec{G} ,

$$\vec{G} = h\vec{A} + k\vec{B}$$

$$= \frac{2\pi}{a} (h\hat{i} + k\hat{j})$$



$$\vec{k} = k_x \hat{i} + k_y \hat{j}$$

$$2\vec{k} \cdot \vec{G} + G^2 = 2 \cdot \frac{2\pi}{a} (hk_x + k^2) + \frac{4\pi^2}{a^2} (h^2 + k^2) = 0$$

$$\Rightarrow \frac{4\pi}{a} (hk_x + k^2) = -\frac{4\pi^2}{a^2} (h^2 + k^2)$$

$$\Rightarrow \boxed{hk_x + k^2 = -\frac{\pi}{a} (h^2 + k^2)}$$

This is the Bragg's Condⁿ of square lattice.

Minimum value of $h, k \rightarrow (0, 0)$ Not possible

$$h = \pm 1, k = 0$$

$$h = 0, k = \pm 1$$

These are the possible values of h & k

Now if $h = \pm 1$, $K = 0$

& if $h = 0$, $K = \pm 1$

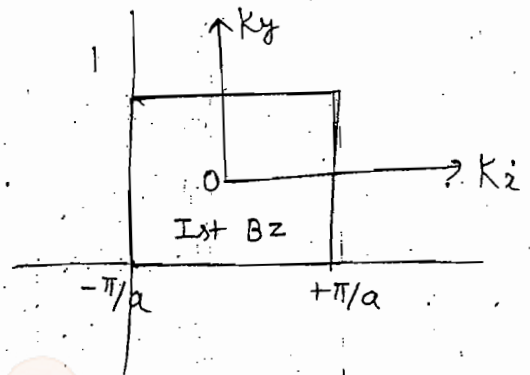
$$\Rightarrow \pm K_x = \frac{\pi}{a}$$

$$\Rightarrow \pm K_y = \frac{\pi}{a}$$

$$K_x = \pm \frac{\pi}{a}$$

$$K_y = \pm \frac{\pi}{a}$$

$K_x = \pm \frac{\pi}{a}$ & $K_y = \pm \frac{\pi}{a}$ enclose the area of 1st B.Z.



BZ are very imp. in electrical as well as magnetic property.

BZ decide the e^- & phonone.

Electric property decide by the motion of e^- in the crystal.

If e^- move freely then crystal is good conductor.

If e^- can not move freely then crystal is insulator.

If band gap is large, then more energy should be provided to free the e^- .

If e^- is moving inside the crystal then it'll have some mom. then by De-Broglie hypothesis, it'll have some

λ

$$\lambda = \frac{h}{p}$$

If Bragg's Condⁿ is satisfied, then wave associated with e^- move in backward dirⁿ instead of forward dirⁿ so band gap arises.

So e^- is free to move in BZ. So e^- will have the energy of V.B. or C.B. If e^- have energy of band gap then it will do back & forth motion \rightarrow standing wave.

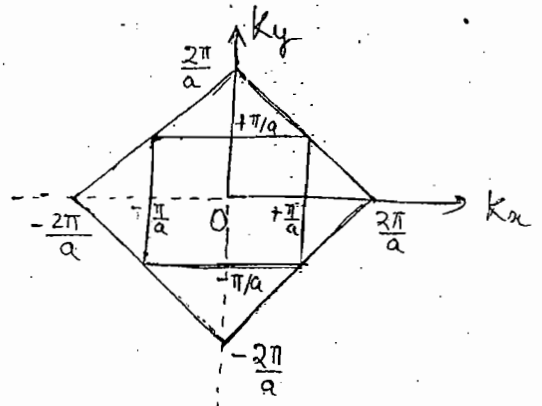
The concept of BZ is also applicable on phonone.

Area of BZ tells that e^- can move freely in this area but if stuck on boundary then phase changes by 180° . & then Standing wave formation occur & band gap arises.

2nd Brillouin Zone

Next condⁿ of k & h , $h = \pm 1$
 $k = \pm 1$

$$\Rightarrow \pm k_x \pm k_y = -\frac{2\pi}{a}$$



Four lines \Rightarrow

$$k_x + k_y = -\frac{2\pi}{a}$$

$$+k_x - k_y = -\frac{2\pi}{a}$$

$$-k_x + k_y = -\frac{2\pi}{a}$$

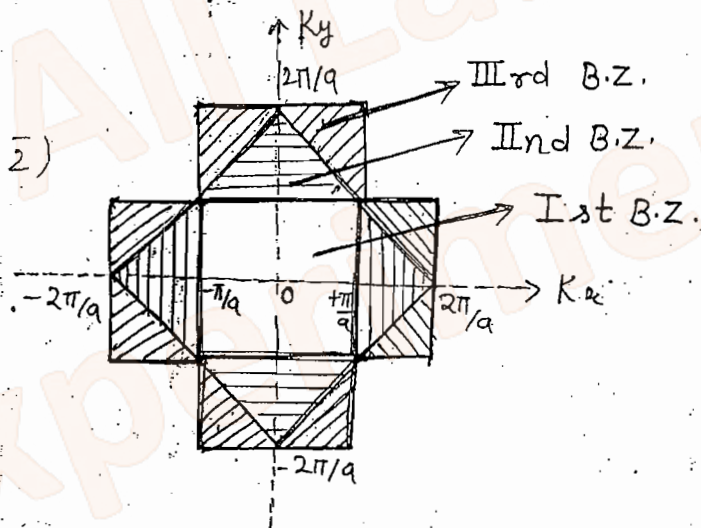
$$-k_x - k_y = -\frac{2\pi}{a}$$

2nd B.Z. is of triangular shape. (4 Δ)

3rd B.Z. :-

(2,0), (0,2), (0,-2)

3rd B.Z. there are 8 Δ .



These are the B.Z. of square lattice.

- Rectangular Lattice \rightarrow shape of I B.Z. is rectangular.
- Hexagonal " \rightarrow shape of I B.Z. is Hexagonal.
- Cube " \rightarrow shape of I B.Z. is Cube.
- Square " \rightarrow " " Square.

Ques :- Which of the following statement about B.Z. for a particular reciprocal lattice are correct.

(i) All B-Z have same length in 1D, same area in 2D & same volume in 3D.

This is true.

(ii) They all have same shape. False

(iii) They all have same symmetry. True



Questions

Q.1:- Interatomic separation of Pb crystal having fcc structure is 3.5 \AA then calculate the no. of atoms in 1 mm^2 square area of

(i) (100) plane

(ii) (111) plane

Q.2:- α -Co has hcp structure with lattice spacing of $a_h = 2.51 \text{ \AA}$ & height $c = 4.07 \text{ \AA}$. & β -Co is fcc with cube sides 3.55 \AA . Calculate the ^{ratio} difference of densities of two forms.

Q.3:- From X-rays data Fe is found to have cubic cell parameter of 2.87 \AA . Its density & atomic mass are 7870 kg/m^3 & 55.85 respectively. Find out the Bravais lattice of Fe & interatomic separation of Fe atoms.

Q.4:- Sodium transforms from bcc to hcp crystal structure at about 23 K without change of density in the cubic phase lattice parameter is $a_c = 4.23 \text{ \AA}$ and in hcp phase $c/a_h = \sqrt{\frac{8}{3}}$. Find out the lattice constant in hcp phase (a_h).

Q.5:- (a) Calculate the diffraction angle for the 1st β peaks in Al powder diffraction pattern. Note that crystal structure of Al is fcc & lattice constant is 4.04 \AA . & X-ray W.L. is 1.54 \AA .

(b) If the lattice const. of Al is larger than 4.04 \AA . Describe how pattern would change.

Q.6:- In powder X-ray diffraction pattern, using X-rays of W.L. 1.54 \AA . Three consecutive 1st order peaks are observed at 2θ value of 60° , 90° & 112° . If system is cubic & peak at 90° corresponds to (220) plane. Calculate

(a) Value of lattice constant a .

(b) Obtain the Miller indices for the rest peaks, & identify the system.



Q.7:- A bcc cell has a lattice const. a . Calculate

(a) Spacing b/w (111) plane

(b) Bragg diffraction angle θ_B for diffraction from (100) plane

(c) if X-rays of W.L. λ are used.

Q.8:- A bcc crystal is used to measure the W.L. of some X-rays. The Bragg angle for the reflection from (110) plane is 20.2° . Calculate the W.L. of X-rays if lattice parameter of the crystal is 3.15 \AA .

Q.9:- The molar mass of Magnesium oxide having NaCl type structure is 40.30 and density is $3.58 \times 10^6 \text{ gm/m}^3$ at 298 K . Calculate (i) lattice parameter of the crystal.

(ii) The values of $\left(\frac{\sin \theta}{\lambda}\right)$ for the planes (100), (110) & (111).

Q.10:- A powder sample of fcc lattice with lattice const. 4.09 \AA is used for X-ray diffraction studies using monochromatic beam of X-ray of W.L. 1.54 \AA . Find the

- (i) lowest value of θ for which the Bragg reflection would be observed.
- (ii) Find the Bragg angle for IIIrd peak.

Q.11 :- A simple cubic structure with cube side 4 \AA is used to scatter X-rays of W.L. 4.8 \AA . Determine the Miller indices of all sets of plane which satisfy the Bragg condition, & for each peak, find the Bragg angle.

Neutron diffraction & e^- diffraction :-

{ X-ray diffraction } * calculate the energy of X-rays, neutrons & electrons corresponding to 1 \AA Wavelength.

$$E_x, E_n, E_{e^-} = ?$$

$$E_x = \frac{hc}{\lambda}$$

$$E_n = \frac{p^2}{2m_n} = \frac{h^2}{2m_n \lambda^2}$$

$$E_e = \frac{p^2}{2m_e} = \frac{h^2}{2m_e \lambda^2}$$



By De-Broglie hypothesis
 $p = h/\lambda$

Even if λ is same, then E_x, E_n, E_e are different. e^- & n are not mass-less. Mass of e^- & n are different.

$$E_x = \frac{6.6 \times 10^{-34} \times 3 \times 10^8}{1 \text{ \AA} = 10^{-10}} = 1.98 \times 10^{-15} \text{ J} = \frac{1.98 \times 10^{-15}}{1.6 \times 10^{-19}}$$

$$E_n = \frac{(6.6 \times 10^{-34})^2}{2 \times 1.67 \times 10^{-27} \times (10^{-10})^2} =$$

$$E_e = \frac{(6.6 \times 10^{-34})^2}{2 \times 9.1 \times 10^{-31} \times (10^{-10})^2} =$$

Depend on Energy, these diffractions are used for different Analysis.

For X-rays, $\lambda \propto \frac{1}{V}$ or $\lambda \propto \frac{1}{\sqrt{V}}$ is correct?

where V is the cube voltage?
 $(eV \propto \frac{1}{\lambda} \Rightarrow \lambda \propto \frac{1}{V})$

For e^- , $\lambda \propto \frac{1}{\sqrt{V}}$ $(eV \propto \frac{1}{\lambda^2} \Rightarrow \lambda \propto \frac{1}{\sqrt{V}})$

for n , No dependency of λ on V bcoz n are chargeless but they can be accelerated by temp.

$$\lambda = \frac{h}{\sqrt{2m_n E_n}} \quad \left\{ \text{from } E_n = \frac{h^2}{2m_n \lambda^2} \right\}$$

thermal energy $E_n = \frac{3}{2}KT$ (3 Dim)

$$\lambda = \frac{h}{\sqrt{3m_n KT}}$$



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Uses :-

(i) X-Ray diffraction :-
X-ray diff used in crystal ^{lattice} structure determination.

(ii) neutron diffraction :-
is used to determine magnetic structure of solid and distribution of nuclei.

(iii) Electron diffraction :-
is used to determine surface morphology i.e. it is used in surface studies of the crystal.

$$E_x > E_e > E_n$$

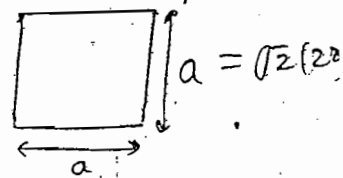
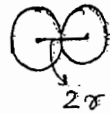
for LA W.L.

$E_e > E_n$ but e^- have -ve charge so it can not penetrate the crystal so used for surface study.

Q.1:- $2r = 3.5$, $a = 4.94 \text{ \AA}$

1 mm^2 Area

for fcc, $a = \sqrt{2}(2r)$
 $= 1.414 (3.5)$
 $= 4.94 \text{ \AA}$



(100):- Area of square = $a^2 = (4.94)^2 \text{ \AA}^2$

No. of atoms in this area = 2

$1 \text{ \AA} = 10^{-7} \text{ mm}$

In $(4.94)^2 \times 10^{-14} \text{ mm}^2$ Area = 2 atoms.

1 mm^2 Area = $\frac{2 \times 10^{14}}{(4.94)^2}$

= 8.16×10^{12} atoms

In (111) plane

Area = $\frac{\sqrt{3}}{2} a^2 = \frac{\sqrt{3}}{2} \times (4.94)^2 \times 10^{-14} \text{ mm}^2$

In this area $\frac{\sqrt{3}}{2} \times (4.94)^2 \times 10^{-14} \text{ mm}^2 = 2$ atoms.

In $1 \text{ mm}^2 = \frac{2 \times 2 \times 10^{14}}{\sqrt{3} (4.94)^2}$

= 9.4×10^{12} atoms

(111) is more closed pack.

(100) plane



Q.2 :-

α -Co	β -Co
hcp	fcc
$a_h = 2.51 \text{ \AA}$	$a_c = 3.55 \text{ \AA}$
$c = 4.07 \text{ \AA}$	

Ratio $\frac{\rho_c}{\rho_h} = ?$

c \rightarrow cubic
h \rightarrow hcp

density $\rho = \frac{\text{No of atom}}{\text{Unit Volume}}$

$$\rho_c = \frac{4}{a_c^3}$$

$$\rho_h = \frac{6}{\frac{3\sqrt{3} a_h^2 c}{2}}$$

$$\frac{\rho_c}{\rho_h} = \frac{4}{a_c^3} \times \frac{3\sqrt{3} a_h^2 c}{6} = \sqrt{3} \frac{a_h^2 c}{a_c^3}$$

$$= \frac{1.732 \times (2.51)^2 \times 4.07}{(3.55)^2} = \frac{44.3596}{44.7388}$$

$$a^3 = \frac{n M_A}{N_A \rho_m}$$

hcp, $\frac{3\sqrt{3} a_h^2 c}{2} = \frac{6 M_A}{N_A \rho_m}$

fcc, $a^3 = \frac{4 M_A}{N_A \rho_m}$



$$\frac{\rho_c}{\rho_h} = 0.99$$

Since hcp & fcc both are closed pack so this ratio should be approx to 1.

Q.3 :-

Fe : $a = 2.87 \text{ \AA}$
 $\rho = 7870 \text{ kg/m}^3$
 $m_A = 55.85$

$$a^3 = \frac{n M_A}{N_A \rho_m} \Rightarrow n = \frac{a^3 N_A \rho_m}{M_A}$$

$$n = \frac{(2.87)^2 \times 6.023 \times 10^{23} \times 7870}{55.85}$$

$$n \approx 2 \text{ for bcc.}$$

$n=1 \rightarrow$ sc
 $n=2 \rightarrow$ bcc
 $n=4 \rightarrow$ fcc
 $= 8 \rightarrow$ dc

Interatomic separation, for bcc

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

$$2r = \frac{\sqrt{3}}{2} \times 2.87 \text{ \AA} = \frac{1.73 \times 2.87}{2}$$

$$2r = \underline{\underline{2.48 \text{ \AA}}}$$

Q.4 :- bcc $\xrightarrow{\text{Na}}$ hcp

$$a_c = 4.23 \text{ \AA} \quad \frac{c}{a_h} = \sqrt{\frac{8}{3}}, \quad a_h = ?$$

for bcc $\Rightarrow \frac{n}{a^3} = \frac{N_A \rho_m}{M_A} = \frac{2}{a^3}$

$$\Rightarrow \frac{2}{a_c^3} = \frac{3\sqrt{3} a_h^2 c}{2 M_A}$$

bcc $\rightarrow a_c^3 = \frac{n m_A}{N_A \rho_m}$

$$a_c^3 = \frac{2 m_A}{N_A \rho_m} \quad \text{--- (1)}$$

hcp $\rightarrow \left(\frac{3\sqrt{3} a_h^2 c}{2} \right) = \frac{6 m_A}{N_A \rho_m} \quad \text{--- (2)}$

Divide (1)/(2) $\Rightarrow \frac{2 a_c^3}{3\sqrt{3} a_h^2 c} = \frac{2}{6}$

$$\Rightarrow 2 a_c^3 = \sqrt{3} a_h^2 c$$

$$2(4.23)^3 = \sqrt{3} a_h^2 (1.633 \text{ \AA})$$

$$\frac{151.373934}{(1.633 \times \sqrt{3})} = a_h^3$$

$$a_h^3 = \frac{151.373934}{2.8284}$$

$$a_h^3 = 53.592 \Rightarrow$$

$$a_h = \underline{\underline{3.7702 \text{ \AA}}}$$



Q.5:- Al \rightarrow fcc

(a) $a = 4.04 \text{ \AA}$
 $\lambda = 1.54 \text{ \AA}$

I, 3 peaks $\rightarrow (111), (200), (220)$

$$2d \sin \theta = \lambda$$

(111), $d_{111} = \frac{a}{\sqrt{h^2+k^2+l^2}}$

$$d_{111} = \frac{4.04}{\sqrt{3}} = 2.33 \text{ \AA}$$

$$2d \sin \theta_1 = \lambda \Rightarrow 2 \times 2.33 \times \sin \theta_1 = 1.54 \text{ \AA}$$

$$\Rightarrow \sin \theta_1 = \frac{1.54}{2 \times 2.33} = 0.3304$$

$$\theta_1 = \sin^{-1}(0.3304) = 19.293^\circ$$

$$\theta_1 \approx 19.3^\circ$$

diff. angle $\boxed{2\theta_1 = 38.6^\circ}$ $\underline{A_1}$

(200), $d_{200} = \frac{4.04}{\sqrt{4+0+0}} = \frac{4.04}{2} = 2.02 \text{ \AA}$

$$2d \sin \theta_2 = \lambda \Rightarrow 2 \times 2.02 \sin \theta_2 = 1.54$$

$$\Rightarrow \sin \theta_2 = \frac{1.54}{4.04} = 0.3812$$

$$\theta_2 = 22.4^\circ \Rightarrow \boxed{2\theta_2 = 44.8^\circ}$$
 $\underline{A_2}$

(220), $d_{220} = \frac{4.04a}{\sqrt{8}} = \frac{4.04a}{2\sqrt{2}} = 2.8567$

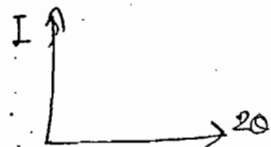
$$2d \sin \theta_3 = \lambda \Rightarrow 2(2.8567) \sin \theta_3 = 1.54 \quad 2 \times \frac{4.04}{2\sqrt{2}} \sin \theta_3 = 1.54$$

$$\Rightarrow \sin \theta_3 = \frac{1.54}{4.04} \times \sqrt{2} = 0.539$$

$$\Rightarrow \theta_3 = 32.61^\circ \Rightarrow \boxed{2\theta_3 = 65.23^\circ}$$
 $\underline{A_3}$

(b) Entire pattern will be shifted to lower diffraction angle.

$a \uparrow, d \uparrow, \theta \downarrow$



Q.6 :- $2d \sin \theta = \lambda$

$2 \times \frac{a}{\sqrt{h^2+k^2+l^2}} \sin \theta = \lambda \Rightarrow \sin \theta = \frac{\lambda}{2a} \sqrt{h^2+k^2+l^2}$

$\sin^2 \theta = \frac{\lambda^2}{4a^2} (h^2+k^2+l^2) \Rightarrow$ A form of Bragg's law

$\sin^2 \theta_1 : \sin^2 \theta_2 : \sin^2 \theta_3 = (h_1^2+k_1^2+l_1^2) : (h_2^2+k_2^2+l_2^2) : (h_3^2+k_3^2+l_3^2)$

2θ	θ	$\sin \theta$	$\sin^2 \theta$	
60°	30°	$\frac{1}{2}$	$\frac{1}{4}$	$\rightarrow 4$
90°	45°	$\frac{1}{\sqrt{2}}$	$\frac{1}{2}$	$\rightarrow 8$
112°	56°	0.829	0.687	$\rightarrow 11$

for $2\theta = 90^\circ$

$(h^2+k^2+l^2) = 8$ for (220)

for $2\theta = 90^\circ$, we'll get 8 when $(\sin^2 \theta \times 16)$ so multiply by 16 in all $\sin^2 \theta \Rightarrow 4, 8, 11$

60° corresponds to (200)

112° " " (311)

$d = \frac{a}{2\sqrt{2}}$

$2d \sin \theta = \lambda \Rightarrow \frac{a}{\sqrt{2}} \sin 45^\circ = \lambda \Rightarrow a = \lambda \times 2 = 1.54 \times 2$

$\Rightarrow a = 3.08 \text{ \AA}$

Q.7 :- (i) bcc $\rightarrow a$

$d_{111} = \frac{a}{2\sqrt{3}}$

(ii) $2d_{100} \sin \theta_B = \lambda \Rightarrow 2 \times \frac{a}{2} \sin \theta_B = \lambda$

$\theta_B = \sin^{-1} \left(\frac{\lambda}{a} \right)$



Q.8 :- bcc, Reflection of (110) $\rightarrow 2\theta = 2^\circ$

$a = 3.15 \text{ \AA}$, $\lambda = ?$

$2d_{110} \sin \theta_B = \lambda$

$\lambda = 2 \times \frac{3.15}{\sqrt{2}} \times 0.34 \text{ \AA}$

$[d_{110} = \frac{a}{\sqrt{2}}]$

$\lambda = 1.538 \text{ \AA}$

Q.9 :- MgO, $M_m = 40.30$
 (NaCl type structure) $\rho_m = 3.58 \times 10^6 \text{ gm/m}^3$

(i) $a = ?$ (ii) $\left(\frac{\sin \theta}{\lambda}\right)$

(i) $a^3 = \frac{n M_A}{\rho_m N_A}$ ($n=4$)

$a^3 = \frac{n_{Na} m_{Na} + n_{Cl} m_{Cl}}{\rho_m N_A} = \frac{4 (m_{Na} + m_{Cl})}{\rho_m N_A}$

$a^3 = \frac{4 \times 40.30}{3.58 \times 10^6 \times 6.02 \times 10^{23}} = \frac{161.1 \times 10^{-29}}{3.58 \times 6.02} = 7.4797 \times 10^{-29}$

$a = 4.21 \times 10^{-10} \text{ m} \Rightarrow \boxed{a = 4.2 \text{ \AA}}$



(ii) $\frac{\sin \theta}{\lambda}$ and $2d \sin \theta = \lambda$

$d_{100} = \frac{a}{2}$

$\sin \theta = \lambda$
 $\frac{\sin \theta}{\lambda} = \frac{1}{a}$

$\frac{\sin \theta}{\lambda} = 0.23 (\text{\AA})^{-1}$

$d_{110} = \frac{a}{2\sqrt{2}}$
 $\frac{\sin \theta}{\lambda} = \frac{2}{\sqrt{2} \times 4.2} = \frac{\sqrt{2}}{4.2}$

$d_{111} = \frac{a}{\sqrt{3}}$
 $\frac{\sin \theta}{\lambda} = \frac{\sqrt{3}}{2 \times 4.2} = \frac{\sqrt{3}}{8.4}$

Q.10 :- (a) lowest value of $\theta \rightarrow$ (111) plane

$d_{111} = \frac{a}{\sqrt{3}} = \frac{4.09}{\sqrt{3}} \text{ \AA}$

$\theta_{\text{lowest}} \Rightarrow 2 \times \frac{4.09}{\sqrt{3}} \sin \theta = 1.54 \text{ \AA}$
 $\Rightarrow \boxed{\theta_{\text{lowest}} = 19.03^\circ}$

(b) Third peak \rightarrow (220)

$d_{220} \rightarrow \frac{a}{2\sqrt{2}}$
 $2 \times \frac{a}{2\sqrt{2}} \sin \theta = 1.54$
 $\boxed{\theta = 32.17^\circ}$

Q.11 :- sc, $a = 4 \text{ \AA}$, $\lambda = 4.8 \text{ \AA}$

for sc \rightarrow all peaks allowed.
 (100) (110) (111) (200) (220)

$2d \sin \theta = n\lambda \Rightarrow \sin \theta = \frac{n\lambda}{2d}$
 $\sin \theta = \frac{\lambda}{2d} \leq 1$ if this condⁿ is satisfied \rightarrow peaks are allowed.

$\sin \theta_{100} = \frac{4.8}{2 \times 4} = 0.6 \Rightarrow \boxed{\theta_{100} = 36.86^\circ}$

$\sin \theta_{110} = \frac{4.8}{2 \times 4/\sqrt{2}} = 0.6 \times \sqrt{2} \Rightarrow \boxed{\theta_{110} = 58.05^\circ}$ $\left\{ \frac{a}{\sqrt{2}} = d_{110} \right.$

$\sin \theta_{111} = \frac{4.8}{2 \times 4/\sqrt{3}} = 0.6 \times \sqrt{3} \approx 1.03 > 1$
 Not possible

So Only 2 peaks \rightarrow (100), (110)

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