Toppersnotes
Unleash the topper in you

CSIR-NET

Council of Scientific & Industrial Research

PHYSICAL SCIENCE

VOLUME - VI

SOLID STATE

SIERRA INNOVATIONS

SOLID STATE

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Solid - State

Matter

solid — liq — Gas — Plasma

↓ Crystalline. — ↓ Non-crystalline. (Amorphous) glass - rubber etc.

In case of solid atoms and molecules are closely packed and forms a condense state of matter Hence interaction among atom or molecules is strongest.

Crystalline - atoms and molecules are regularly arranged or periodically arranged

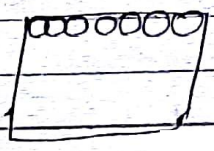
We consider atom as a hard sphere and hence have fixed radius, same size and repeate itself after 2r distance each of atoms are a atomic plane and layer are also have periodical arrangement.

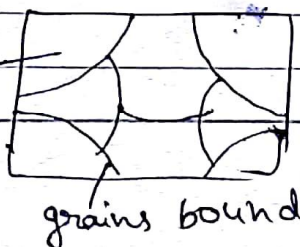
So a solid which has regular or periodic arrangements of atoms or molecules.

Amerphous :- which has irregular or random arrangement of molecules.

Crystalline

↙ Single crystal — ↘ Poly crystalline





Only one type of arrangement throughout the solids

(Diamond)
(Quartz)

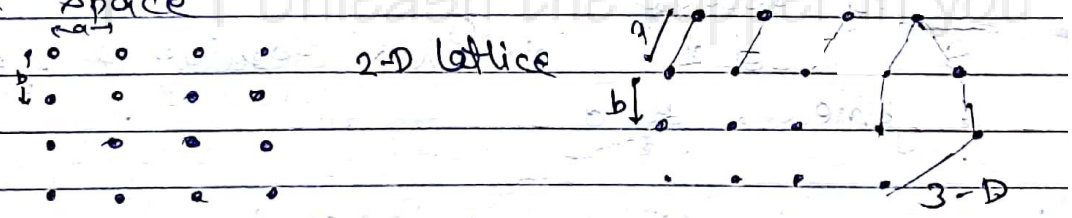
poly crystalline can be consider as a agreegiate of large number of single crystal
its properties depends upon size of grain
(Gold, Cu, Ag, Al)

Arrangements of atom decide the physical property of solid.

Crystallography

Arrangements of atoms or molecules in a crystalline solid.

Lattice: lattice is a set of periodically arranged points in space



lattice parameter is the distance forever two consiquence lattic points.

In square lattice a=b

A lattice could be space lattice or bravice lattice only if each lattice point has identical surroundings.

Crystal System	lattice parameter	Bravious lattice	lattice syste
Cubic	$a=b=c$ $\alpha=\beta=\gamma=90^\circ$	S.C., BCC, FCC	P, I, F
Tetragonal	$a=b\neq c$ $\alpha=\beta=\gamma=90^\circ$	SC, BCC	P, I
Orthorohmbic	$a\neq b\neq c$ $\alpha=\beta=\gamma=90^\circ$	Sc, BCC, FCC, EC	P, I, F, C
Trigonal or Rhombohadral	$a=b=c$ $\alpha=\beta=\gamma=120^\circ$	SC	
Hexagonal	$a=b\neq c$ $\alpha=\beta=90^\circ$ $\gamma=120^\circ$	SC	
Monoclinic	$a\neq b\neq c$ $\alpha=\gamma=90^\circ$, $\beta\neq 90^\circ$	SC, EC	
Triclinic	$a\neq b\neq c$ $\alpha\neq\beta\neq\gamma\neq 90^\circ$	SC	

Effective No. per unit cell / lattice point per unit cell -

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{8}$$

N_i - Interior atom
N_f = atom of face
N_c = atoms at corner

	S.C.	BCC	FCC	HCP	diamond
Effective No/ lattic Point (N)	1	2	4	6	8
Co-ordinate No/ nearest neighbour atom	6 $(\pm a,0,0)$ $(0,\pm a,0)$ $(0,0,\pm a)$	8 $(\pm a/2, \pm a/2, \pm a/2)$	12 $(\pm a/2, a/2, 0)$	12 $(\pm a/2, \pm a/2, 0)$	4 $(a/4, \pm a/4, \pm$
Atomic (2r) Diameter (Nearest Neighbour distance)	a	$\frac{\sqrt{3}a}{2}$	$\frac{a}{\sqrt{2}}$	a	$\frac{\sqrt{3}}{4}a$
Volume of unit cell	a^3	a^3	a^3	$3\sqrt{2}a^3$ $3\sqrt{3}a^2c$ $\left(c/a = \sqrt{8/3}\right)$	a^3
Vol^m of the primitive cell	a^3	$\frac{a^3}{2}$	$\frac{a^3}{4}$	$\frac{3\sqrt{2}a^3}{6}$	$\frac{a^3}{8}$
Vol^m of the atoms in unit cell	$\frac{\pi a^3}{6}$	$\frac{\sqrt{3}\pi a^3}{8}$	$\frac{\sqrt{2}\pi a^3}{6}$	πa^3	
Packing fraction	$\pi/6$ 52%	$\sqrt{3}/8\,\pi$ 68%	$\sqrt{2}/6\,\pi$ 74%	$\pi/3\sqrt{2}$ 74%	34%

Miller-Bravais indices for Hexagonal crystal system -

$(h,k,l) \longrightarrow (h,k,i,l)$

h,k,l – miller indices

i – Bravais indices

$$\boxed{i = -(h+k)}$$

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

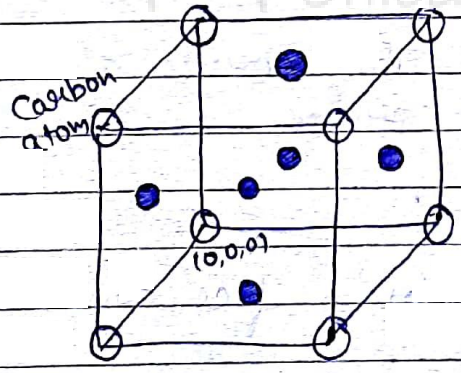
hcp → $(0\,0\,1) \longrightarrow (0\,0\,0\,1)$ closed packed plane.

5. Diamond cubic (DC) → (tetrahedral)

Diamond cubic structure has fcc lattice with two atom basis. If one atom occupies (0,0,0) position then other atom occupies $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ position

Or

Diamond cubic structure can be consider as interpenetration of two fcc unit cell. If corner of one unit cell is at (0,0,0) then corner of other unit cell would be at $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$



2nd unit cell effective no.
3 Face + 1 corner

1 No. of atom per unit cell $\boxed{n = 8}$

4 + 4 → due to 2nd unit cell

due to 1st unit cell

Co-ordination no. – 4

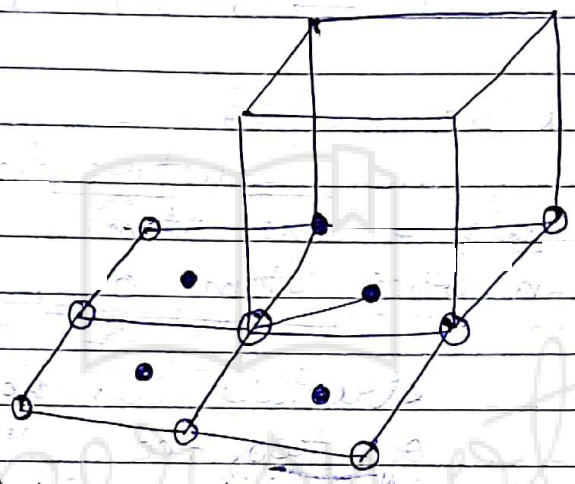
plane – loose packed

Nearest neighbour distance -

$2r = \frac{1}{4} \times \sqrt{3}\, a$ ($\frac{1}{4}$ of body diagonal)

$$2r = \frac{\sqrt{3}}{4} a$$

4. No. of 2nd nearest neighbour - 12.



5. 1st nearest neighbour distance for fcc = 2nd nearest neighbour distance for DC.

(1st nearest neighbour - 1st cubic corner and 2nd cubic corner)

2nd nearest neighbour -

In 1st cubic - 1st cubic's face centered atom

5. Volume of unit cell - a^3

6. Volume of primitive unit cell - $a^3/4$

7. lattice point - 4
atom - 8.

8. Atomic density $8/a^3$

9. APF (packing fraction) -

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

$$= \frac{\sqrt{3}\pi}{16} = 34\%$$

10. loose packed structure. (<96% , 94%)

11. Ex - diamond, Si, Ge, Sn etc.

(Octahedral)

6. ZnS (Zinc-Sulphide or Zinc blende) Structure :-

This structure similar to diamond cubic structure except if one of the Fcc unit cell is made of Zinc atom than other unit cell is made of Sulpher atom.

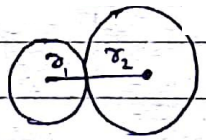
lattice - Fcc with two atom basis

basis (1Zn + 1S) and vise-versa

(0,0,0) $(\frac{1}{4},\frac{1}{4},\frac{1}{4})$

this is a molecular structure.

Interatomic distance



$r = r_{Zn} + r_S$

No of atoms per unit cell -

4Zn + 4S

= 4ZnS molecule.

this is a molecular structure so we write it in terms of molecule not in atoms.

Nearest neighbour distance.

$$r_{Zn} + r_S = \frac{\sqrt{3}\,a}{4}$$

No. of second nearest atom = 12

Second nearest neighbour distance = $a/\sqrt{2}$

Volume of unit cell = a^3

Volume of perimitive unit cell = $a^3/4$

Molecular density = $4/a^3$

A.P.F. $= \dfrac{\left(4 \times \frac{4}{3}\pi r_{Zn}^3\right) + \left(4 \times \frac{4}{3}\pi r_S^3\right)}{a^3}$

$$= \frac{4 \times \frac{4}{3}\pi}{a^3}\left(r_{Zn}^3 + r_S^3\right)$$

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

$$= \frac{\sqrt{3}\,\pi}{4}\left(\frac{\frac{r_{Zn}^3}{r_S^3} + 1}{\left(\frac{r_{Zn}}{r_S} + 1\right)^3}\right)$$

ex - GaAS, C

It is loosed packed plane.

NaCl Structure (Sodium Chloride structure) or Rock salt :-

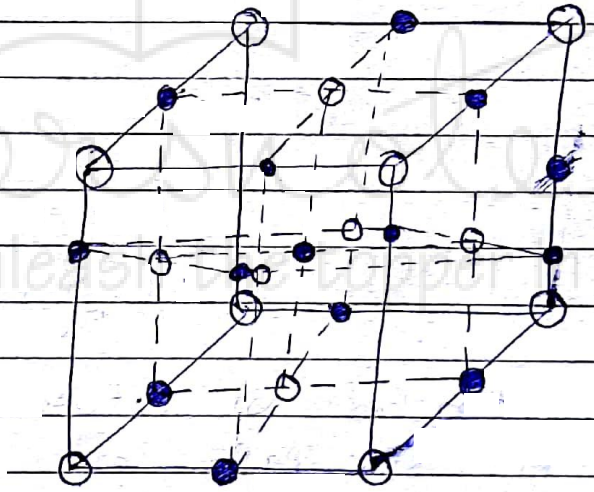
NaCl structure have FCC lattice with two atoms basis (1 Na + 1 Cl)

If Na occupies (0,0,0) position then Cl occupies ($\frac{1}{2}$,0,0), (0,0,$\frac{1}{2}$) or (0,$\frac{1}{2}$,0) or vise-versa.

Or

Nacl structure can be consider as interpenitration of two FCC lattic. If one unit cell has origen at (0,0,0) and another unit cell has origen at ($\frac{1}{2}$,0,0) or (0,$\frac{1}{2}$,0) or (0,0,$\frac{1}{2}$)

O - Cl
● - Na
Side center - $\frac{1}{4}$
body center - $\frac{1}{2}$



1. No. of atoms per unit cell

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

$1 + \frac{1}{4} \times 12 = 4$ (Na)

4 NaCl molecule.

2. Co-ordination no. - 6

3. $r_{Na} + r_{Cl} = a/2$

4. No. of second nearest neighbour = 12
5. of second nearest neighbour distance = $a/\sqrt{2}$

6. Volume = a^3
7. Volume of unit cell $a^3/4$
8. Molecular density $4/a^3$

9. Packing fraction

$$= \frac{4\left(\frac{4}{3}\pi r_{Na}^3 + \frac{4}{3}\pi r_{Cl}^3\right)}{a^3}$$

$$= \frac{4 \cdot \frac{4}{3}\pi \left(r_{Na}^3 + r_{Cl}^3\right)}{2^3 (r_{Na} + r_{Cl})^3}$$

$$= \frac{2\pi}{3} \frac{\left[1 + \left(\frac{r_{Na}}{r_{Cl}}\right)^3\right]}{\left(1 + \frac{r_{Na}}{r_{Cl}}\right)^3}$$

10. loose packed structure.
11. Ex - KCl, KBr, AgBr etc.

CsCl Structure :-

CsCl has simple cubic lattice with two atoms basis (1Cs + 1Cl)

If Cs atom occupies (0,0,0) position and Cl occupies at (½, ½, ½) position and vise-versa.

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Or

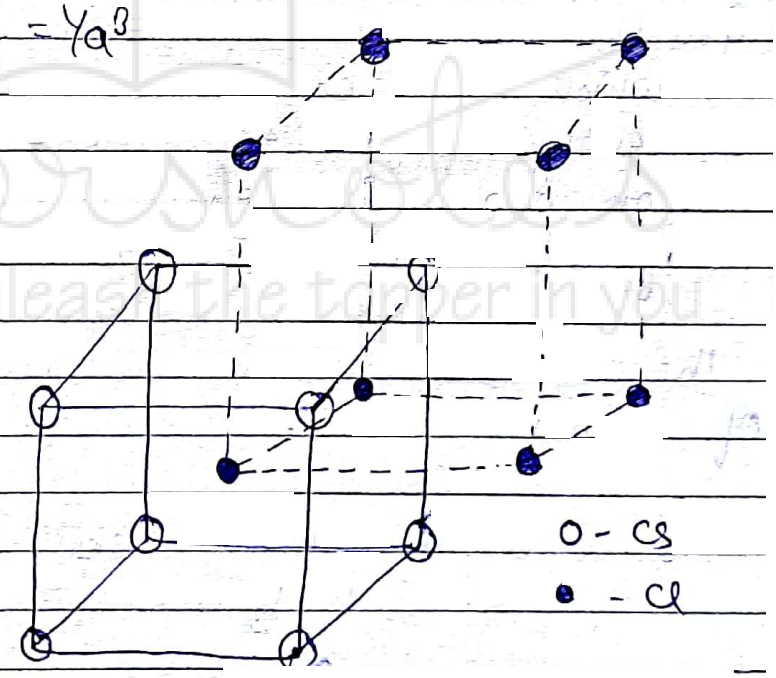
CsCl structure can be consider a interpenetration of two S.C. unit cell if one unit cell origen at (0,0,0) then other origen at (½, ½, ½)

1. No. of atoms - 2 (1 Cs + 1 Cl)
   = 1 CsCl molecule
2. No. of nearest atom - 8
3. $r_{Cs} + r_{Cl} = \frac{\sqrt{3}}{2} a$
4. No. of second nearest atom - 6
5. second nearest neighbour distance = a
6. Volume of unit cell a^3
7. Volume of perimitive cell - a^3
8. Molecular density = $1/a^3$
9. APF =

$$= \frac{\frac{4}{3}\pi r_{Cl}^3 + \frac{4}{3}\pi r_{Cs}^3}{a^3}$$

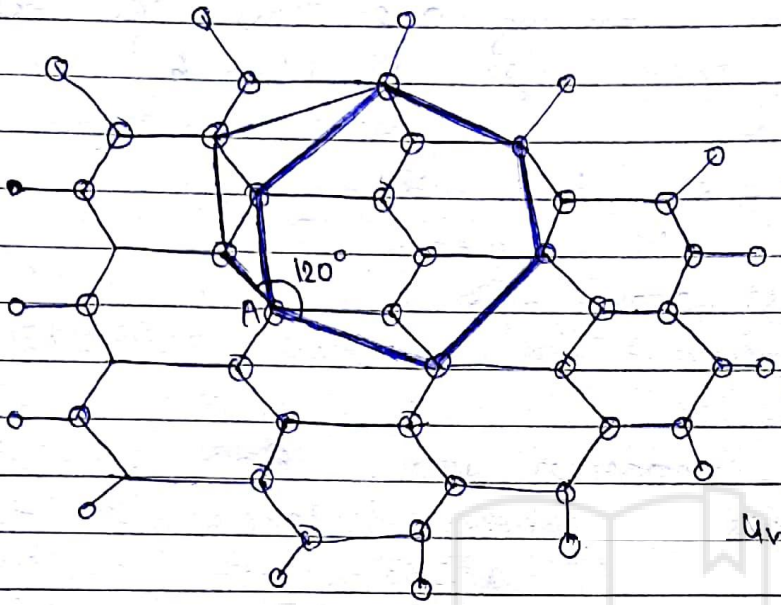
$$= \frac{\frac{4}{3}\pi \left(r_{Cl}^3 + r_{Cs}^3\right)}{\left(\frac{2}{\sqrt{3}}\right)^3 \left(r_{Cs} + r_{Cl}\right)^3}$$

$$= \frac{\sqrt{3}\pi}{2} \frac{\left[\left(\frac{r_{Cs}}{r_{Cl}}\right)^3 + 1\right]}{\left(1 + \frac{r_{Cs}}{r_{Cl}}\right)^3}$$

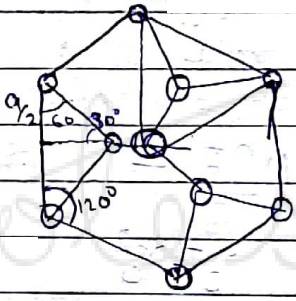


10. loose packed structure
11. ex - CsCl, CsBr, RbCl. etc.

Graphene :-



Unit cell of Graphene.



Graphen is a 2-D structure in which each carbon atom is covalently bounded to 3 near by carbon atom. Graphene has 2-D hexagonal structure with 2 atom basis.

This structure is known as Honey.

The Graphaide structure is made up of stracking of graphite sheet.

1. No. of atom per unit cell

$$n = 1/3 \times 6 + 4 = 6$$

2. No. of nearest atom (co-ordination no) = 3

3. $a/2 = 2r \cos 30°$

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

No. of primitive unit cell = 2

4. No. of second nearest neighbour = 6
5. Second nearest neighbour distance = a
6. Area of unit cell $\frac{\sqrt{3}}{4} a^2 \times 6$

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

7. Area of primitive unit cell = $\sqrt{3}/2\, a^2$
($\frac{1}{3}$ area of unit cell)

8. Atomic density (No. of atom per unit area)

$\frac{6}{\frac{3\sqrt{3}}{2} a^2} = \frac{4}{\sqrt{3} a^2}$

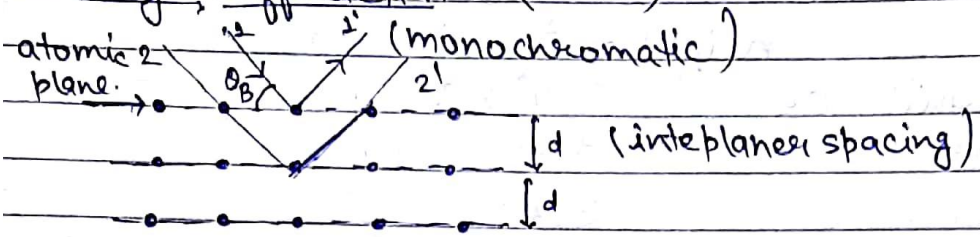
9. Packing fraction

$= \frac{\text{area of atoms}}{\text{area of atoms per unit cell}}$

$= \frac{6 \times \pi r^2}{\frac{3\sqrt{3}}{2} a^2} = \frac{\pi}{3\sqrt{3}} = 60.5\%$

10. loosed packed structure.
ex Graphene.
Graphene & Graphaite are conductors.
Graphite is also made by Graphene.
Co-ordination no. is 3 (covalent bonds)
Valancy of carbon - 4
free e^- - 1 so it is conductor.
In diamond e^- per carbon atom free so it behave like electric insulator.

X-ray differaction :- (XRD)



(monochromatic)

(interplaner spacing)

X-rays are EM waves of very short wavelength (1-10 A°)
~~typical order~~ (1~1A°)

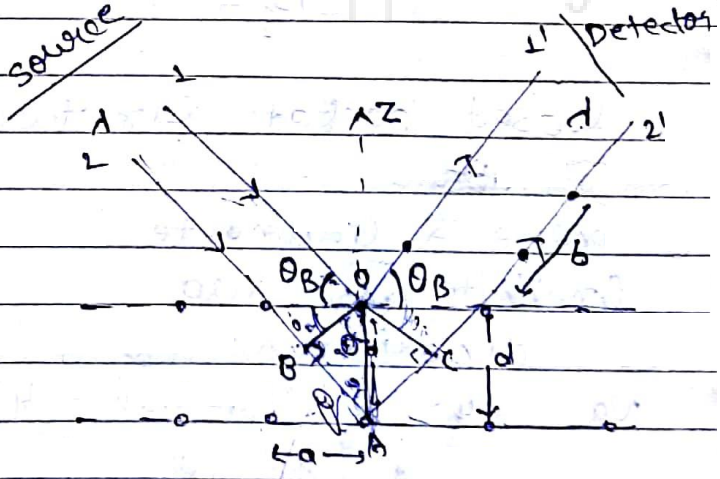
White light cann't be used in the determination of crystal structure because wavelength of white light is not be comparable to interatomic distance

A plane differaction grating cann't differect x-rays.

A crystal is behaving as a natural grating of x-rays.

One atomic plane differects only $10^{-3} - 10^{-5}$ part of incident intensity.

no. of planes to differects all part of incident intensity is $10^3 - 10^5$



Angular speed of source and detector should be same

1' and 2' are in the position of infere

Condition of inference

1- same

$\Delta\phi$ - const.

Path difference = AB + AC

= $n\lambda$

$\boxed{2d_{hkl}\sin\theta_B = n\lambda}$ Bragg's law.

Bragg's law is consequence of periodicity of lattice.

θ_B - Bragg's angle

n - order of differaction (n = 1, 2, 3 ...)

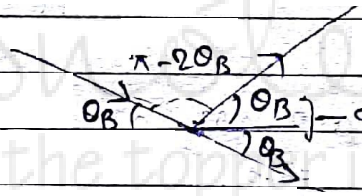
λ - wavelength of incident x-ray.

For the numericle purpose n=1 until n value is not mention in the que.

Angle of differaction :-

angle b/w incident x-ray and diffracted x-ray beam. = $2\theta_B$

(angle is always b/w vector of tail-tail and head-head always never in heal-tail .)



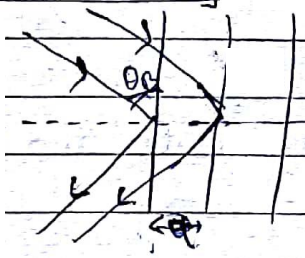
If and θ_B is measured in x-y plane then Bragg's law

$2d\sin\theta_B = n\lambda$

If θ_B is measured in x-z plane then $2a\sin\theta_B = n\lambda$

" " y-z " $2b\sin\theta_B = n\lambda$

$\boxed{2a\sin\theta_B = n\lambda}$



$\boxed{2b\sin\theta_B = n\lambda}$