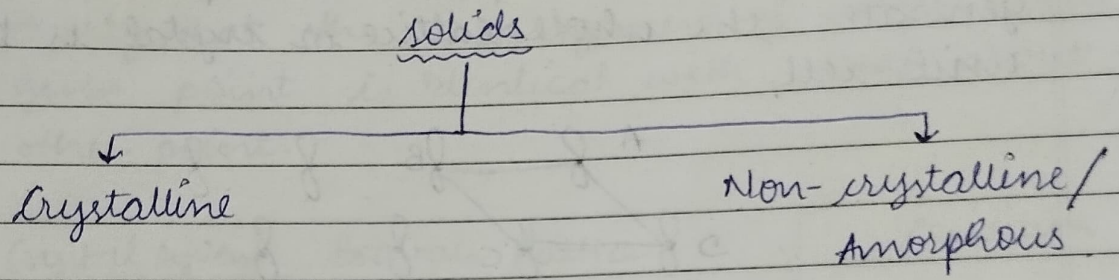
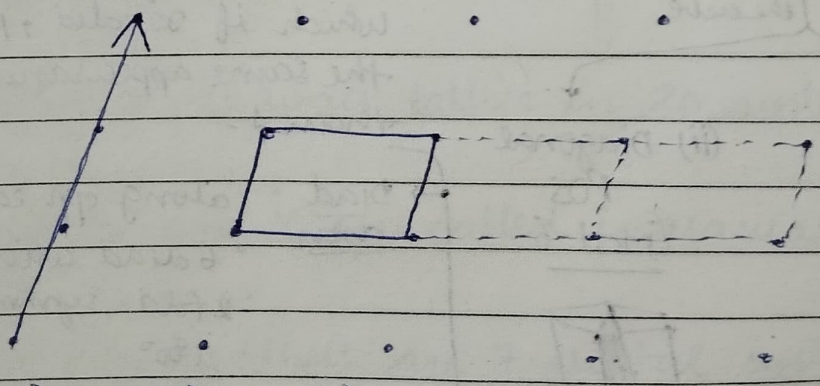
Unit-III

Crystal structure and semiconductor

Crystalline substances are those in which the arrangements of units of matter (ions, atoms, cluster of ions) inside the solid is regular or periodic whereas in amorphous solid, there is no definite order in the arrangement of units.



Lattice: Any ideal crystal is constructed by the definite regular repeatative of identical structural units in space so that the environment of each point is the same. These is known as lattice. Each point in the lattice is called a lattice point and it has a highest probability of finding an atom or an ion.



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

$\vec{a}$, $\vec{b}$ and $\vec{c}$ are fundamental translational vectors.

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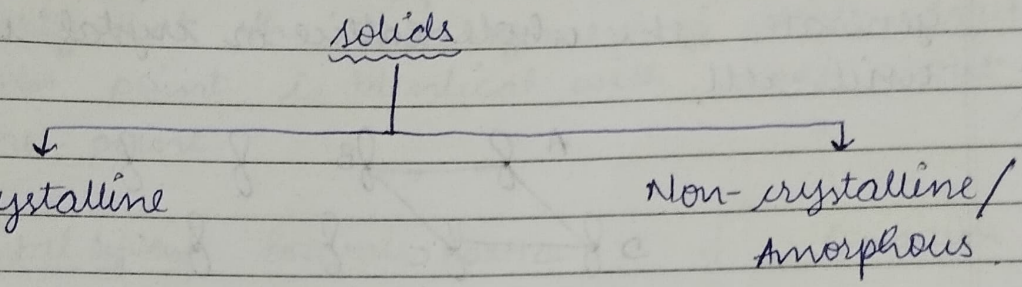

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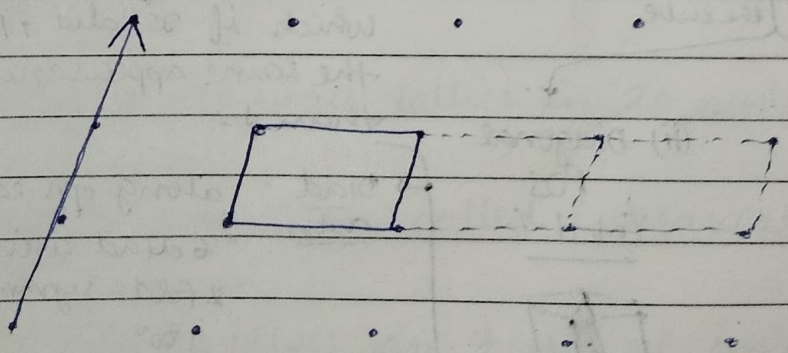


$$\vec{T} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c}$$

$\vec{a}$, $\vec{b}$ and $\vec{c}$ are fundamental translational vectors.

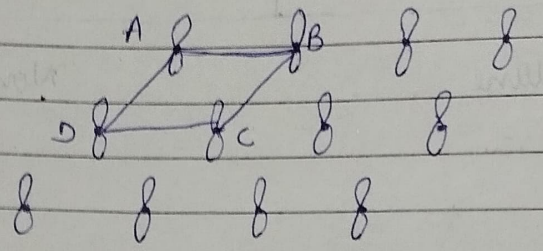
n_1, n_2, n_3 are integers.

★ Basis :-

In a crystal structure every lattice point is associated with an assembly of atom which is called basis.

Crystal structure = lattice + Basis.

★ **Unit cell :-** The smallest unit of lattice or crystal which on continous repeatation can generate the whole lattice or crystal is known as unit cell.



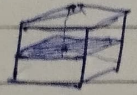
ABCD is a unit cell here.

(pdf in ppt) ★ **Symmetry in crystal:**

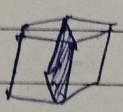
① Mirror Plane of Symmetry

Plane -
(i) passes through origin
(ii) divides equally the cube

(i) POS
Total - 3



(ii) Diagonal POS
Total - 6



② Rotation Axis of symmetry

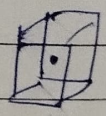
→ an axis of line about which if rotated, presents the same appearance more than 1.

→ Diad axis : · along opp. edge
· 6 diad axis
· 2 fold symm.
· 180°

→ Triad axis : · along diagonal
· 4 triad axis
· 3 fold
· 120°

→ tetra axis : · along opp. faces

③ Centre of Symmetry



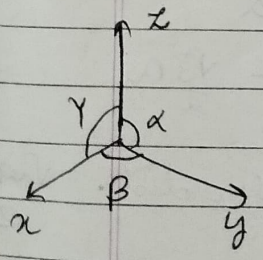
A point group about a lattice point is defined as the collection of symmetry ~~EMo~~ operation (mirror plane of symmetry, centre of symm., Rotational axis of symm.). which way applied about the lattice point. it leaves the lattice invariant.

Bravais Lattice :- It is defined as an infinite (space lattice) no. of points in the space with a property that the arrangement of point about the given point is identical with that about any other point.

∴ 2D

	Crystal System	Bravais Lattice	Condition
①	Square	Square	$\|\vec{a}\| = \|\vec{b}\|$, $\gamma = 90°$
②	Rectangular	(i) Rectangular Primitive (ii) Rectangular centered	$\|\vec{a}\| \neq \|\vec{b}\|$, $\gamma = 90°$
③	Hexagonal	Hexagonal	$\|\vec{a}\| = \|\vec{b}\|$, $\gamma = 120°$.
④	Oblique	Oblique	$\|\vec{a}\| \neq \|\vec{b}\|$, $\gamma \neq 90°$

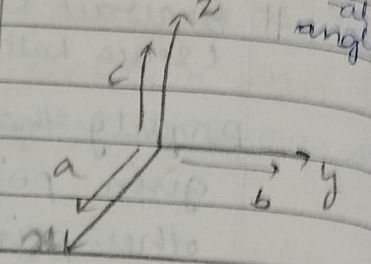
→ There are total 5 bravais lattice in 2D system.



α, β and γ are called interaxial angles.

→ In 3D their are 7 crystal system with 14 Bravais lattice.

Crystal system	Bravais lattice	condition
Cubic	(i) Simple cubic (SC) (ii) Body centred cubic (BCC) (iii) Face centred cubic (FCC)	$a=b=c$ Lattice parameters $\alpha=\beta=\gamma=90^\circ$ Interaxial angles



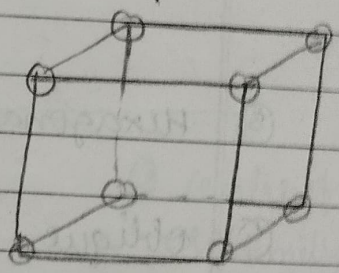
Coordination Number :- The no. of nearest neighbour atoms or ions surrounding an atom or ion.

(i) No. of atoms present per unit cell

a. $8 \times \frac{1}{8} = 1 \longrightarrow$ SC.

b. $8 \times \frac{1}{8} + 1 = 2 \longrightarrow$ BCC

c. $8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 4 \longrightarrow$ FCC.



(ii) Co-ordination Number - 6 (6 nearest atoms to 1 atom)

SC $\longrightarrow$ 6 ; Nearest neighbour dist. = a

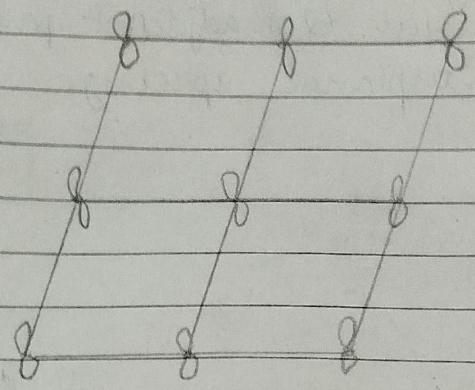
BCC $\longrightarrow$ 8 ; Nearest neighbour dist. = $\frac{\sqrt{3}}{2}a$

FCC $\longrightarrow$ 4 + 4 + 4 = 12 ; Nearest neighbour dist. = $\frac{\sqrt{2}a}{2}$

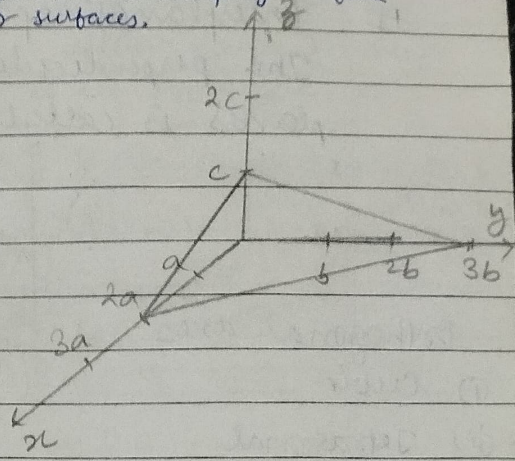
$= \frac{a}{\sqrt{2}}$.

The orientation of a surface may be defined by considering how the plane intersects the main crystallographic axes of the solid. The application of set of rules leads to the assignment of miller indices (hkl) which are set of no. which quantity the intercepts & thus may be used to uniquely define the plane or surfaces.

Millers Indices :-



represented in set of (h, k, l)



Method :

1. Determine the coordinates of the ~~intercepts~~ intercepts made by the plane along the 3 crystallographic axes (x, y, z) . (2a, 3b, c)
2. Express the intercepts as multiples of the unit cell dimensions or lattice parameters along the axes,

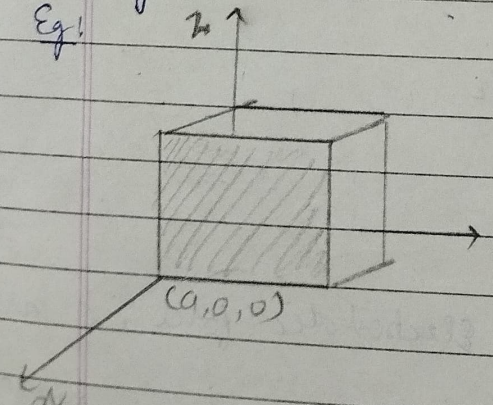
i.e	$\frac{2a}{a}$	$\frac{3b}{b}$	$\frac{c}{c}$
	2	3	1.

3. Get the reciprocals of these numbers i.e.

$\frac{1}{2}$, $\frac{1}{3}$, 1.

4. Reduce the reciprocals to the smallest set of integral no. and enclose them in bracket (LCM=6). Multiply by LCM. (3 2 6) ← Millers indices.

Eg:

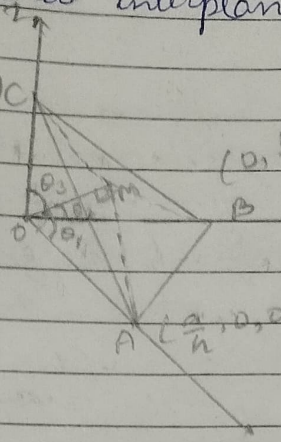


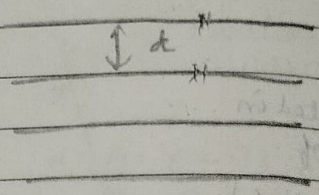
	x	y	z
Intercepts →	a	∞	∞
	$\frac{a}{a}$		
	1	∞	∞
Reciprocal	1	0	0

Millers indices (100)

Interplanar spacing

The perpendicular dist. b/w adjacent parallel lattice planes is called interplanar spacing.





OM - $d_{(hkl)}$ - interplanar spacing.

* Let (h, k, l) will be miller indices of plane ABC

Orthogonal axes
(i) Cubic
(ii) Tetragonal
(iii) Orthorhombic.

* Direction cosines:

$\cos\theta_1$ = First direction cosine
$\cos\theta_2$ = second direction cosine
$\cos\theta_3$ = Third direction cosine.

$$\cos\theta_1 = \frac{d_{hkl}}{a/h}$$

$$\cos\theta_2 = \frac{d_{hkl}}{b/k}, \quad \cos\theta_3 = \frac{d_{hkl}}{c/l}$$

From property of direction cosines:

$$\cos^2\theta_1 + \cos^2\theta_2 + \cos^2\theta_3 = 1$$

substituting values of $\cos^2\theta_1$, $\cos^2\theta_2$, $\cos^2\theta_3$.

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

$$d^2_{hkl}\left(\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right) = 1$$

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

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

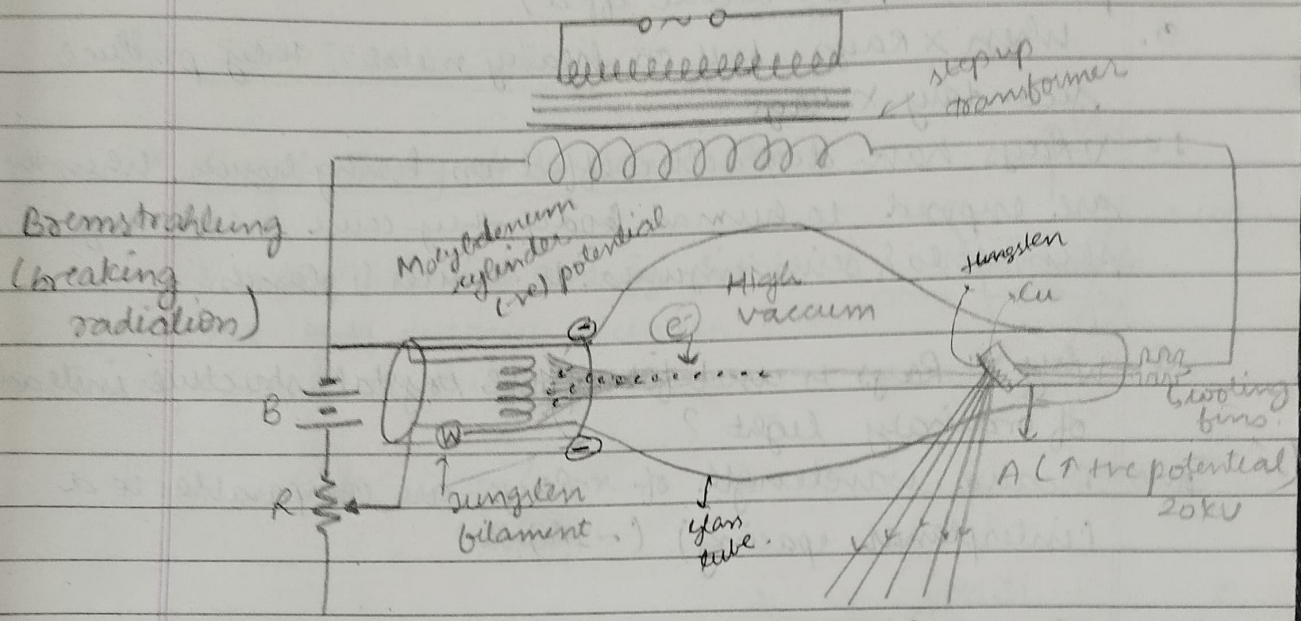
Production of X-rays:-

- When Thermal vibrations > Electrostatic force; e^- are released.
- Why only Tungsten: (M.P.)↑ (At. no.↑ = 74), so that it is not melted due to the bombardment of fast-moving e^-, which cause lot of heat
  M.P. = 3422°C.

X-Ray are produced when a beam of fast moving cathode rays that is e^- strike a heavy target materials such as tungsten or molybdenum

- Why Cu as Target material? (at no. ↑ - does not allow hard x-rays to be produced.)
  - gives shortest λ above 1Å.

→ e^- are released from tungsten by thermionic emission



X-Ray Coolidge tube

Properties of x-Rays ($\lambda = 0.01 - 10nm$)

1. X-Rays are ~~EM~~ waves of very short wavelength. They travel in straight lines with the velocity of light. They are invisible to eyes.
2. Under suitable conditions, x-rays are reflected & refracted like ordinary light.
3. They exhibit the property of interference, diffraction & polarisation like ordinary light.
4. They are not reflected by electric & magnetic fields.
5. X-rays ~~are~~ can penetrate through the substances which are opaque to ordinary light, eg. wood, flesh, thick paper, thin sheets of metals.
6. They cause fluorescent in many substances like barium, cadmium, tungsten, zinc sulphide etc
7. X-rays can ionise a gas through which they pass

(When a beam of x Rays is passed through a gas, the gas molecules are broken in the +ve & -ve charged particles & the gas becomes conducting ie the gas is ionised)

8. When x Rays face on certain metals, they liberate photo e⁻ (photo electric effect).

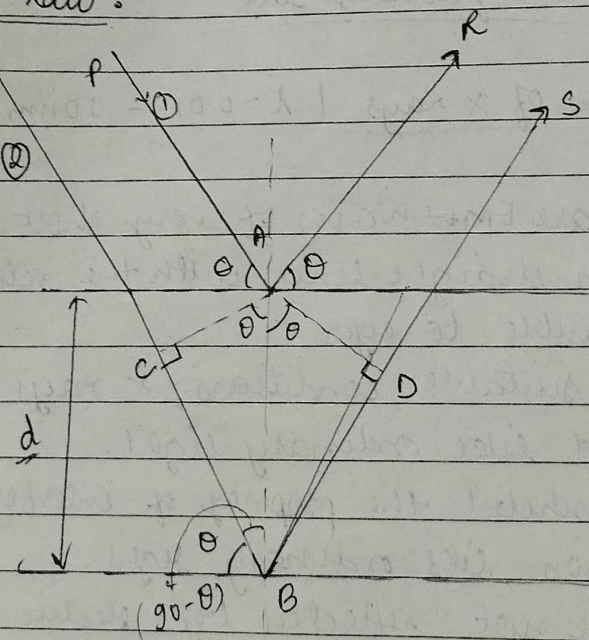
9. When x Rays fall on heavy metal, they produce secondary x-Rays

10. x-Rays have destructive effect on living tissues. When they are exposed to human body, they cause reddening of skin, sores & series injuries to tissues & glands.

Q. Why x-Rays is used for probe crystal structure instead of ordinary light?

Ans Because wavelength of x-Rays are comparable to d (interplanar spacing) (~1Å)

Bragg's Law:-



Here the path According to

path difference = nλ

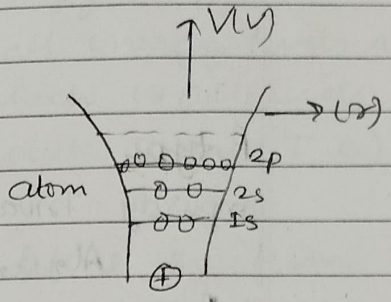
CB + BD = nλ —①

$CB = BD = d\sin\theta$ —— (2)

$\boxed{2d\sin\theta = n\lambda}$, where $n = 1, 2, 3 \ldots$

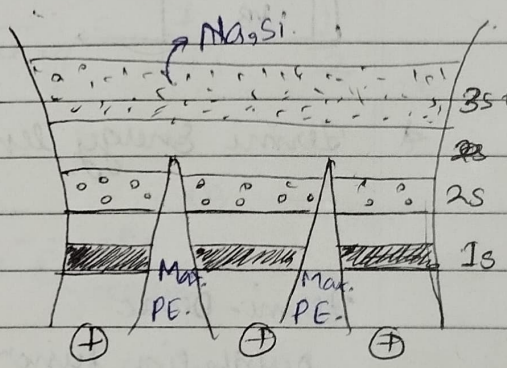
SEMICONDUCTOR :-

★ Band theory of semiconductor :-



V is the potential energy & r is the ~~diff~~ distance between e⁻ and its nucleus.

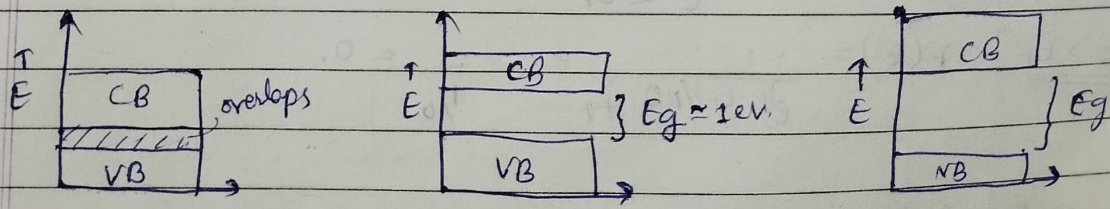
$$PE = \frac{-Ze^2}{4\pi(z)r}$$



The Band which is completely occupied or having highest occupied band energy is valence band.

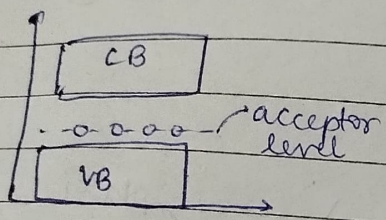
The lowest unfilled or partially filled energy band is conduction band.

→ forbidden band energy gap — Si - 1.1eV
Ge - 0.7eV.

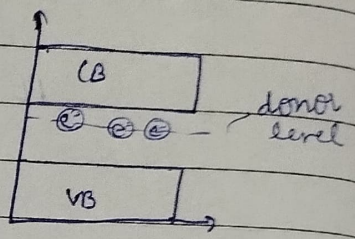


conductor semi-conductor insulator.

P-type
impurity - Trivalent
Al, B, Ga



N-type
Pentavalent impurity
P, As, Sb, Bi.



* Fermi Energy level :-

Fermi-Dirac Distribution func^n → $P(E) = \frac{1}{e^{(E-E_f)/KT} + 1}$ $KT \to K_BT$

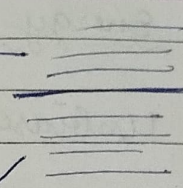
Probability of occupation of the particle in energy E.

(1) At T=0K. , $E > E_f$
$E < E_f$

$E > E_f$ $P(E) = \frac{1}{e^{(E-E_f)/K0} + 1} = \frac{1}{1/0} = 0.$

$E < E_f$ $P(E) = \frac{1}{e^{(E-E_f)/K0} + 1} = \frac{1}{1/0} = \frac{1}{e^{-\infty} + 1} = \frac{1}{1/e^{\infty} + 1} = \frac{e^{\infty}}{e^{\infty} + 1} = 1.$

level above the fermi energy level are all unfilled with e⁻



level below the fermi energy level all level are filled with e⁻.

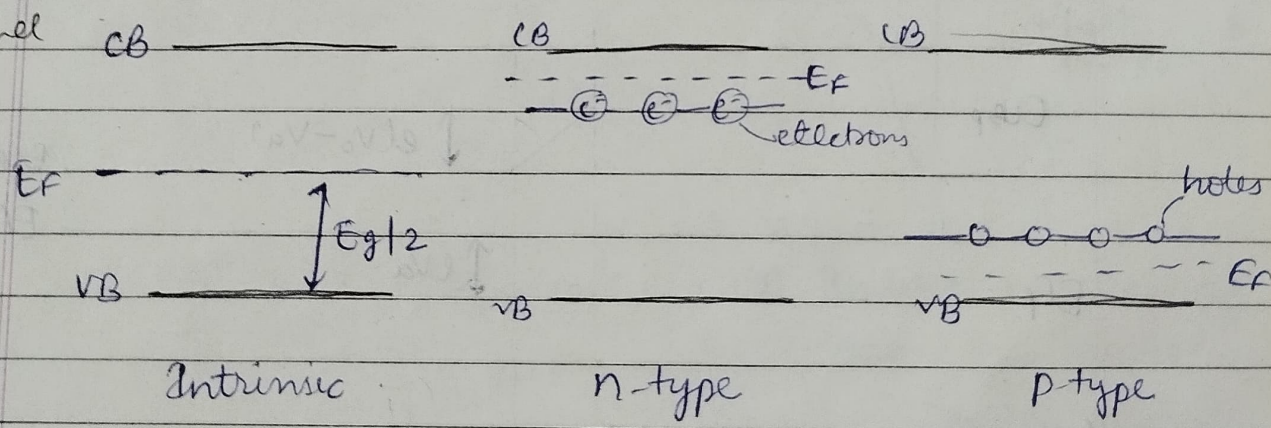
★ From this we can define fermi energy level as a particular state, below which all energy levels are completely filled and above which all levels are completely empty at absolute Temp (T=0).

At T≠0, In this case, we can define the fermi energy state as the state whose probability of occupation of the particle is 1/2 at T≠0.

↳ T≠0, E = Ef

$$P(E) = \frac{1}{e^{0/kT}+1} = \frac{1}{1+1} = \frac{1}{2}$$

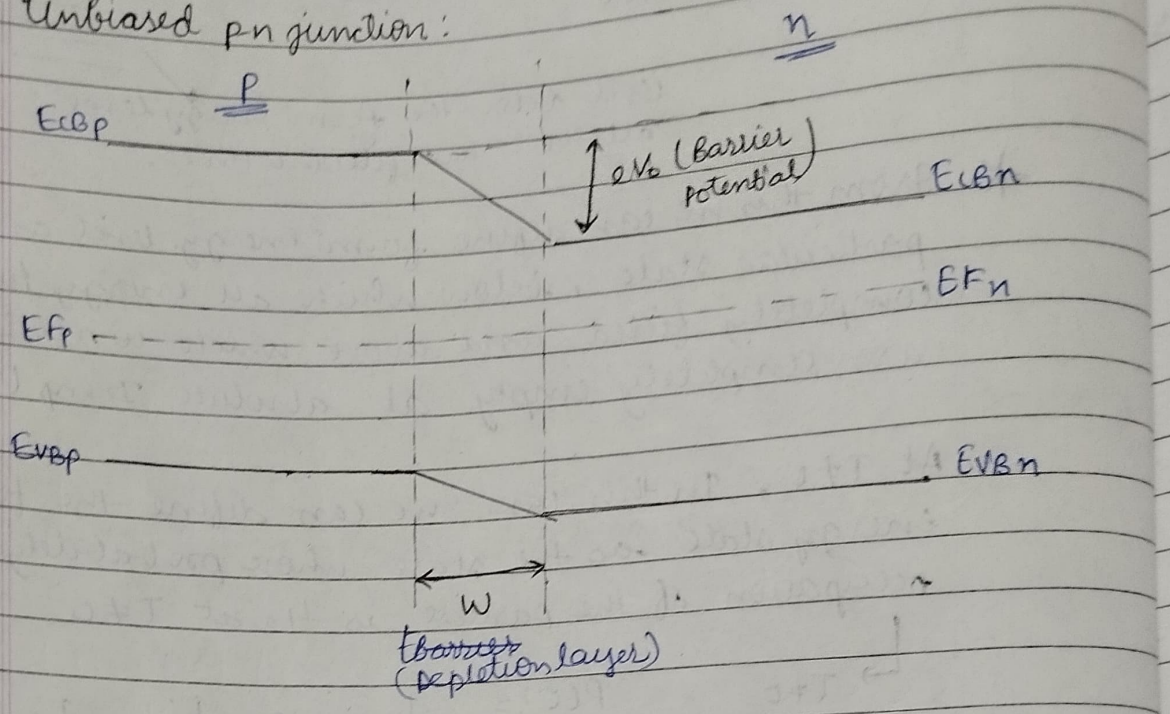
position of Fermi level



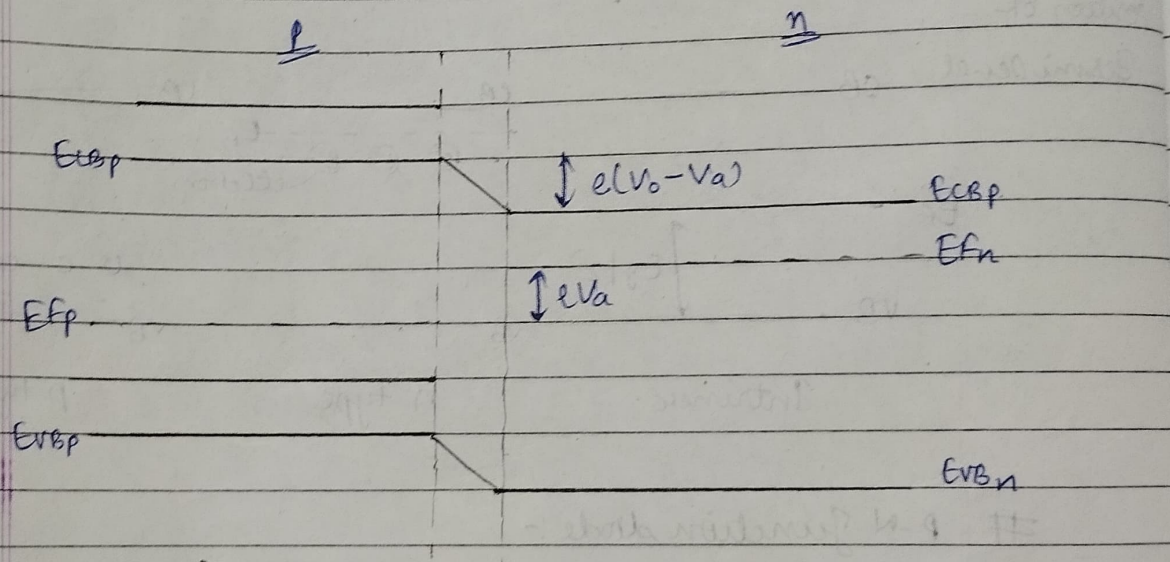
P-N Junction diode :-

* Energy band diagram:

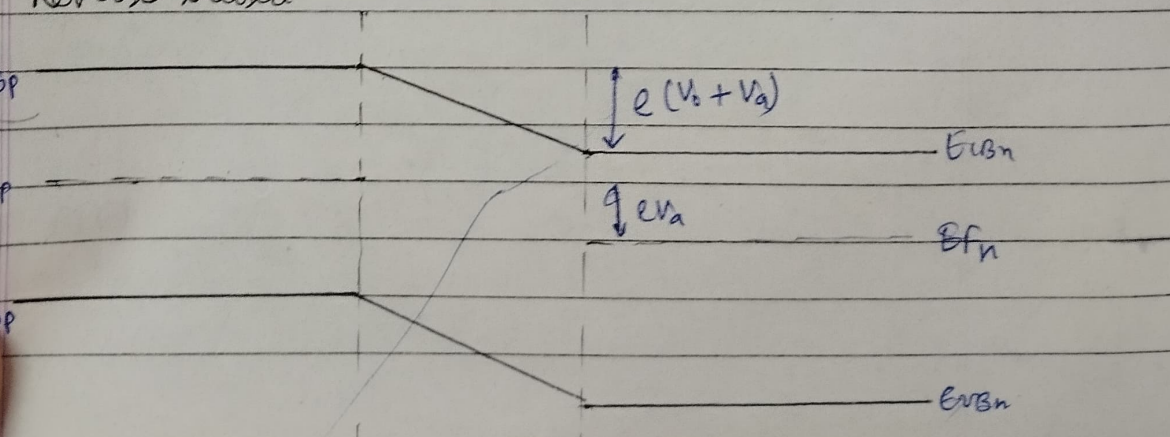
① Unbiased pn junction:

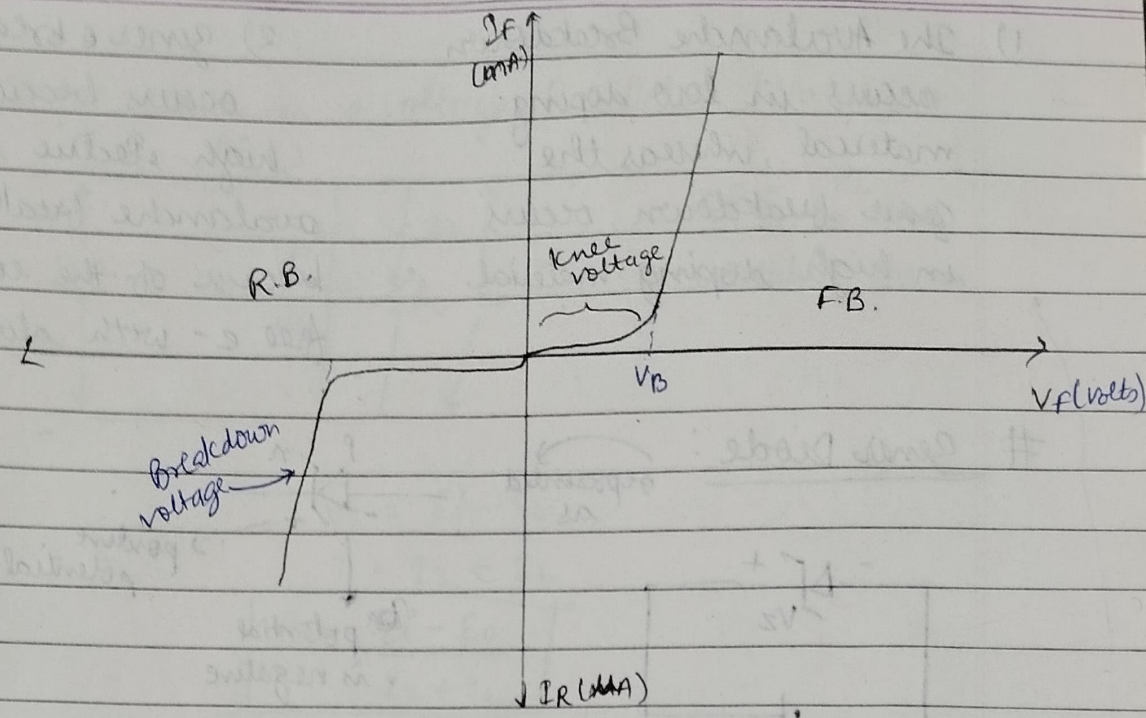


② Forward biased:

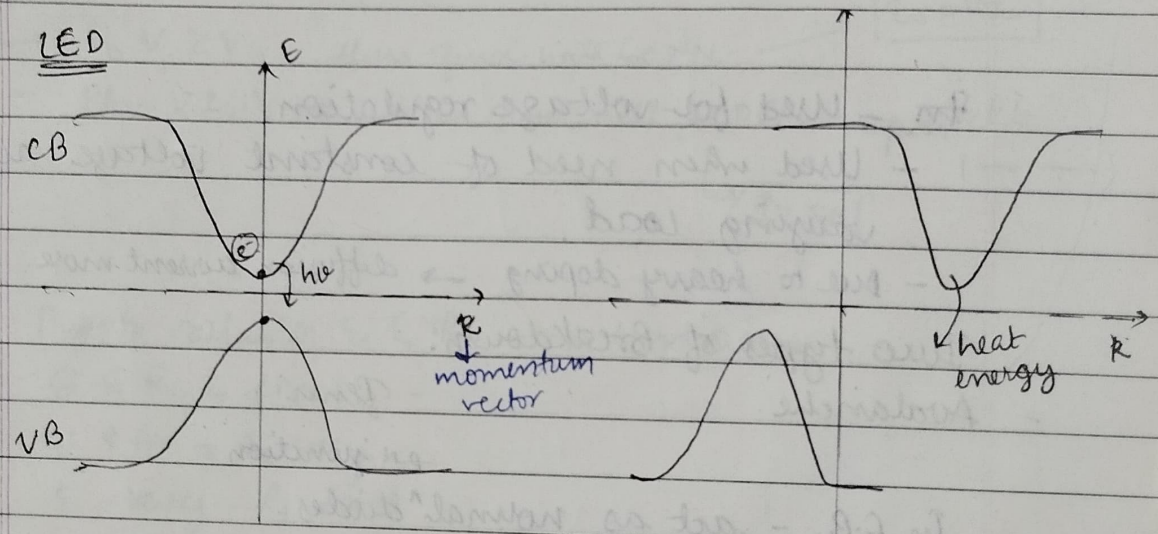


③ Reverse biased





LED



(a) Direct Band energy gap.
Eg: GaAs
↓
here photon energy releases

(b) Indirect Band energy gap. Eg: Si, Ge.
↓
here heat energy releases.

$$E = \frac{hc}{\lambda} \Rightarrow \lambda = \frac{hc}{E_g} = \frac{12400 \text{ eV-Å}}{E_g(\text{eV})}$$

Difference b/w Avalanche & Zener Breakdown:-
→ The difference b/w these two is based on mechanism of occurrence.