Material science

(16smbeph1)

(Brief notes for reference)

By

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Note: Students are instructed to refer book for study and reference respectively for further elaborate points as prescribed by the University.

'UNIT-1'

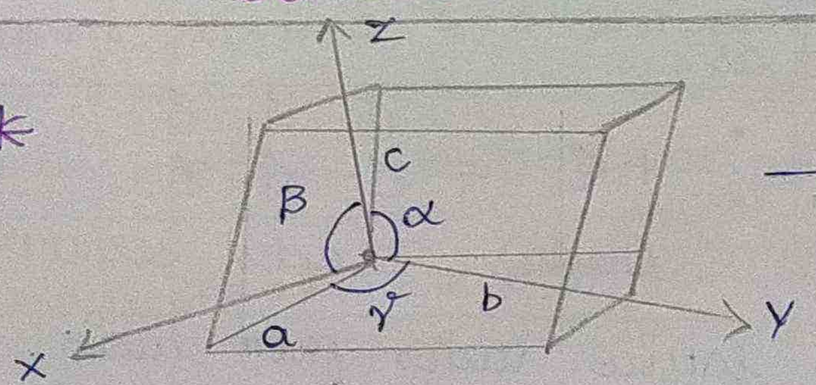
- 'CRYSTAL STRUCTURE'

TWO MARK QUESTIONS :-

1) Define unit cell :

* unit cell is the smallest portion of a crystal lattice.
* It is the simplest repeating unit in a crystal structure.
* The entire lattice is generating by the repetition of the unitcell in different directions.
* The unit cell has 6 parameters. They are three edges - a, b, c and the angles between the edges be α, β and γ.
* The unit cell is divided into types namely,
  1) Primitive unit cell
  2) centred unit cell
     - Body centered unit cell
     - Face centered unit cell.
     - End centered unit cell.

*



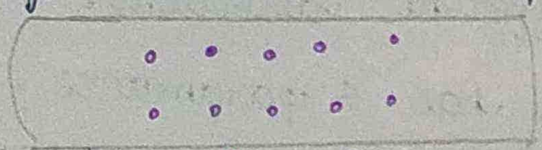
→ which represent 3 edges & 3 angles

2) Define lattice and how it varies from basis?

* The crystal **lattice** is the symmetrical three dimensional structural arrangements constituent particle inside a crystalline solid as points.

* In a crystal lattice each atom or molecule is represented by single points. These points are called lattice site or lattice points. These points are joined by a straight line is crystal lattice.

* The crystal lattice is represented by



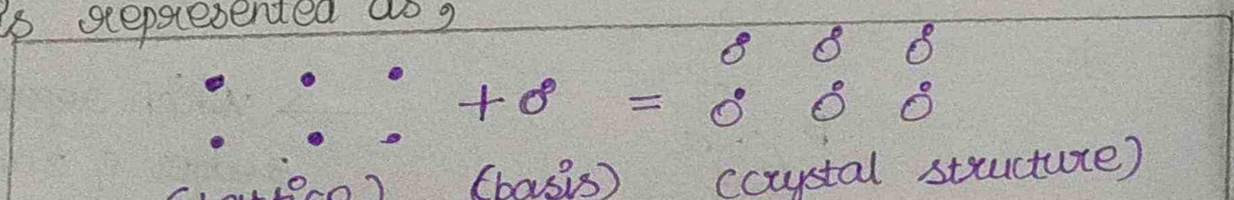
* The crystal basis is the arrangement of atoms. that is particular to the mineral being considered.

LATTICE DIFFER FROM BASIS :

* The lattice which is periodic arrangement of point in space it describe the structure of crystal

* The basis is a collection of atoms in particular fixed arrangement in space.

It is represented as,



This is how the lattice varies from basis.

3) What do you mean by Bravais lattice?

* Bravais lattice is a set of all equivalent atoms in a crystal that are able to brought back into themselves when they are displaced by the length of the unit vector in a direction ll to a unit vector.

* There are 14 types of Bravais lattices. They are not always primitive. They are classified according to symmetry and space rotation into the seven crystal systems.

* They are represented as, P, I, F & C. P-Primitive, I - BCC, F - FCC, C - End centered.

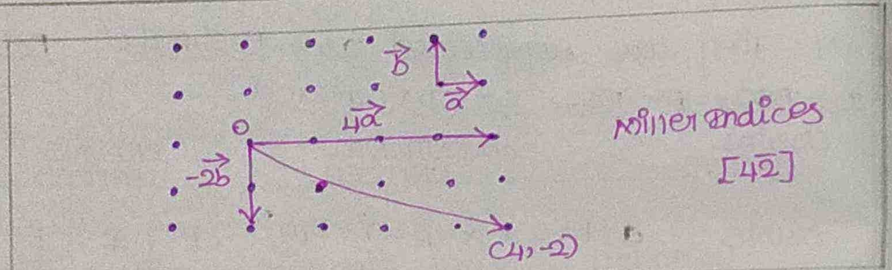
CRYSTAL SYSTEM	CONVENTIONAL UNIT CELL	BRAVAIS LATTICES			
cubic	$a=b=c$, $\alpha=\beta=\gamma=90^\circ$	P	I	F	
Tetragonal	$a=b\neq c$, $\alpha=\beta=\gamma=90^\circ$	P	I		
orthorhombic	$a\neq b\neq c$, $\alpha=\beta=\gamma=90^\circ$	P	I	F	C
Hexagonal	$a=b\neq c$, $\alpha=\beta=90^\circ$, $\gamma=120^\circ$	P			
Trigonal	$a=b=c$; $\alpha=\beta=\gamma\neq 90^\circ$	P			
monoclinic	$a\neq b\neq c$; $\alpha=90^\circ$, $\gamma=90^\circ$ $\beta\neq 90^\circ$	P			C
Triclinic	$a\neq b\neq c$; $\alpha\neq\beta\neq\gamma$	P			

4) What are Miller Indices ?

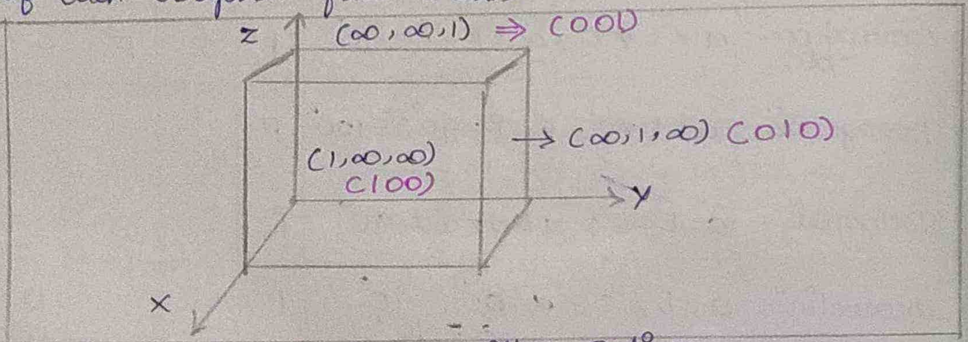
* Miller Indices are a method of describing the orientation of a plane or set of planes with in a lattice in relation to the unit cell.

* It is a symbolic vector representation for the orientation of an atomic plane in a crystal lattice and are defined as the reciprocals for the fractional intercepts which the plane makes crystallographic axes.

MILLER INDICES FOR DIRECTION AND PLANE EXAMPLES :-



* Miller Indices are the reciprocals of the parameters of each crystal face thus,



* These are called as Miller Indices.

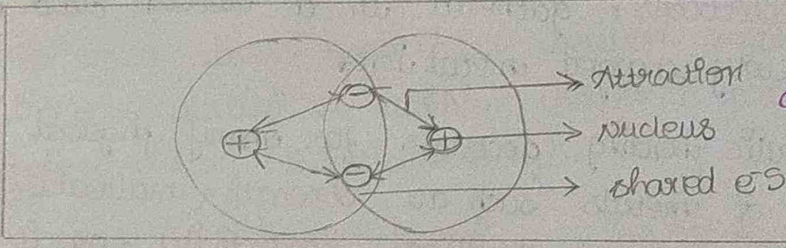
5) Define Covalent Bonding :-

* In 1916, "Lewis" suggested the covalent bonding phenomenon.

* A covalent bond is formed by equal sharing of electrons from both the participating atoms. The pair of electrons participating in this type of bonding is called shared pair or bonding pair.

* The covalent bonding among atoms in the sharing of electrons in their valance shells to attain the nearest noble gas configuration and to contribute the stability.

* The sharing will be among similar or dissimilar atoms. Bonding takes place between atoms with small differences in electronegativity which are close to eachother in periodic table (between metals and nonmetals).



Formation of covalent bond.

* EXAMPLES :-

1) H • + • C̈l : ⟶ H — C̈l : ⇒ HCl

2) Ö = C = Ö ⇒ CO_2

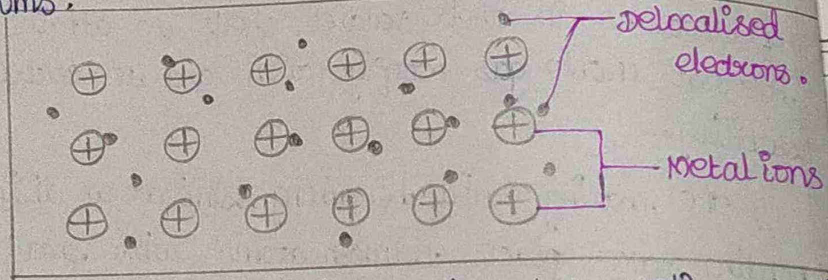
3) :Ö• + :Ö• ⟶ •Ö::Ö: or <O=O> ⇒ O_2

6) Write about Metallic bonding ?

* In metals each atom loses all its valance electrons and becomes a positively charged ion.

* The free electrons form a electron cloud.

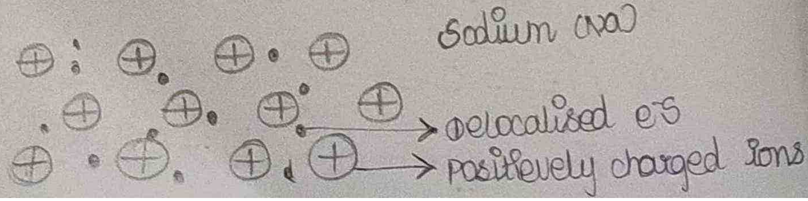
* The electrons are like sea and the metal closely packed ions are immersed in the sea. The valance electrons move freely in the sphere of influence of other atoms.



* Metallic bond constitutes the electrostatic attractiv forces between the delocalized electrons called conduction electrons, gathered in a electron cloud and the positively charged metal ion.

* Metallic bonding accounts for many physical properties of metals such as strength, malleability, ductility, thermal and electrical conductivity, opacity and luster.

Eg:-



* The factors that affect metallic bond strength are,

1) The number of e-s delocalised from the metal: the greater the number of delocalized electrons the stronger the bond.

2) Size of the cation the smaller the ionic radius, the greater the effective nuclear charge acting on the electron sea.

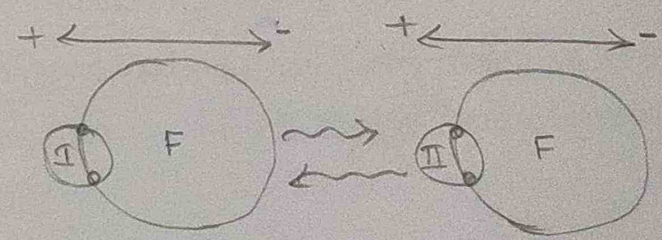
7) Write short note on hydrogen bonding:

* A hydrogen bond is the attractive interaction of a hydrogen atom and a electronegative atom. such as nitrogen, oxygen or fluorine, that comes from another molecule or chemical group.

* The hydrogen has a polar bonding to another electronegative atom to create the bond.

* These bonds can occur between molecules (intermolecularly) or within different parts of a single molecule (intramolecularly).

Eg:-

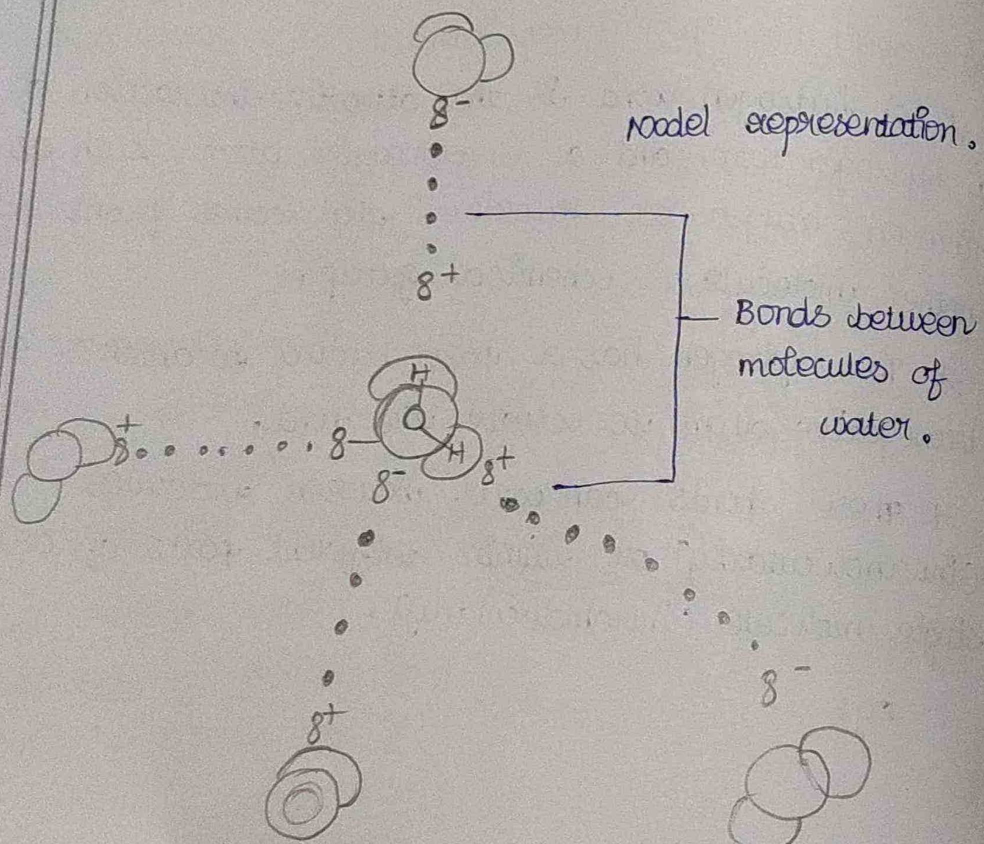


Hydrogen bond in HF.

* The hydrogen bond is stronger than a vanderwaal interaction, but weaker than covalent or ionic bonds.

* This types of bond occur in both inorganic molecules such as water and organic molecules like DNA.

* Another Example be the hydrogen bond between molecules of water.



PART-B

WRITE ABOUT TYPES OF BRAVAIS LATTICES :-

* Bravais lattice is a set of all equivalent atoms in a crystal that are able to brought back into themselves when they are displaced by the length of the unit vector in a direction ⫽ to a unit vector.

* There are 14 types of Bravais lattices. They are not always primitive. They are classified according to symmetry and space rotation into the seven crystal system.

* A bravais' lattice is an infinite array of discrete points with an arrangement and orientations that appears exactly a same, for whichever of the point array is viewed.

* A (3D) Bravais lattice consist of all points with position vectors R of the form,

$$R = n_1 a_1 + n_2 a_2 + n_3 a_3 \longrightarrow (1)$$

* Here, a_1, a_2 and a_3 are any three vectors not all in the same plane. n_1, n_2 and n_3 range through all integral values.

* Thus the point $\sum n_i a_i$ is reached by moving n_i steps of length a_i in the direction of a_i for $i = 1, 2, 3$

* The vectors a_i are called primitive vectors and are said to generate or span the lattice.

* They are represented as P, I, F and C.

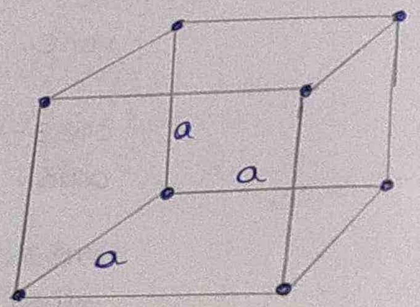
P - primitive, I - BCC, F - FCC, C - end (or) Base centered

CRYSTAL SYSTEM	CONVENTIONAL UNIT CELL	BRAVAIS LATTICES		
CUBIC	$a=b=c, \alpha=\beta=\gamma=90^\circ$	P	I	F
TETRAGONAL	$a=b\neq c, \alpha=\beta=\gamma=90^\circ$	P	I	
ORTHORHOMBIC	$a\neq b\neq c, \alpha=\beta=\gamma=90^\circ$	P	I	F
HEXAGONAL	$a=b\neq c, \alpha=\beta=90^\circ$, $\gamma=120^\circ$	P		
TRIGONAL	$a=b=c, \alpha=\beta=\gamma\neq 90^\circ$	P		
MONOCLINIC	$a\neq b\neq c; \alpha=90^\circ \neq \beta$, $\gamma=90^\circ$	P		
TRICLINIC	$a\neq b\neq c, \alpha\neq\beta\neq\gamma$	P		

SYSTEM	BRAVAIS LATTICE	CHARACTERISTICS OF SYMMETRY ELEMENTS.
simple (cubic)	simple, Body-centered, Face-centered	Four 3-fold rotation axes (along cube diagonal)
Tetragonal	simple, Body centered	one-4 fold rotation axis.
orthorhombic	simple, base-centered, body centered and Face centered.	Three mutually orthogonal 2-fold axis of rotation.
Monoclinic	simple, Base centered	one 2 fold axis of rotation.
Triclinic	simple	None
Trigonal	simple	one 3-fold rotation axis.
Hexagonal	simple	one 3-fold rotation axis.

2) WRITE ABOUT SIMPLE CUBIC CRYSTAL WITH EXAMPLE

* Simple or primitive cubic lattice csc or cubic has one lattice point at the each corner of the unit cell.
* It has unit cell vectors $a=b=c$ and inter-axial angles $\alpha=\beta=\gamma=90^\circ$
* The simplest crystal structures are those in which there is only a single atom at each lattice point.
* In the sc structures the spheres fill 52% of the volume.
* The number of atoms in a unitcell is 1



* Let a' be the edge length of the unit cell and r be the radius of sphere.
* As spheres are touching eachother.

* Therefore $a = 2r$. Number of spheres per unit cell $= \frac{1}{8} \times 8 = 1$
* Where the the co-ordination number and packing factor be,
* Each corner of the atom touches four atoms in its horizontal plane, and two atoms one vertically above it and one vertically below it.
* So there are six equally spaced nearest neighbour atoms at each distance 'a' from the atom. Therefore, the co-ordination number is six.

$$CN = 6.$$

$$\text{Packing factor} = \frac{\text{volume of all atoms in the unitcell}}{\text{volume of the unitcell}}$$

$$= \frac{\text{No. of atoms in unitcell} \times \text{volume of one atom}}{\text{volume of unitcell}}$$

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

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

$$= \frac{\pi}{6} = 0.52$$

Packing factor = 52%.

* It is a loosely packed structure.

Example :

* Polonium.
* Two adjacent Po atoms contact each other, so the edge length of this length of is equal to two Po atomic radii : $l = 2r$.
* Therefore, the radius of Po atomic radi : $l = 2r$
* Density is given by density $= m/V$
* The density of polonium can be found by determining the density of its unit cell (the mass contained within a unit cell divided by the volume of the unit cell)
* Since, Po unit cell contains one-eighth of a Po atom of each of its eight corners of a unit cell contain one Po atom.
* The mass of Po atom is - 3.47×10^{-22} g
* The volume of Po is - 3.79×10^{-23} cm^3
* Therefore, the density of Po = 9.16 g/cm^3
* The atomic radius r of the a simple cubic (SC) structure.

$$2r = a$$

$$\boxed{r = a/2}$$

DIFFERENCE BETWEEN ELECTROVALENT AND COVALENT BOND.

COVALENT	ELECTROVALENT
• A covalent bond is a type of chemical bond that is formed due to electron sharing between two atoms.	• Electrovalent bond is a type of chemical bond that can be defined as an electro-static attraction between two atoms.
• The Nature of a covalent bond is a direct chemical bond between two atoms.	• The nature of electrovalent bond is a type of electro-static attraction between two atoms.
• The difference in the electronegativity values of the atoms should be lower than 1.7 in order to form a covalent bond.	• The difference in the electro-negativity values of the atoms should be higher than 1.7 in order to form an electrovalent bond,
• The ions are not involved in the formation of a covalent bonds (only atoms)	• Ions are involved in the formation of a electrovalent bond.
• They have high polarity.	• They have low polarity.

- They have a definite shape.
- On which the liquid or gas will be at room temperature.
- The melting and boiling points are high due to internal energy. Many covalent bonds must be broken if the solid is to be melted but a large amount of thermal energy is required.
- These are mostly poor conductors because electrons are held either on the atoms or within the covalent bonds. They cannot move through the lattice.
- Most covalent substances are brittle.

- They donot have a definite shape.
- On which the solid will be at a room temperature.
- very high melting points due to strong bonding among atoms due to internal energy.
- solid compounds do not conduct electricity when a potential is applied because there are no mobile charge particles.
- Most substances are brittle.

EXAMPLE :

CO_2 :

:Ö + C + Ö:

⇓

:Ö : : C : : Ö:

(or)

:Ö = C = Ö:

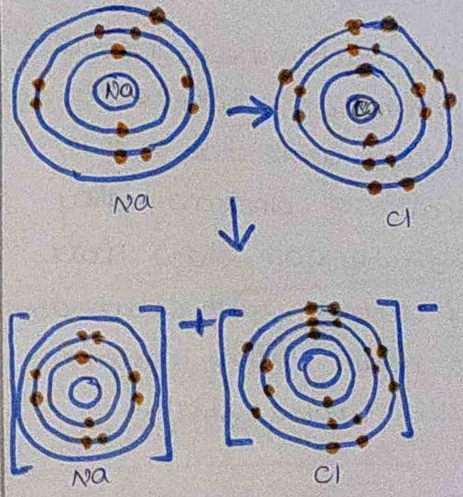
- They are soluble in non-polar solvents

Example explanation :

- The Lewis structure of CO_2 in double bond the CO_2 has total 1 carbon atom and 2 oxygen atoms.
- Each oxygen atom has a valance electrons whereas the carbon atom only has the

EXAMPLE :

NACl :



- They are soluble in polar solvents like water due to strong attraction among ions.
- when sodium loses its one valance e's gets smaller in size, while cl goes larger when it gains an additional valence electrons.
- After the reaction takes place the charged Na^+ & Cl^- ions are held together by

- 4 valance electron to satisfy the octet rule.

- carbon need 4 more valance e-s. since each oxygen atoms has 3 lone pairs of electrons, they can be each share 1 pair of electrons with carbon as a result, filling carbon's outer valance shell.

- electrostatic force form a ionic bond.

- when they approach closely the orbits of electrons ion being overlap eachother then electrons repel each other by virtue of the repulsive electro-static coloumb force.

4) DESCRIBE MILLER INDICES WITH EXAMPLES:-

- Miller indices are used to specify directions and planes.
- These directions and planes could be in lattice or in crystals.
- The number of indices will match with the dimension of the lattice or the crystal.
- Eg. in 1D there will be two (one) index and 2D there will be two indices.
  - [hkl] - represents a direction.
  - <hkl> - represents a family of directions.
  - (hkl) represents a plane
  - {hkl} represents a family of planes.

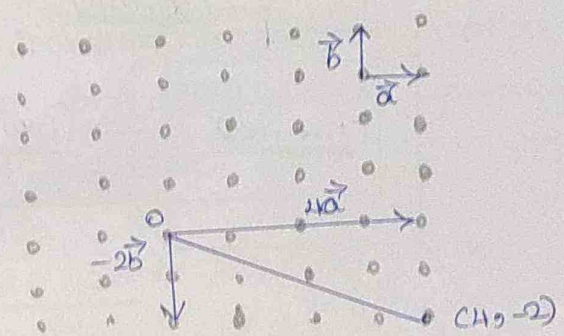
MILLER INDICES FOR DIRECTION :-

- A vector r passing from the origin to a lattice point can be written as,

$$r = r_1 a + r_2 b + r_3 c$$

where, a, b, c - basic vectors and (r_1, r_2, r_3) - miller indices.

- Fractions in (r_1, r_2, r_3) are eliminated by multiplying all components by their common denominator.
- eg. $(1, 3/4, 1/2)$ will be expressed as $(4, 3, 2)$



Miller indices → $[4\bar{2}]$

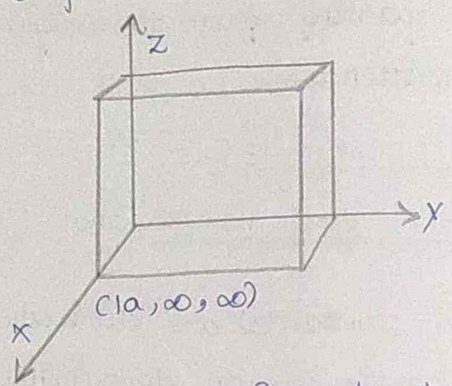
MILLER INDICES FOR PLANES

* Consider the plane which is one of a infinite number of parallel plane each a consistent distance (a)

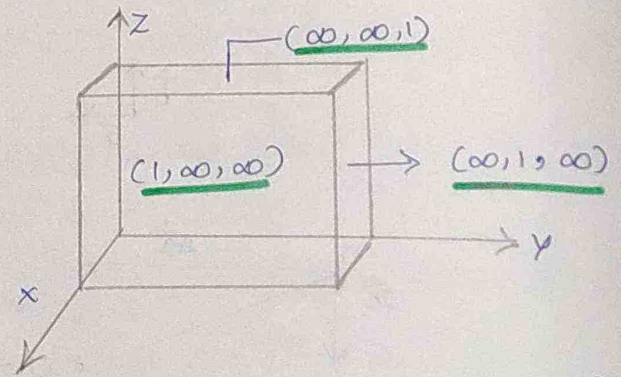
away from the origin.

* The plane intersects the x axis at point a. It runs parallel along y and z axes.

* Thus, this plane can be designated as (1, ∞, ∞)



Likewise it can be designated the ~~left~~ right side as (∞, 1, ∞) and the upper plane can be written as (∞, ∞, 1)



* where, (1, ∞, ∞) = (100), (∞, ∞, 1) = (001) and (∞, 1, ∞) = (010)

* The intercepts of the lattice planes along the x, y and z axes, then take the reciprocals of the intercepts and obtain their lowest integer ratios.

FAMILY OF DIRECTIONS:-

It is a set of directions related by symmetry operations.

Index	Members in family for cubic lattice.
$\langle 100\rangle$	[100], [$\bar{1}$00], [010], [0$\bar{1}$0], [001], [00$\bar{1}$]
$\langle 110\rangle$	[110], [$\bar{1}$10], [1$\bar{1}$0], [$\bar{1}\bar{1}$0], [101], [$\bar{1}$01], [10$\bar{1}$], [011], [0$\bar{1}$1], [01$\bar{1}$], [0$\bar{1}\bar{1}$].
$\langle 111\rangle$	[111], [$\bar{1}$11], [11$\bar{1}$], [$\bar{1}\bar{1}$1], [$\bar{1}$1$\bar{1}$], [1$\bar{1}\bar{1}$], [$\bar{1}\bar{1}\bar{1}$]

IMPORTANCE OF MILLER INDICES :-

* It is important to have a notation system for atomic planes since these planes influence.
  - optical properties
  - Reactivity
  - surface tension
  - dislocations.

* This is called as Miller Indices. It is used as a symbolic representation for the orientation of an atomic plane in a crystal lattice and are defined as the reciprocals for the fractional intercepts.

Some of the multiplicity factors are,

cubic	hkl	hhl	hk0	hh0	hhh	h00	
	48	24	24	12	8	6	
Hexagonal	hk.l	hh.l	h0.l	hk.0	hh.0	h0.0	00.l
	24	12	12	12	6	6	2
Tetragonal	hkl	hhl	h0l	hk0	hh0	h00	00l
	16	8	8	8	4	4	2
orthorhombic	hkl	hk0	h0l	0kl	h00	0k0	00l
-bic	8	4	4	4	2	2	2

5) WRITE ABOUT VANDERWAALS BONDING:-

* A weak dipole-dipole interaction is the origin of the vanderwaals bond, which is therefore charac-terized by a low cohesive energy and so low melting temperatures.

* Also spontaneous dipole formation in one atom may induce an equal and opposite dipole in another atom nearby,

* Another type of vanderwaals bonding is observed for certain polar molecules that have permanent dipole

The vanderwaals potential energy can be approximated as

* $$E(r) = \frac{a}{r^n} \quad \frac{B}{r^m}$$

- 2nd term - classical dipole dipole interaction αr^{6}.
- 1st term - repulsion for small r.

* In the equation, a & b are empirical parameters as in n if we equilibrium we have r_0 and $E(r_0)$ are the equilibrium seperation and energy for a stable bond to form $E(r_0)$ must be negative thus

$m<n$. $\frac{dE}{dr} = 0 \quad \therefore r_0 \left[\frac{na}{mB}\right]^{\frac{1}{n-m}}$ and

$$E(r_0) = \frac{B}{r_0^m}\left[\frac{m}{n} - 1\right]$$

Some Lennard Jones potential - in which the minimum interaction energy and its distance.

*

	r_0 (a)	E(J)
He	2.2	1×10^{-22}
H_2	2.7	4
ar	3.2	15
n_2	3.7	13
CO_2	4.5	40

* Once a random dipole is formed in one atom an induced dipole is formed in the adjacent atom, this is the type of bonding present in N_2 molecules and it is known as vanderwaals bonding.

* Vanderwaals force include attractions and repulsions between atoms, molecules and surfaces as well as other intermolecular forces. They differ from covalent and ionic bonding in that they are caused by correlation in the fluctuating polarizations of nearby particles.

* Hydrogen bonds occur in inorganic molecules such as water and organic molecules such as DNA and proteins.

* Vanderwaals attractions can occur between any two or more molecules and are dependent on slight fluctuations of the electron densities.

* Three types of vanderwaals force.
1) dispersion, dipole-dipole and hydrogen.

* Vanderwaals interaction is the weakest of all intermolecular attractions between molecules.

* However, with a lot of vanderwaals force interacting between two object, the interaction can be very strong.

* Spontaneous dipole formation is one atom may induce an equal & opposite dipole in another atom nearby so causing attraction. This is the vanderwaals bond.

* Another type of vanderwaals bonding is observed for certain polar molecules that have a permanent dipole moment.

* Although unionized atoms are electrically neutral electrons with them are in a constant state of motion and so may momentarily from small charge dipoles.

+e - - - - - - - - -e

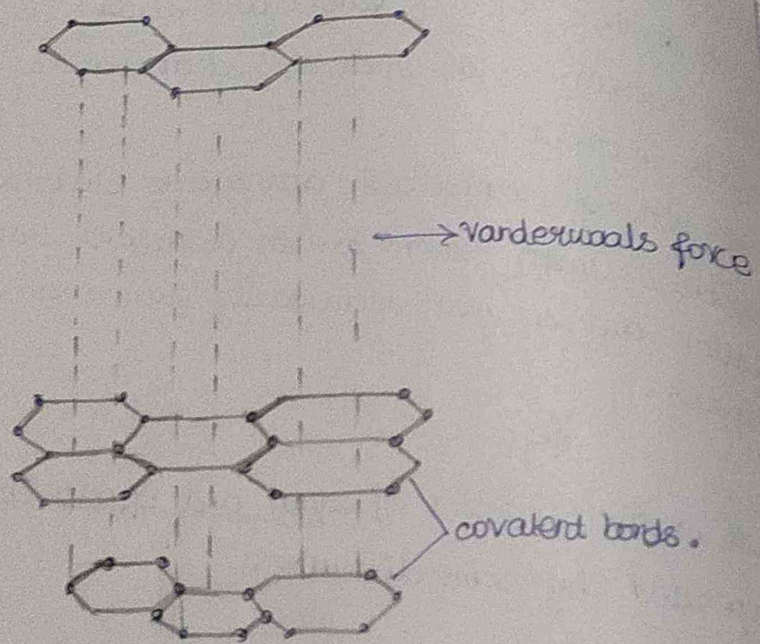
* A dipole consist of equal and opposite charges seperated by some distance.

* A charge dipole may spontaneously form in a neutral atom due to the motion of electrons around the nucleus.

* The direction and magnitude of this dipole constantly fluctuates but may induce similarly fluctuating dipoles in other atoms.

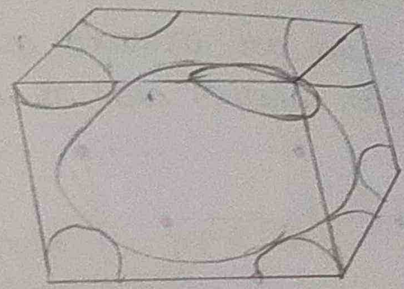
Graphenes bonding forces in Graphite :-

* weak forces between graphenes suggest that they are the vanderwaals forces.

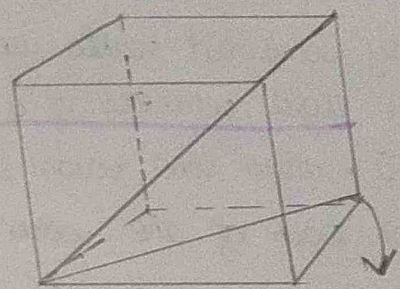


Structure include lithium, sodium, potassium, chromium, barium, vandium, alpha iron or tungsten.

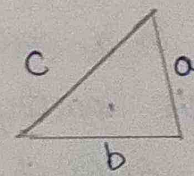
* Metals have a bcc structure are usually harder and less malleable than close-packed metal such as gold.



Derivation of unit cell length and atomic radius for BCC?



diagonal

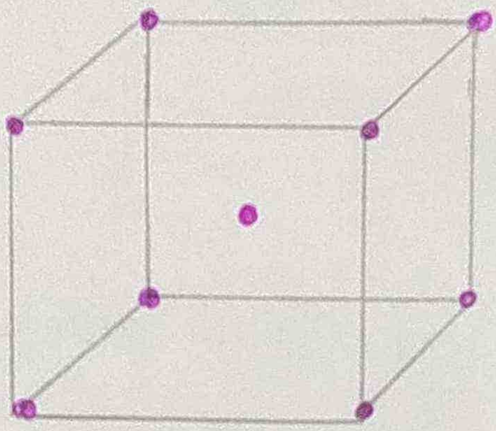


right angle triangle

1) Describe Bcc and Fcc with Examples :

BODY CENTERED CUBIC :

* The atoms are arranged at the centers of the cube with another atom at the cube centre.



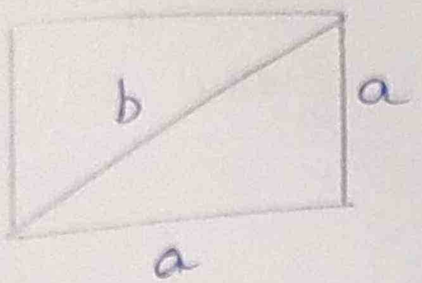
8 corner atoms one atom at the centre.

* The body centered cubic unit cell has atoms at each of the eight corners of a cube. (like the cubic unit cell) plus one atom in the centre of the cube ie) Each of the corner atoms in the corner of another cube so the corner atoms are shared among eight unit cell.

* The volume of atoms in a cell per the total volume of cell is called the packing factor. The bcc unit cell has a packing factor of 68 %.

* some of the materials that have a bcc

But at the base, the diagonal is,



$b^2 = a^2 + a^2$

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

$\boxed{b = \sqrt{2}a}$

For c, $c^2 = a^2 + b^2 = a^2 + (\sqrt{2}a)^2$

$c^2 = a^2 + 2a^2 = 3a^3$

$c^2 = 3a^2$

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

$\boxed{c = \sqrt{3}a}$

The diagonal $c = \sqrt{3}\,a$

$c = 4R$

$c = \sqrt{3}a$

$a = \frac{4}{\sqrt{3}}R$

$\boxed{\text{The atomic radius } a = \frac{4}{\sqrt{3}}R}$

The atomic packing factor for BCC :-

* The atomic packing factor for BCC structure

is given by,

$$APF = \frac{\text{Total number of atoms}}{\text{volume of unit cell.}}$$

we know that,

$= 1$ body atom $+ 8$ corner atoms

$= 1 + 8\,(1/8)$

$= 1 + 1$

$= 2$ atoms

$$\boxed{a = 4R/\sqrt{3}\,a}$$

$$APF = \frac{2 \text{ atoms } \left(\frac{4}{3}\pi R^3\right)}{a^3}$$

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

applying it we get,

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

$$= \frac{\frac{8}{3}\pi R^3}{\frac{4^3 R^3}{(\sqrt{3})^3}}$$

$$= \frac{8\pi (\sqrt{3})^3}{3(4^3)}$$

$= 0.68$

$= 6.8\%$

$= 68\%$

the Atomic packing factor of a unit cell is ie) the volume of space occupied is 68%

BCC structures stronger and brittle ?

* Although BCC materials have higher number of slip systems than FCC, the slip planes are not closely packed in FCC, the slip planes are not closely packed it is at the same homologous temperature.

* Ductile and brittle are relative terms, since the deformation of a material and the corresponding mode of failure depends on the many conditions in addition to crystal structure such as stress, rate of loading and ambient temperature among things.

* BCC metals they do have slip systems, consisting of the {110}, {123} and {112} family of planes, each with their own preferred direction of slip fail to exhibit the extent of ductility as shown by FCC metals.

* This is because BCC structure is not a close packed one the slip planes are of the highest planar density but not close packed.

* This leads to increased activation energies for dislocation motion along a slip direction as compared to FCC.

* However, at elevated temperatures, they typically brittle BCC transitions into a relatively ductile material.

* At temperatures below the ductile - brittle transition temperature of the facture toughness is exceeded before the stress is sufficient to induce dislocation motion and brittle fracture is observed.

* These observed reasons shows that BCC are strong and brittle.

EXAMPLES :

- one of the example for bcc is chromium (Cr).
- chromium is a metal in group VIB of the periodic table with atomic number 24, an atomic weight of 5.1996 and a density of 7.19. It has a melting temperature of 1875°c.
- The electronic configuration for chromium is $(Ar)(3d)^5(4s)^1$ and it has an atomic radius of 0.13nm. (0.130nm).
- At room temperature chromium has a bcc crystal structure with a basis of one Cr atom.

E = 248 GPa.

Formula → Cr

lattice type → Body centered cubic

group → group 6

Melting point → 2180 K (1907°c, 3465°F)

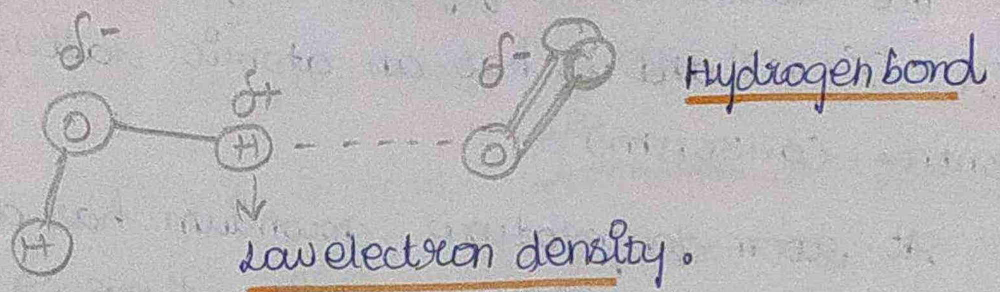
Boiling point → 2944K (2671°c, 4840°F)

Density → 7.19g/cm^3

- Some other example of bcc be (Cr, W), Fe(α) Ta, Mo. etc..

2) Describe in detail about hydrogen bonding:

* A hydrogen bond is a dynamic attraction between a pair typically electronegative atoms involving a hydrogen atoms located between them. Hydrogen bonds are responsible for the life-giving properties of water.

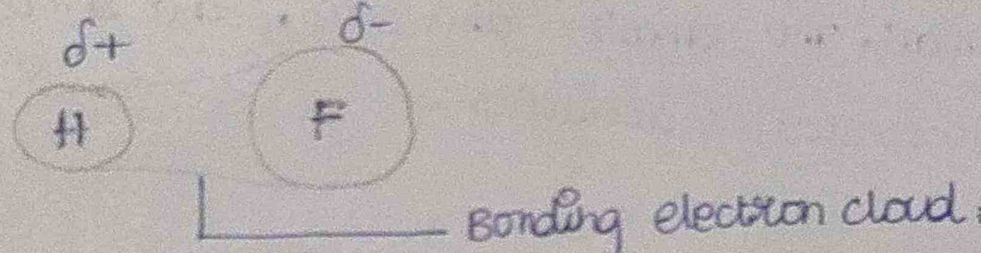


* polar molecule such as water molecules have a weak, partial negative charge at one region of the molecule (the oxygen atom in water) and a partial positive charge elsewhere (the hydrogen atoms in water).
* The water molecule (O-H) bond is highly polar bond.
* Hydrogen has no inner shell electron and is very small in size, the positive charge density developed is high.
* The nucleus of hydrogen atom is exposed to attraction by nearby electron cloud, a lone pair of

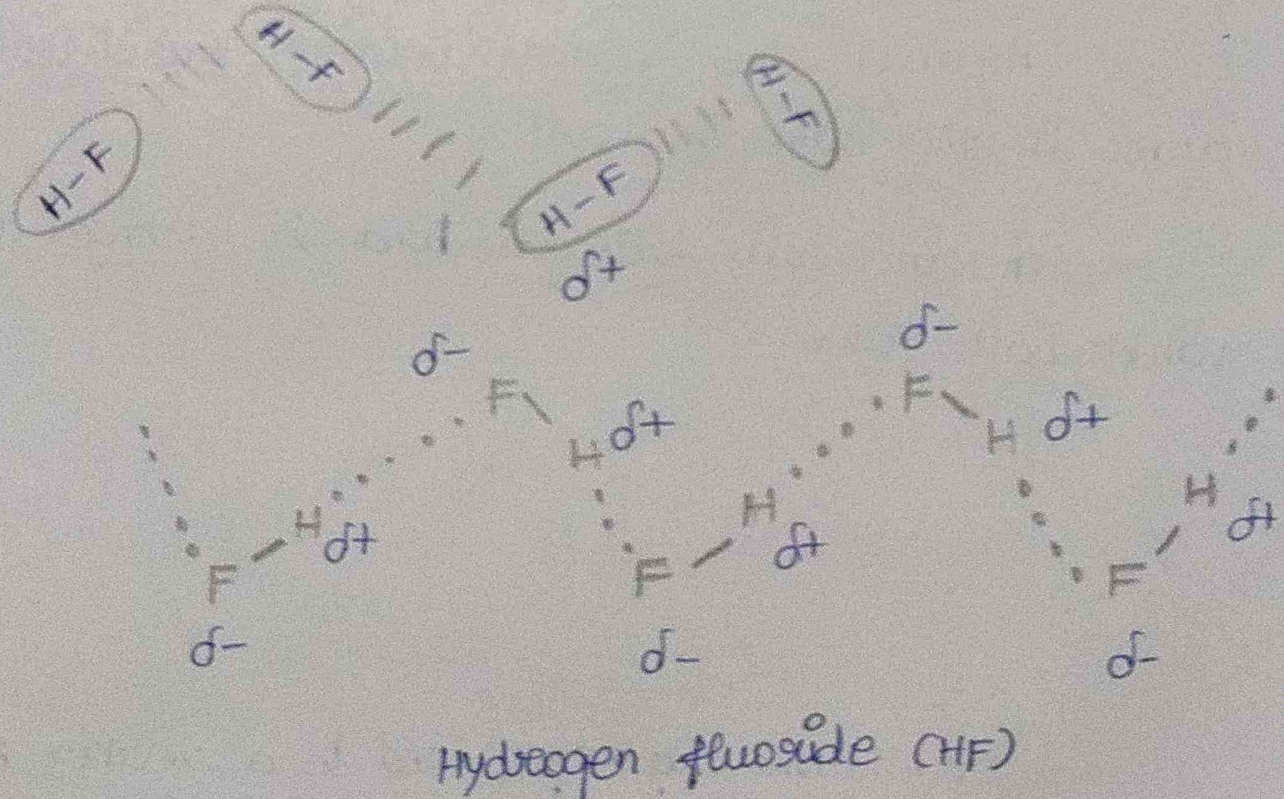
electrons on the electronegative atom

* Hydrogen bonding is a special case of dipole - dipole interactions.

* when hydrogen bonded to a highly electronegative atom (such as nitrogen, oxygen, fluorine), the bonding electron pair is drawn towards the electronegative atom.



Hydrogen bonding in Hydrogen fluoride :



Hydrogen fluoride (HF)

condition for H-Bonding :-

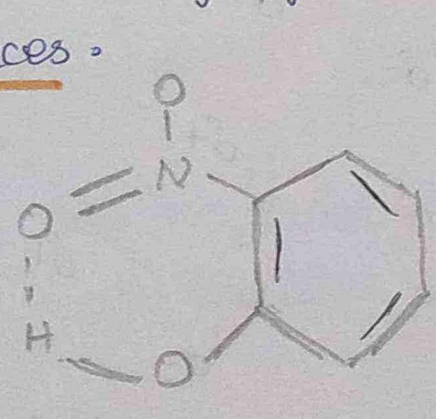
- A hydrogen atom must be directly bonded to a highly electronegative atom (eg. F, O and N)
- An unbonded pair of electrons (lone pair electrons) is presented on the electronegative atom.
- The size of the electronegative atom should be small. The smaller the size, the greater is the electrostatics attraction.

Intermolecular hydrogen bond :-

- Hydrogen bond formed between two molecules.

Intramolecular hydrogen bond :-

- Hydrogen bond formed between two different atoms in the same molecule.
- Intermolecular hydrogen bond is stronger than a vanderwaal's forces.



- Eventhough hydrogen bond is a weaker bond.

Strength of hydrogen bond:

- Hydrogen bonding is very weak bond. The strength of hydrogen bond is intermediate between the weak vanderwaal's forces and the strong covalent bonds. Thus whereas the bond dissociation energy of a covalent bond is 209-418kj/mol. That for H-bond is only 12.62-41.8 kj/mol.

Explanation:

* In H_2O_2 there are intermolecular hydrogen bonds between molecules.

* However. in H_2S, H_2Se and H_2Te the interaction between molecules is dipole-dipole interactions.

* The strength of hydrogen bond is stronger than dipole-dipole interactions.

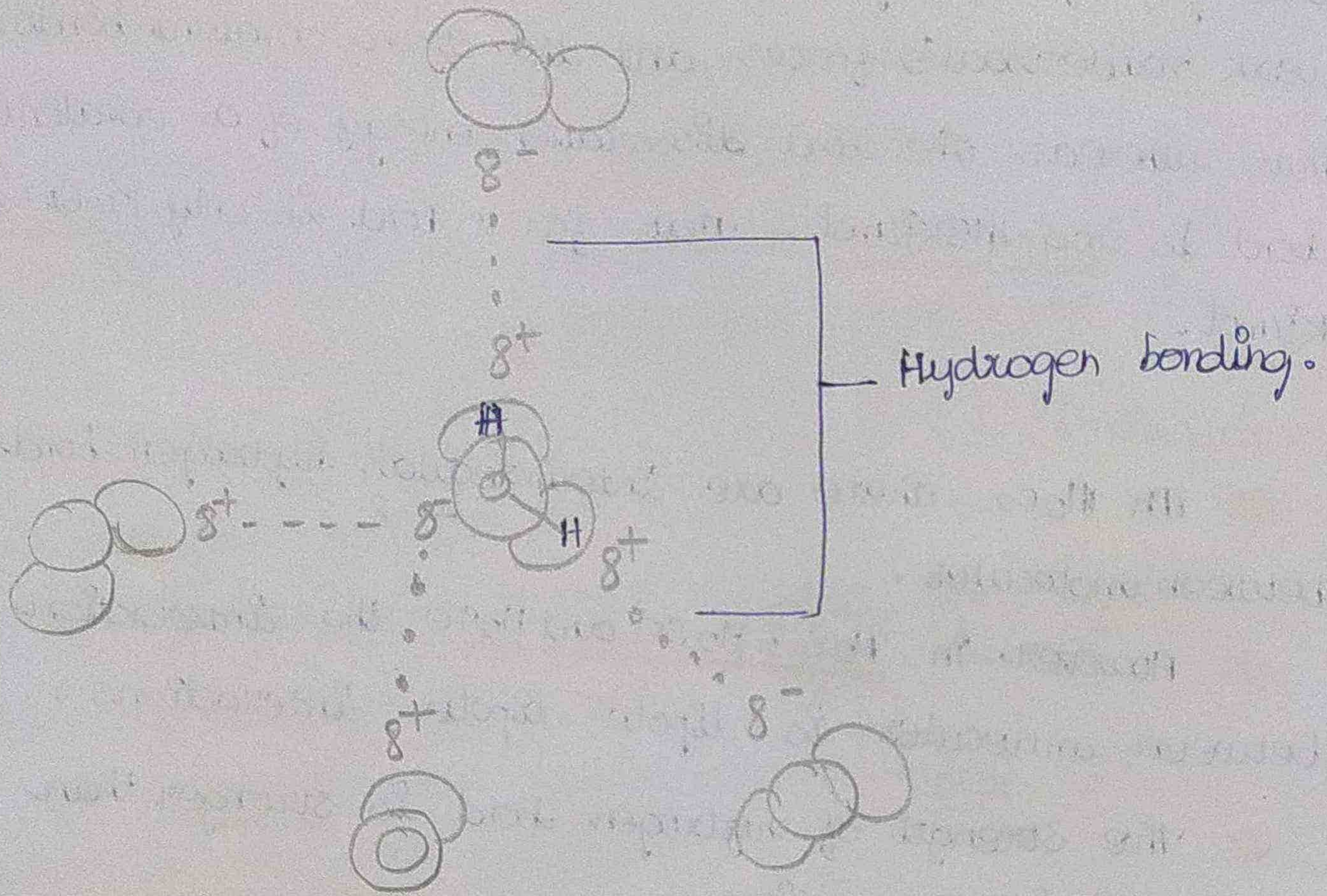
* To break the hydrogen bonds, more energy is required.

* H_2O has the largest enthalpy change of vaporization.

Consequences of H-bond:

- High melting and boiling points:
- The compound having H-bond show abnormally high melting and boiling point.

• Due to the containing hydrogen bond to the fact that some extra energy is needed to break these bonds.



* As hydrogen attached to carbon atom can also participate in hydrogen bonding when the carbon atom is bound electronegative atoms as in the case in chloroform $CHCl_3$.

* The electronegative atom attracts the electron cloud from around the hydrogen nucleus and by decentralizing the cloud, leaves the atom with a

positive partial charge.

* Because of the small size of hydrogen relative to other atoms and molecules.

* The resulting charge through only partial represent a large density.

* A hydrogen bond results when this strong positive charge density.

* Attracts a lone pair of electrons on another heteroatom which becomes hydrogen-bond acceptor.

properties:

1) Hydrogen bonds are directional
2) These bonds have low melting points.
3) They are good insulators.
4) They are soluble in polar and non-polar solvents
5) They are transparent to light.
6) These are stronger than dispersion bond
7) solids may be crystalline or non-crystalline.

UNIT - 2 : 'TWO MARK QUESTIONS'

1) what is meissner's effect ?

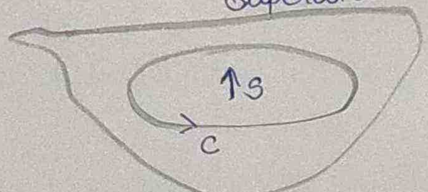
* when the superconducting material is place in a magnetic field under the condition when $T \le T_c$ and $H \le H_c$, the flux lines are excluded from the material. It explains as follows,

* There is another much more fundamental characteristics which distinguishes the super conductor from a normal but ideal conductor.

* the superconductor expels magnetic flux. ie,

$$\boxed{B = 0}$$

superconductor.



The nature of superconducting $C_S \sim e^{-B\Delta}$

$$0 = IR = V = \oint \varepsilon \cdot dl$$

$$= \int_S \nabla \times \varepsilon \cdot ds$$

$$\boxed{V = -\frac{1}{c}\int_S \frac{\partial B}{\partial t} \cdot ds}$$

* since s and c are arbitrary.

$$0 = -\frac{1}{c} B \cdot S$$

$$\boxed{B = 0}$$

Thus, for an ideal conductor, it matters if its field cooled or zero field cooled.

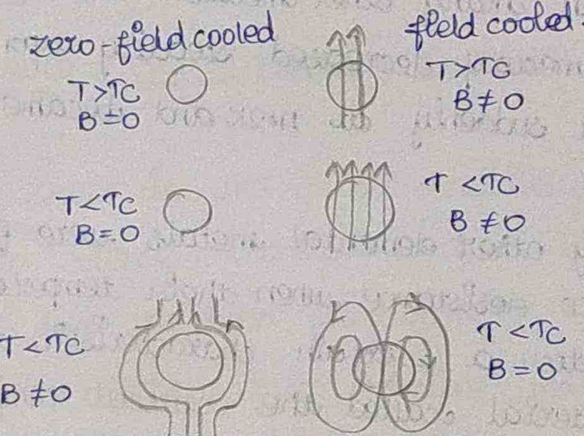
$$B = \mu H = 0 \Rightarrow \mu = 0$$

$$M = \chi H = \frac{\mu - 1}{4\pi} H$$

$$\boxed{\chi_{SC} = -\frac{1}{4\pi}}$$

$$\boxed{M = -\frac{1}{4\pi} H_{ext}.}$$

Ideal conductor



2) What do you mean by superconductivity ?

* The phenomenon of superconductivity in which the electrical resistance of certain materials completely vanishes at low temperature is one of the most interesting and sophisticated condensed

matter in physics.

* It was discovered by the Dutch physicist Heike Kamerlingh Onnes, who was the first to liquefy helium (which boils at 4.2 kelvin at std pressure).

* In 1911 Kamerlingh Onnes and one of his assistants discovered the phenomenon of superconductivity while studying the resistance of metal at low temperatures.

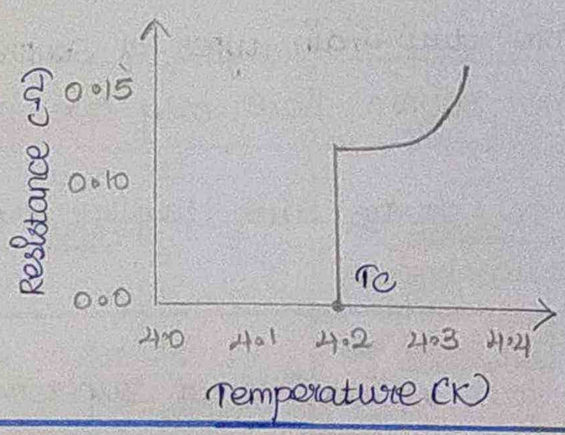
* They studied mercury because very pure samples could easily be prepared by distillation.

* As in many other metals, the electrical resistance of mercury decreased steadily upon cooling, but dropped suddenly at 4.2K and became undetectably small.

* Many other elemental metals were found to exhibit zero resistance when their temperatures were lowered below a certain characteristic temperature of the material called the critical temperature T_c

High-Tc superconductor	Tc(K)
• $Tl_2Ba_2Ca_2Cu_3O_{10+x}$	125
• $HgBa_2Ca_2Cu_3O_{8+x}$	135
• $Hg_{0.8}Tl_{0.2}Ba_2Ca_2Cu_3O_{8.33}$	134

* "The phenomenon of losing resistivity when sufficiently cooled to a very low temperature."

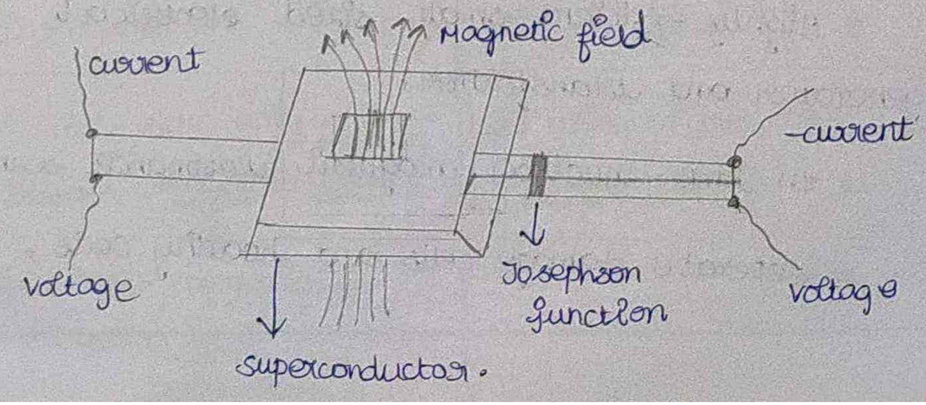


3) Define SQUID :-

* SQUID - Superconducting Quantum Interference Devices.

* A SQUID is the most sensitive type of detector known to science. Consisting of a superconducting loop with two Josephson junctions.

* SQUIDs are used to measure magnetic fields.



* It has a principle of small change in magnetic field produces variation in the flux quantum.
* There are two main types of SQUIDS
  1) RF SQUIDS have only one Josephson Junction.
  2) DC SQUIDS have two or more junctions.

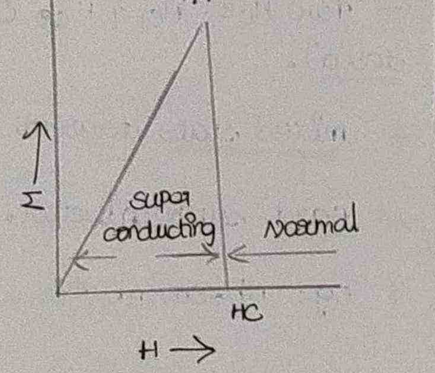
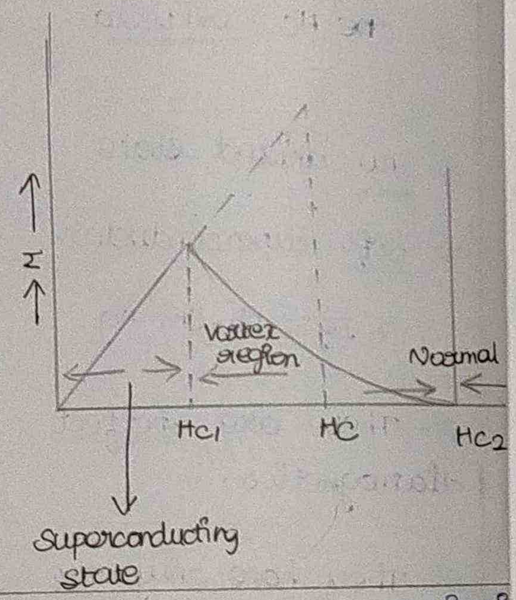
4) Write any four applications of superconductors:

- Larger distance power transmission (e-0)
- Switching device (easy destruction of super conductivity).
- Sensitive electrical equipment (small variation → large constant current).
- memory / storage element (persistent current)
- Highly efficient small sized electrical generator and transformer.
- In NMR - nuclear magnetic resonance scanning.
- seperate damage cells and healthy cells.

'FIVE MARK QUESTIONS'

1) Difference between Type I and Type II superconductors.

Type-I	Type-II
* Sudden loss of magnetisation.	* Gradual loss of magnetisation.
* Exhibit Meissner's effect.	* Does not exhibit Meissner's effect.
* one Hc - 0.1 tesla	* Two Hcs - H_{c1} & H_{c2} (≈30 tesla).
* no mixed state	* mixed state present
* soft superconductor • Eg: Pb, Sn, Hg	* Hard superconductor. • Eg: Nb-Sn, Nb-Ti
* These are perfect diamagnetics.	* These are not perfect diamagnetics.
* They have only one critical magnetic field.	* They have two critical magnetic field.
* These materials undergoes a sharp transition from the	* These materials undergoes a gradual transition from

superconducting state of the normal state at the critical magnetic field.	the superconducting state to the normal between the two critical magnetic fields.
* The highest value of critical magnetic field is 0.1wb. * Applications are very limited.	* The upper critical field can be of the order of 50wb * They are used to generate very high magnetic field.
TYPE-I 	TYPE-II 
* As seen from magnetization curve, transition at Hc is reversible. i.e) if field is again lowered below Hc the material again becomes superconductor. • Eg:- Pb, Sn, Hg	* As seen from magnetization curve, transition at Hc is not reversible. • Eg:- Nb-Sn, Nb-Zr.

2) Write notes on High temperature superconductors:-

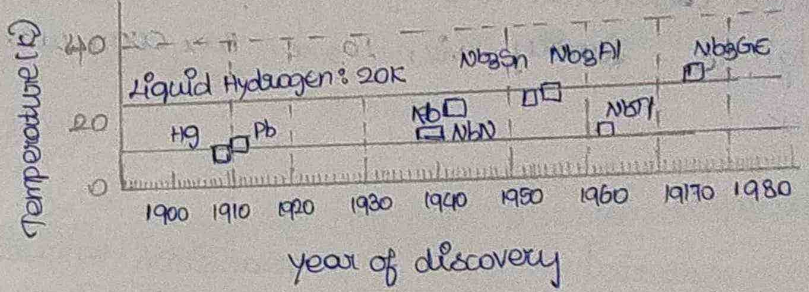
Superconductivity:-

* The phenomenon of losing resistivity when sufficiently cooled to a very low temperature.

* It was discovered by H.kamerlingh onnes, Leiden (1908). → for liquification of Helium.

* The superconductivity: Ideal conductivity was discovered by him in 1911.

* Many metals becomes superconducting at low temperatures.



High Temperature Superconductors:-

* It has been long dream of scientist working in the field of superconductivity.

* To find a material that becomes a superconductor at room temperature.

* A discovery of this type will revolutionize every aspect becomes a superconductor at room of modern day technology such as power transmission and storage, communication, transport and even the type of computers we make.

* Any superconductor with a transition temperature above 30K is in general called high T_c superconductor.

* Till the year 1986, the highest known transition temperature T_c was 23K in the Nb_3Ge alloy.

* Till the year 1986 the Bednorz and Muller discovered the first superconductor of the high T_c - family viz, $La_{2-x}Ba_xCuO_4$ with T_c of ~ 35K

Examples :-

Material		Transition temperature (T_c)
• $La_{1.85}B_{0.15}CuO_4$	–	36
• $YBa_2Cu_3O_7$	–	90
• $Tl_2Ba_2Ca_2Cu_3O_{10}$	–	125

Characteristics :

* They have high transition temperatures (T_c) accompanied by high critical currents (I_c) and high critical magnetic field (H_c)

* They have a modified perovskite crystal structure. The structure is highly anisotropic.

* They are oxides of copper in combination with other elements. They have a layered structure consisting of one or more CuO_2 layers.

* The most important characteristic of high T_c superconducting oxides is their metallic properties.

* The conductivity is metallic in the CuO_2 planes, the conductivity is much smaller in a direction perpendicular to CuO_2 planes.

Preparation of High T_c ceramic superconductor $YBa_2Cu_3O_{7-x}$.

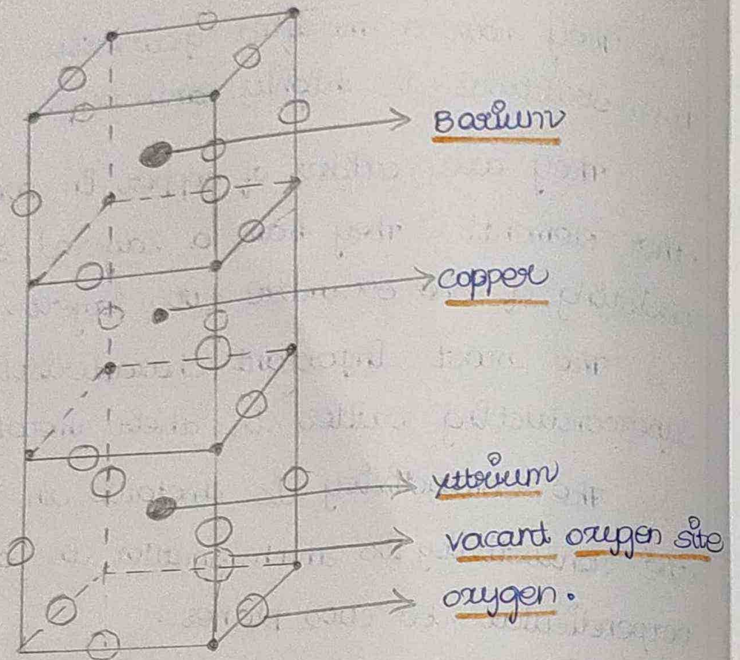
* The preparation of yttrium barium copper oxide superconductor by the shake and bake method. This method involves a four step process.

1) Mixing the chemicals
2) calcination (initial firing).

3) The intermediate firing

4) The final oxygen annealing.

Crystal structure of ($YBa_2Cu_3O_{7-x}$)



* Three body centered cubic unit cells are stacked one above another:

* The atom distributions in the unit cell are

• copper atom at body corners $= 8 \times \frac{1}{8} \times 3 = 3$

• Barium $= 1 \times 2 = 2$, yttrium $\Rightarrow 1 \times 1 = 1$

• oxygen atom at midpoint of edges

$12 \times \frac{1}{4} \times 3 = 9$

Some oxygen positions are vacant such that their number is between 6.5 and 7.

* The superconducting properties appear to be a sensitive function of the oxygen content and therefore of the partial pressure of oxygen during heat treatment.

Applications:

• large distance power transmission (e-σ)

• switching device (easy destruction of superconductivity)

• sensitive electrical equipment (small variation (V) → large constant current).

• memory / storage element (persistent current)

• Highly efficient small sized electrical generator and transformer.

---

3) Derive London equation:

* On Meissner's effect that one of the condition for the superconducting state is the magnetic flux density $(B) = 0$.

* On this condition, inside the superconductor that is the magnetic flux cannot penetrate.

* The magnetic flux does not suddenly drop to zero inside the surface.

* The phenomenon of flux penetration inside the superconductors was explained by H. London and F. London.

London first equation :-

* Let n_s and v_s be the number density and velocity of superconducting state & electrons.

* The equation of motion or acceleration of electrons in the superconducting state is given by,

$$m(dv_s/dt) = -eE$$

(or)

$$dv_s/dt = -eE/m \longrightarrow ①$$

m - mass of electrons, e - charge

current density ⇒ $J_s = -n_s e v_s$

* Differentiate it with respect to time,

$$dJ_s/dt = -n_s e(dv_s/dt) \Rightarrow (-\frac{eE}{m})$$

* Put equation ① in above equation we get,

$$dJ_s/dt = (n_s e^2 E)/m$$

$-n_s e(dv_s/dt)$

$-n_s e(-\frac{eE}{m})$

$n_s e^2 E/m$

$$dJ_s/dt = (n_s e^2 E)/m \longrightarrow ②$$

Equation ② is known as London's First equation.

London second equation :-

* Take curl (that is cross or vector product) of London's first equation we get,

$$\nabla \times dJ_s/dt = [(n_s e^2)\nabla \times E]/m \longrightarrow ③$$

* By differential form of faraday's law of electromagnetic induction (or Maxwell's third equation).

$$del \times E = -dB/dt$$

$$\nabla E = -dB/dt$$

Substitute in ③ we get,

$$\nabla dJ_s/dt = -[(n_s e^2(dB/dt))/m]$$

* Integrate both sides with respect to time, weget,

$$\nabla J_s = -[n_s e^2(B)/m] \longrightarrow ④$$

* This is known as London's second equation.

Flux penetration from London equation:-

* To explain Meissner effect from london equations consider the differential form of Ampere's circuital law.

$$\nabla B = \mu_0 J_s$$

where, B is magnetic flux density

J_s is current density.

Take curl on both sides of above equation,

$$\nabla \times (\nabla B) = \mu_0 (\nabla \times J_s) \longrightarrow (5)$$

As, $\nabla \times (\nabla \times B) = \nabla(\nabla \cdot B) - \nabla^2 B$

Putting the above equation and London second equation in (5) we get:

$$\nabla \times (\nabla \times B) = \mu_0 (\nabla \times J_s)$$

$$\nabla(\nabla \cdot B) - \nabla^2 B = -[(\mu_0 n_s e^2 (B)/m]$$

* But $\nabla \cdot B = 0$

(Maxwell's second equation of Gauss law for magnetism).

* Therefore, above equation becomes,

$$\nabla^2 B = I(\mu_0 n_s e^2 (B)/m] \longrightarrow (6)$$

where, $\lambda_1^2 = m/\mu_0 n_s e^2$ $(\text{del}^2 B = B/\lambda_1^2) \rightarrow$ (

(or) $\lambda_1 = (m/\mu_0 n_s e^2)^{1/2}$

where, λ_1 is known as London's penetration depth and it has units of length.

$$\nabla^2 B = B/\lambda_1^2 \longrightarrow (7)$$

The solution of differential equation (7) is,

$$B = B(0)\, e^{-x/\lambda_1} \longrightarrow (8)$$

where,

* B(0) is the field at the surface and x is the depth inside the superconductor.

The equation (8) shows that a uniform magnetic field equal to zero can not exist in a superconductor, which is Meissner effect.

In the pure superconducting state the only field allowed in the exponentially decreasing field as the flux penetrated from external surface and it is given by (8).

Suppose $x = \lambda_1$

Equation (8) becomes,

$$\boxed{B = B(0)/e}$$

London penetration depth :-

* The London penetration depth is the distance inside the surface of a superconductor.

* at which the magnetic field reduces

to 1/e times its value at the surface.

* The London penetration depth depends strongly on the temperature and becomes much larger as T approaches critical temperature T_C.

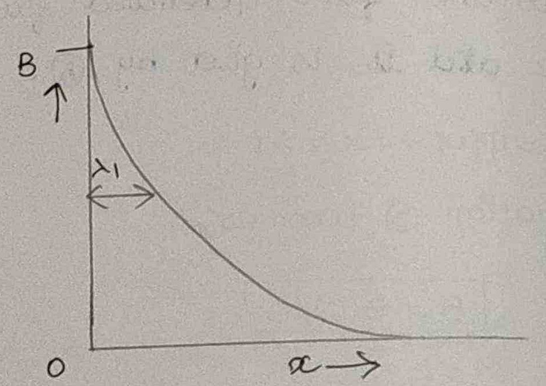
* The relation is,

$$\lambda_1(T)/\lambda_1(0) = [1 - T/T_C^4]^{-1/2}$$

where,

- $\lambda_1(T)$
- $\lambda_1(0)$

} London penetration depth at (T) kelvin and 0 respectively.



* The flux vanishes in the interior of the superconductor.

* The value of λ_1 found experimentally range from 30nm to 300nm.

'TEN MARK QUESTIONS'

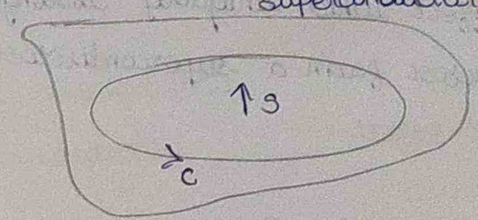
1) Explain in detail about Meissner's effect :-

* When the superconducting material is place in a magnetic field under the condition when $T \leq T_C$ and $H \leq H_C$, The flux lines are excluded from the material. It explains as follows,

* There is another, much more fundamental characteristics which distinguishes, the superconductor from a normal, but ideal, conductor.

* The superconductor expels magnetic flux, $B = 0$ within the bulk of a superconductor.

* This is fundamentally different than an ideal conductor, for which $B = 0$ since, for any closed path.



* A closed path and the surface it contains within a superconductor.

$$0 = IR$$
$$= V$$
$$V = \oint E \cdot dl$$
$$= \int_S \nabla \cdot E \cdot ds$$
$$= -\frac{1}{c} \int_S \frac{\partial B}{\partial t} ds \longrightarrow (1)$$

since, S and c are arbitary.

$$0 = -\frac{1}{c} B \cdot S$$

$$B = 0 \longrightarrow (3)$$

* Thus for an ideal conductor, it matters if it field cooled or zero field cooled.
* where as for a superconductor, regardless of the external field and its history.
* If $T < T_c$, then $B = 0$ inside the bulk.
* This effect which uniquely distinguishes an ideal conductor from a superconductor, is called the Meissner effect.

$$B = \mu H = 0$$
$$\mu = 0$$

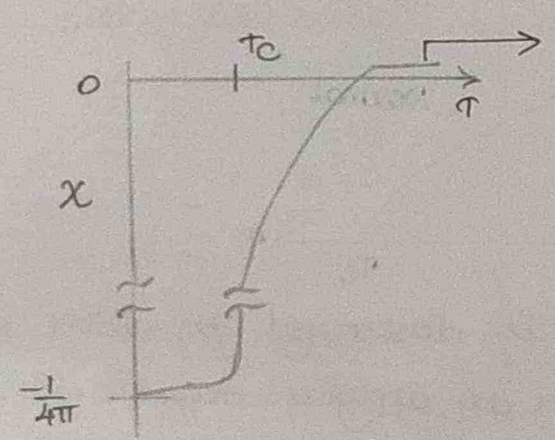
$$M = \chi H$$

$$M = \frac{\mu - 1}{4\pi} H \longrightarrow (4)$$

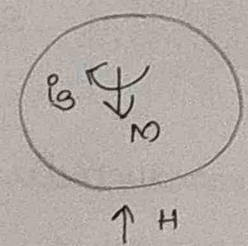
$$\chi_{SC} = -\frac{1}{4\pi} \longrightarrow (5)$$

ie) the measured χ in a superconducting metal is very large and negative (diamagnetic). This can also be interpted as the present of persistent surface currents which maintain a magnetization of

$$M = -\frac{1}{4\pi} H_{ext} \longrightarrow (6)$$



Magnetic susceptibility versus temperature.



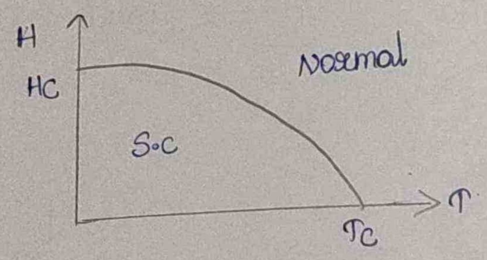
surface currents on a superconductor are induced to expel the external flux.

* The magnetization of in the interior of the superconductor in a direction opposite to the applied field.

* The energy associated with this currents increases with Hext.

* At some point it is then more favorable (ie, a lower energy is obtained) if the system return to a normal metallic state and these screening current abate.

Thus there exists an upper critical field H_c.



* Superconductivity is destroyed by either raising the temperature or by applying magnetic field.

* The meisner effect can be understand from classical electron magnetic theory as a consequence of farday's law,

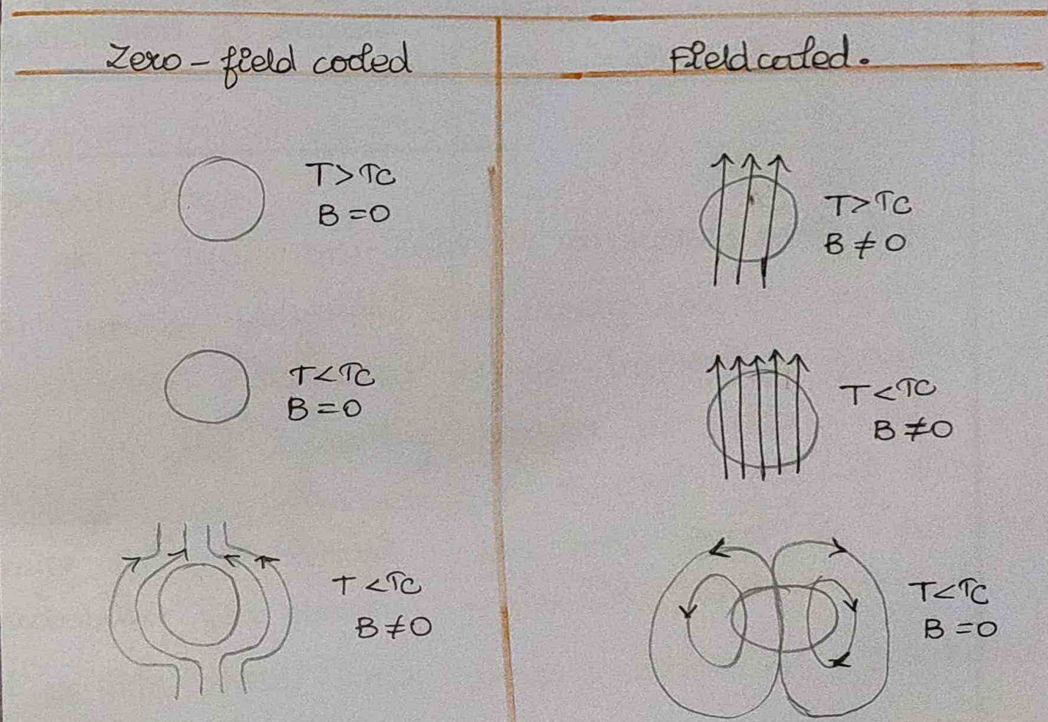
$$emf = \oint \vec{E} \cdot \vec{dl} = -\frac{\partial \phi_B}{\partial t} \rightarrow ⑦$$

$$\frac{\partial}{\partial t}\left\{\frac{m_s}{q_s^2 n_s}\oint \vec{J} \cdot \vec{dl}\right\} = -\frac{\partial \phi_B}{\partial t} \rightarrow ⑧$$

$$\frac{\partial}{\partial t}\left\{\frac{m_s}{q_s^2 n_s}\oint \vec{J} \cdot \vec{dl} + \phi_B\right\} = \frac{\partial}{\partial t}\{\phi_J + \phi_B\} = 0 \rightarrow ⑨$$

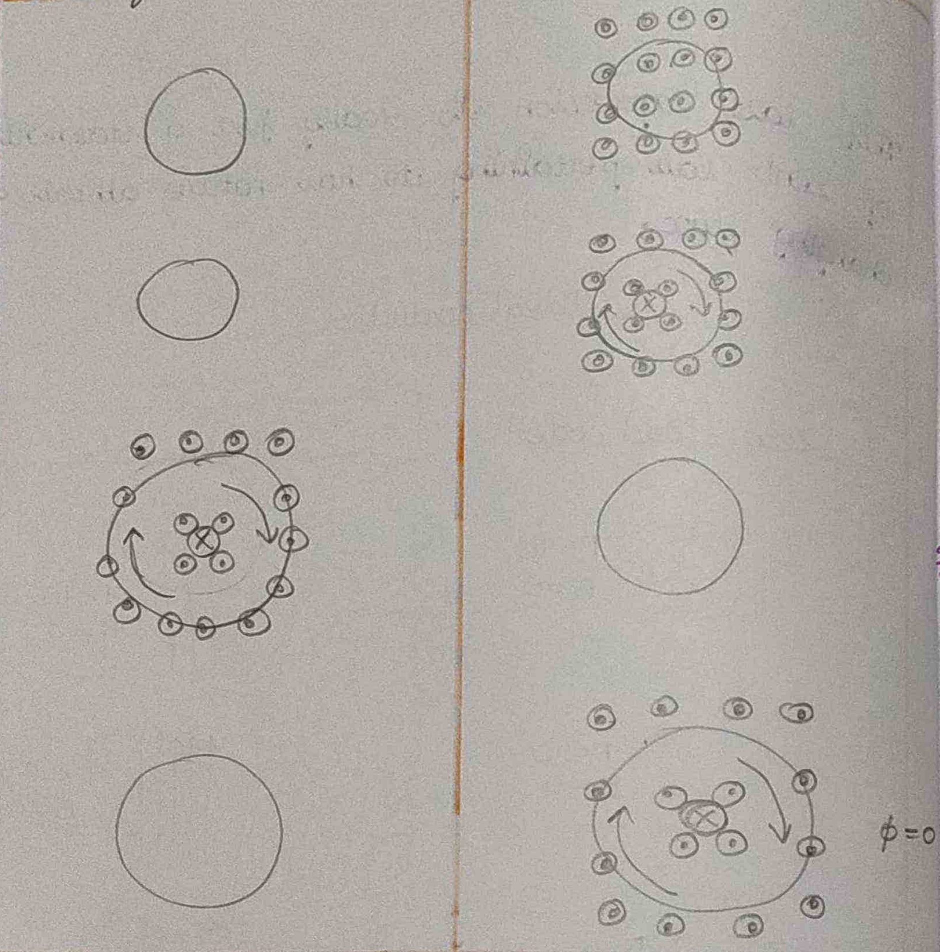
This last expression is really just a statement of len'z law pertaining to how nature abhorbs a changing flux.

Ideal conductor



Superconductor

Zero-field cooled	field cooled.



Application of Meisner's effect :-

* This effect of superconductivity is used in magnetic loviation.

* which is the base of modern high speed bullet trains.

* In superconducting state (phase), due to expulsion of external magnetic field, the sample of super-conducting material levitates above magnet or vise versa.

* Modern high-speed bullet train use the phenomenon of magnetic levitation.

2) Josephson Effect Ac and DC :-

Introduction :-

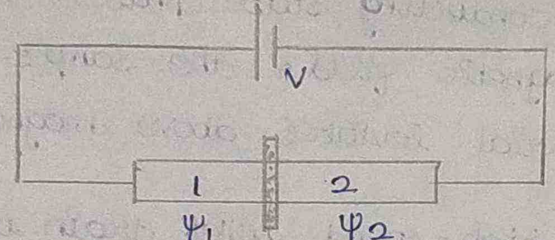
* In 1962, B.D. Josephson analysed what happens at Junction between two closely spaced super conductors, seperated by an insulating barrier.

* If the insulating barrier is thick, the electron pairs can not get through; but if the layer is thin enough (appr 10nm) there is a probablity for electron pairs to tunnel.

* This effect later became known as 'Josephson Tunnelling'.

* Besides, displaying a broad range of interesting macroscopic quantum mechanical properties,

* The Josephson function offers a vast survey of possible application in analog and digital electronics such as SQUID detectors, oscillators, mixers & amplifiers.



* Two superconductors seperated by a thin insulator.

AC and DC effect :-

* The main concept used to discuss the Josephson effects is that of the phase of the paired electron

* The idea of spatial correlation of electrons with the idea of the existence of cooper pairs.

* cooper pairs are set of two electrons that are attracted to one another because an electron attracts positive ions.

* when an electron has attracted a positive ion to a displaced position. we can imagine the

electron as moving out of the area while the +ve ion remains displaced for a time.

* In the region of crystal where the +ve ion is displaced the crystal has a more positive charge than usual and so this region can attract another electron.

* Cooper pairs of electrons are formed because of the virtual exchange of phonons between the electron.

* Returning to the coupling of superconductors through an oxide layer, we write a sort of time dependent. 'Ginzburg-Landau equations' that allow for coupling.

$$i\hbar \frac{\partial \psi_1}{\partial t} = H_1\psi_1 + \hbar U \psi_2 \longrightarrow (1)$$

$$i\hbar \frac{\partial \psi_2}{\partial t} = H_2 \psi_2 + \hbar U \psi_1 \longrightarrow (2)$$

We assume $H_1 = H_2 = 0$,

$$i\hbar \frac{\partial \psi_1}{\partial t} = \hbar U \psi_2 \longrightarrow (3)$$

$$i\hbar \frac{\partial \psi_2}{\partial t} = \hbar U \psi_1 \longrightarrow (4)$$

$$\psi_1 = \rho_1 \exp(i\phi_1) \longrightarrow (5)$$

$$\psi_2 = \rho_2 \exp(i\phi_2) \longrightarrow (6)$$

using (3) & (4) we get,

$$i\dot{\rho}_1 - \rho_1\dot{\varphi}_1 = U\rho_2 \exp(i\Delta\varphi) \longrightarrow (7)$$

$$i\dot{\rho}_2 - \rho_2\dot{\varphi}_2 = U\rho_1 \exp(-i\Delta\varphi) \longrightarrow (8)$$

where,

$$\Delta\varphi = (\varphi_2 - \varphi_1) \longrightarrow (9)$$

Phase difference between the electrons on two sides

$$\dot{\rho}_1 = U\rho_2 \sin\Delta\varphi \longrightarrow (10)$$

$$\rho_1\dot{\varphi}_1 = -U\rho_2 \cos\Delta\varphi \longrightarrow (11)$$

$$\dot{\rho}_2 = -U\rho_1 \sin\Delta\varphi \longrightarrow (12)$$

$$\rho_2\dot{\varphi}_2 = -U\rho_1 \cos\Delta\varphi \longrightarrow (13)$$

Assume $\rho_1 \approx \rho_2 \approx \rho$

$$\frac{d_1}{dt}(\varphi_2 - \varphi_1) = 0 \longrightarrow (14)$$

$$\varphi_2 \equiv \varphi_1 = \text{constant} \longrightarrow (15)$$

$$\rho_1 \equiv \rho_2 \longrightarrow (16)$$

current density J is,

$$J \propto \frac{d}{dt}\rho_2^2 = 2\rho_2\dot{\rho}_2 \longrightarrow (17)$$

so, $$J = J_0 \sin(\varphi_2 - \varphi_1) \longrightarrow (18)$$

Ac :

$q = 2e$ with $\hbar qV$

$$i\hbar \frac{\partial \psi_1}{\partial t} = \hbar U \psi_2 - eV\hbar \psi_1 \rightarrow (19)$$

$$i\hbar \frac{\partial \psi_2}{\partial t} = \hbar U \psi_1 + eV\hbar \psi_2 \rightarrow (20)$$

Again,

$$i\dot{e}_1 - e_1\dot{\phi}_1 = Ue_2 \exp(i\Delta\phi) - eVe_1 \rightarrow (21)$$

$$i\dot{e}_2 - e_2\dot{\phi}_2 = Ue_2 \exp(-i\Delta\phi) + eVe_2 \rightarrow (22)$$

Seperate real and imaginary parts

$$\dot{e}_1 = Ue_2 \sin \Delta\phi \rightarrow (23)$$

$$\dot{e}_2 = -Ue_1 \sin \Delta\phi \rightarrow (24)$$

$$\dot{e}_1 \approx -\dot{e}_2 \rightarrow (25)$$

$$e_1\dot{\phi}_1 = -Ue_2 \cos \Delta\phi + eV \rightarrow (26)$$

$$e_2\dot{\phi}_2 = -Ue_1 \cos \Delta\phi - eV \rightarrow (27)$$

Remembering $e_1 \approx e_2 \approx e$

$$\dot{\phi}_2 - \dot{\phi}_1 \cong -2eV \rightarrow (28)$$

$$\Delta\phi \approx (\Delta\phi)_0 - 2eVt \rightarrow (29)$$

current density.

$$J = J_0 \sin [(\Delta\phi)_0 - 2eVt] \rightarrow (30)$$

$$\omega_J = 2eV = 2e \frac{\text{voltage}}{\hbar} \rightarrow (31)$$

For AC Josephson effect which occurs when

$$\omega = \frac{q}{\hbar} \text{voltage} \longrightarrow (32)$$

These experiments also contributed to better accuracy in the determination of fundamental constants.

Purpose of Josephson effect :-

* working of a SQUID

'UNIT-3'

-'NANOMATERIALS'

'TWO MARKS'

1) Write about Nanomaterials.

* Nanomaterials are commonly defined as materials with an average grain size less than 100 nanometers.

* Nanomaterials have extremely small size which having at least one dimension 100nm.

* one billion nanometers equal one meter.

* The average width of human hair is on the order of 100,000 nanometers.

* A single particle of smoke is in the order of 1,000 nanometers.

* Two principal factors cause the properties of nanomaterials to differ significantly from bulk materials.
  - Increased relative surface area
  - Quantum effects

* 1 nanometer = 10 angstroms, 1nm there may be 3-5 atoms.

2) Write any four properties of nanomaterials

* The mechanical properties of nanomaterials increase with decrease in size, because smaller in size, lesser is the probablity of finding imperfections such as dislocations, vacancies, grain boundaries.

* The optical properties is the reduction of material dimension has pronounced effect on these properties. The size dependence is due to,
  - surface plasmon Resonance (SPR).
  - Quantum size effects.

* Magnetic properties of nanomaterials differ to that of bulk.

* For a ferromagnetic material, total energy is,

$$E_{tot} = E_{exc} + E_{ani} + E_{dem} + E_{app}$$

* where, E_{exc} - exchange energy, E_{ani} - Anisotropic energy, E_{dem} - demagnetization energy, E_{app} - energy due to applied magnetic field.

$$\boxed{E_{tot} = \mu_0 H} \quad , \quad \boxed{D_{cr} = \frac{9\gamma_B}{\mu_0 M_s^2}}$$

* Surface scattering, change of electronic structure quantum transport, Effect of microstructure plays important role in electrical properties.

3) What is fullerence ?

* It was discovered by 1985, Kroto smalley and curl.

* It is a carbon allotropes.

* Hollow sphere (bucky ball), ellipsoid, tube (bucky tube, nanotube).

* Similar structure to graphite :
  - Hexagons
  - pentagons (curvature).

* Euler : 12 pentagons to make sphere.

EXAMPLES :

* C_{60} - Buckminster fullerence.
  - Smallest structure with no pentagons touching.
  - ~.7nm diameter
  - Melting point ~550K

* Bucky onions - one fullerence inside another.
  - upto 70 layers observed.
  - Nanotube generation normally produces some onions

* These fullerence are useful because of size, stability, hydrophobia.

4) Write about CNT?

* Carbon nanotubes are tubular forms of carbon that can be envisaged as graphene sheets rolled into cylindrical form.

* These nanotubes have diameters of few nano-meters and their lengths are up to several micrometers.

* Each nanotube is made up of a hexagonal network of covalently bonded carbon atoms.

* Carbon-nanotubes are of two types,
  - single-walled.
  - multi-walled.

* A single walled carbon nanotube (SWNT) cons of a single graphene cylinder.

* Whereas, a multi-walled carbon nanotubes (MWNT) comprises of several concentric graphene cylinders.

* Depending on the way of rolling of graphene sheets in which single & multiwalled tubes are of different types, viz, armchair, zig-zag and chiral could be produced.

) What are Metallic glases?

* It shares the property of both metals and alloys.

* Metallic glasses are metal alloy that are amorphous. that is they don't have long range atomic order.

* The major advantages of such glasses are that they are generally homogeneous in composition, offer strong and superior corrosion resistance.

* Metallic glasses are two types based on their base material used in preparation.

  1) Metal-Metal glasses:
     - Eg: Ni-Nb, Mg-Zn and Cu-Zr

  2) Metal-metalloid glasses:
     - Eg: Fe, Co, Ni and metalloids like B, Si, C and P are used.

* There is no grain boundaries and dislocations.

* They have TCP [Tetrahedral closely packed structure].

* The metallic glasses are strong and ductile.

* This is known as metallic glasses.

6) What are ceramics?

* ceramic once referred purely to poetry and to articles made by firing materials extracted from Earth.

* ceramics are generally thought of as inorganic and nonmetallic solids with a range of useful properties, including very high hardness and strength extremely high melting points and good electrical and thermal insulations.

* The best known ceramics are pottery, glass, brick, procelain and cement.

* ceramics a nonmetallic and inorganic solid is so broad that it covers a much wide range of materials.

* ceramic include simple materials such as graphite and diamond, made up from different crystalline arrangements of the element carbon.

* Alumina, silicon carbide, silicon nitride, zirconia and sapphire are the types of ceramics.

'FIVE MARK QUESTIONS'

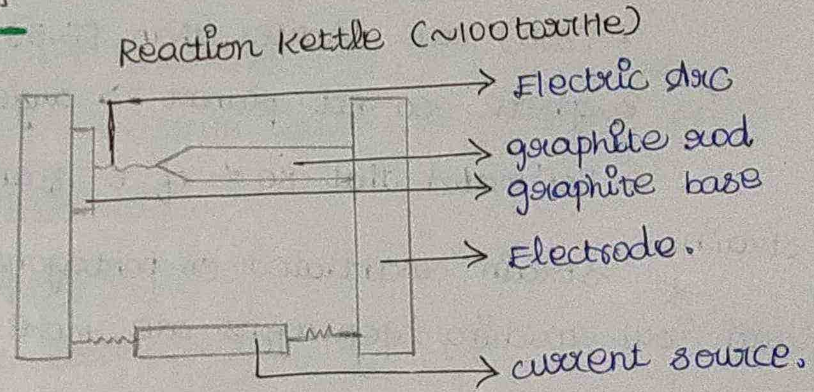
Write the properties of fullerence :-

Fullerence :-

* It is a carbon allotropes.
* It is a hollow sphere (bucky ball), ellipsoid, tube (bucky tube), (nanotube)
* similar structure to graphite :
    - Hexagons
    - pentagons (curvature).
* Euler : 12 pentagons to make sphere.

Production :-

*

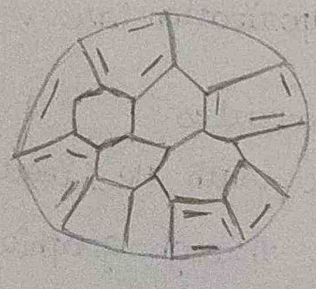


- Before : vaporization laser.
- 1990.
- Graphite electrodes
- Fill chamber with He (inert gas), ~100 torr
- Run current through graphite.

- Get black soot
- ~10% C_{60}
- Some larger fullerenes.

Properties :-

* Stable, but not totally unreactive
* In graphite,
  - sp^2 bonding
  - planar, 120°
* Fullerenes :
  - [6,6] double bonds, hexagons.
  - [6,5] single bonds, pentagons to hexagons
  - [6,6] are shorter than [6,5]
  - sphere, so not planar → angle strain
  - Estimated that 80% of E- formation due to strain.
* strain concentrated on pentagons → structures with out touching pentagons are more stable (C_{60}).



* Slightly soluble in some solvents.
  - Toluene, carbon disulfide etc.
  - In water : large clusters (nC_{60}) of 250-350 nm.
* Toxic ?
  - 2004 : found increase in cellular damage to fish with ~.5ppm in water.
  - 2005 : computer simulation found deformation of DNA by C_{60} in water.
* wave-particle duality with $\lambda = 3pm$, 1999.
* Examples :- C_{60} :-
  - Buckminster fullerene
  - smallest structure with no pentagons touching
  - ~.7nm diameter.
  - Melting point ~550K.
  - It is arranged as 12 pentagons and 20 hexagons.

Physical properties :-

* Do not dissolve in water.
* cannot conduct electricity.
* Soft and slippery.
* Brittle.

* Low melting point solids

chemical properties :

* Fullerenes are stable but not totally unreactive

* The sp^2- hybridized carbon atoms, which are at their energy minimum in planar graphite, must be bent to form the closed sphere or tube, which produces angle strain.

* Fullerene is electrophilic addition at 6,6-double bonds which reduces angle strain by changing sp^2- hybridized carbons into sp^3 hybridized ones.

* The change in hybridized orbitals causes the bond angular to decrease from about 120° in the sp^2 orbitals to about 109.5° in the sp^3 orbitals.

* This decrease in bond angles allows for the bonds to bend less when closing the sphere or tube and thus the molecule becomes more stable.

* Fullerenes are sparingly soluble in many solvents - aromatic such as toluene and carbon disulfide

---

Write properties of CNT's :

* **Strength :**
  - carbon nanotubes are the strongest, flexible and stiffest materials yet discovered in terms of tensile strength and elastic modulus respectively.

* **Hardness :**
  - The hardness (152 GPa) and bulk modulus (462-546 GPa) of carbon nanotubes are greater than diamond, which is considered the hardest material.

* **Electrical properties :**
  - Because of the symmetry and unique electronic structure of graphene, nanotube has a very high current carrying capacity.

* **Thermal conductivity :**
  - All nanotubes are expected to be very good thermal conductors along the tube.

* **EM wave absorption :**
  - There has been some research on filling MWNTs with metals, such as Fe, Ni, Co, etc.,... to increase the absorption effectiveness of MWNTs in the

microwave regime.

* **Thermal properties :**

- All nanotubes are expected to be very good conductors and insulators laterally to the tube axis.

* **Mechanical properties of engineering fibre :**

material	sp. den	yen	strength	strain break
carbonnanotube	1.3-2	1	10-60	10
HS steel	7.8	0.2	4.1	<10
carbon fibre - PAN	1.7-2	0.2-.6	1.7-5	0.3
carbon fibre - pitch	2-2.2	0.4-0.96	2.2-3.3	0.27 0.6
E/S - glass	2.5	0.07-0.08	2.4-4.5	4.[illegible]
kevlar - 49	1.4	0.13	3.6-4.1	2.[illegible]

* **properties of conductive Materials :**

Materials	Thermal conductivity	Electrical conductivity
carbon Nanotube	>3000	$10^6 - 10^7$
copper	400	6×10^7
carbon fibre - pitch	1000	$2-8.5 \times 10^6$
carbon fibre - PAN	8 - 105	$6.5 - 14 \times 10^6$

Application of CNT'S

It's applications are,

* carbon Nanotube Membranes for Transdermal Drug delivery
* For cancer treatment
* For cardiac Autonomic Regulation
* Tissue regeneration
* platelet activation.
* In drug delivery.

Electronic Applications :

* conductive composites
  - Electron emitters.
  - Nanoprobes.
  - sensors – Biomedical Industry, automotive Industry Food Industry, Environmental Monitoring.
  - FED display
  - Template.

Mechanical field :

* CNT Based Actuator :
  - High technology applications, Including humanoid robots, artificial and damaged hearts, artificial limbs,

medical prosthetic devices etc,

CNT based composites :-

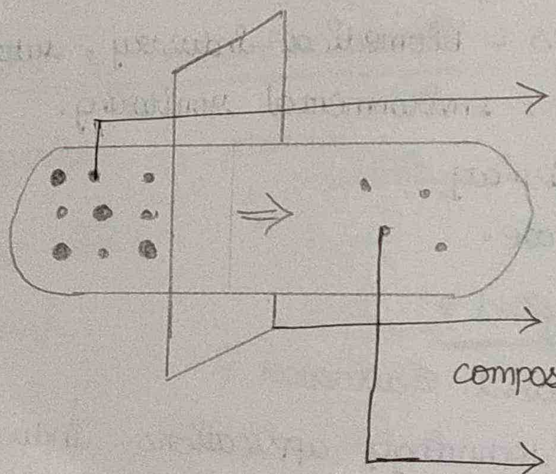
* polymer matrix composite.
* ceramic matrix composite.

Medical field :-

* In drug delivery and cancer therapy
* CNT'S as Biosensors.

Other applications :-

* As thermal Materials.
* Air and water filtration
* Hydrogen storage
* energy storage.



TEN MARKS QUESTIONS

1) **Write in detail about CNT and its properties :-**

CNT

* Carbon nanotubes (CNT) are the basis of nanotechnology.
* carbon with an atomic number of 6 plays a pivotal role in nanotechnology.
* They were discovered by Iijima accidentaly while studying the surface of graphite electrode used in electric and discharge.
* The accidental observation laid a foundation of exciting field of nanotechnology and started a new direction in the carbon research.
* A CNT is a hexagonal array of carbon atoms rolled up into a long, thin, hollow cylinder and are known for the, size, shape and remarkable physical properties.
* they can be mainted (manipulated) chemically and physically for their application in material science, electronics, energy management, biomedical application and many more.

Structure of Nanotubes :

* A carbon nanotube is a tube shaped material made of carbon and has diameter on the nanometer scale.

Two types of carbon nanotubes are observed single walled nanotubes (SWNT) and multiwalled nanotubes (MWNT).

SWNT :

* They have diameter close to 1 nanometer and tube length may vary millions of times longer.

* They can be formed in three different forms- archair, zigzag and chiral forms on basis of rolling of graphene sheet into a seamless cylinder. Each form has a special effect on electrical property of nanotubes.

MWNT :

* The discovery of C_{60} motivated the researchers to search for other carbon compounds containing curved graphenes.

* This led to the discovery of multiwalled nanotubes were made of concentric cylinders of rolled up graphene sheets capped with semi-fullerene

* The length of a tube was in the range of few μm, the diameter was (10-20nm)

* As the size increases, these structures exhibit properties between fullerenes and graphite.

Properties of carbonanotubes :

strength :

* carbon nanotubes have higher tensile strength than steel and kevlar.

* The strength originates from sp^2 bonds between the individual carbon atoms.

* carbon nanotubes are not strongly, they are also elastic.

* upon application of force, nanotube can bend and returns to its original shape when the force is removed.

* A nanotube's elasticity does not have a limit and under very strong forces, it is possible to permenantly weakened by defects in the structure of nanotube.

* A nanotube's strength can be weakned by defects in the structure of the nanotube.

* A nanotube's strength can be weakened by defects in the structure of the nanotube.

* Defects occur a from atomic vaccancies or a rearrangement of the carbon bonds.

* Defects in the structure can cause a small segment of the nanotubes to become weaker, which in turn cause the tensile strength of the entire nanotube to weaken.

* The tensile strength of a nanotube depends on the strength of the weakest segment in the tube similar to the way the strength of a chain.

Electrical properties :-

* The sp^2 bonds between carbon atoms results in conducting nature of carbon nanotubes.

* They also withstand strong electric currents because of the strong nature of bonds.

* Single walled nanotubes can route electrical signals at speeds up to 10GHZ, when used as inter-connects on semi-conducting devices.

* The electronic properties can be manipulated application of external magnetic field, mechanical for[ce] etc.

Thermal stability :-

* carbon nanotubes are able to withstand high temperatures, thus acting as very good thermal conductors.

* The temperature stability of carbon nanotubes. Is estimated to be upto 2800 C and about 750 C in air.

* the carbon nanotubes are shown to transmit over 15 times the amount of watt per minute as compared to copper wires.

* This property has special application in field emission flat - panel displays and cold - cathode guns used in microscopes.

* In nanoelectronics SWNTs have been used to fabricate transistors that can function at room temperature and are potential for devices operating at tetrahertz (THz) frequencies.

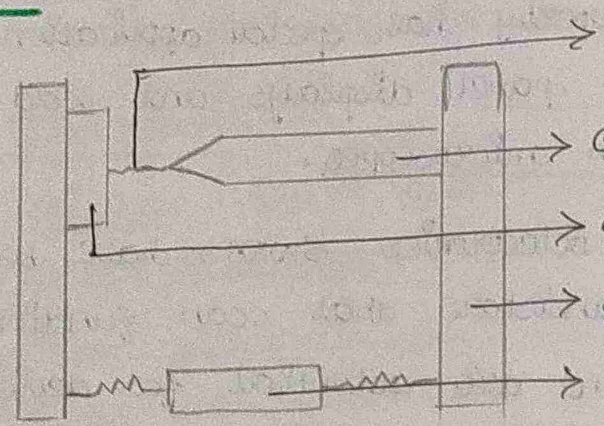
* These are the properties of carbonnanotubes.

* In which the products containing carbon nanotubes are crushed or incinerated in a waste dump.

2) what is fullerene ? write its properties :-

* Discovered 1985, Kroto, smalley and curl.
* It is a carbon allotropes.
* Hollow sphere (buckyball), ellipsoid, tube (buckytube, nanotube).
* Similar structure to graphite.
    - Hexagons
    - pentagons.
* Euler - 12 pentagons to make sphere.

Production :-



- Before - vapourization laser
- 1990
- Graphite electrode
- Fill chamber with He (inert gas) ~ 100 torr
- Run current through graphite.

* Get black soot
* ~10% C_{60}
* Some larger fullerenes.

Properties:

* stable but not totally unreactive.

* In graphite:
  * sp^2 bonding
  * planar 120°

* Fullerenes:
  1) [6,6] double bonds, hexagons.
  2) [6,5] single bonds, pentagons to hexagons.
  3) [6,6] are shorter than [6,5]
  4) Sphere, so not planar → angle strain.
  5) Estimated that 80% of E- formation due to strain.
  6) strain concentrated on pentagons → structures with out touching pentagons are more stable (C_{60}).

* slightly soluble in some solvents
* toluene, carbon disulfide etc.
* in water : large clusters (nC_{60}) of 250-350n[m]
* Toxic ?
  - 2004 - found increase in cellular damage to fish with ~.5ppm in water.
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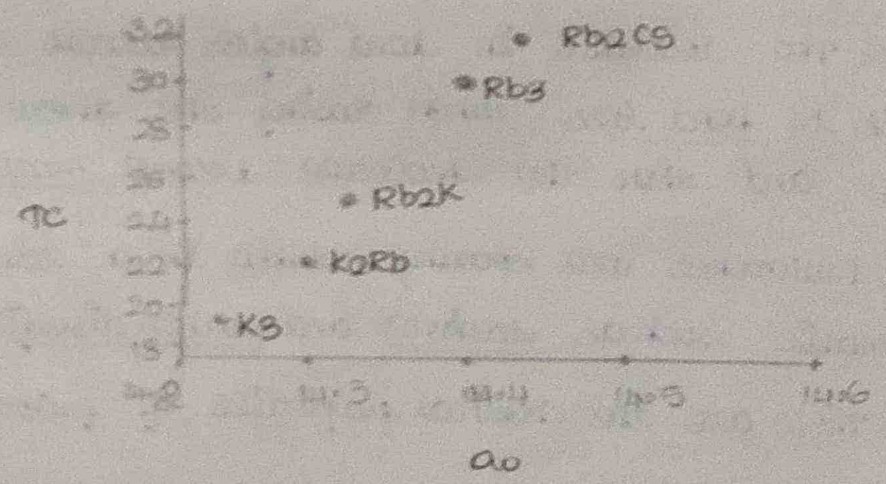
C_{60} :
- Buckminster fullerence
- smallest structure with no pentagons touching
- ~.7nm diameter
- melting point ~550K

Bucky onions :
- one fullerene inside another
- upto 70 layers observed
- nanotube generation normally produces some onions.

Fullerite :
- bulk solid C_{60}
- FCC structure.

ultrahard fullerite :

* 310 ± 40 GPa hardness
* Diamond : < 240 GPa (sometimes 150 GPa).
* A_3C_{60}, A_6C_{60}
* Alkali metal cations for each sphere.
* 3 metal holes occupy per sphere (blue)
* A_3C_{60} - conductor
* A_6C_{60} - Insulator at room temperature.
* A_3C_{60} becomes a super conducting
* lattice constant a_0 changes to accomodate the metal cation.
* different Tc.



Physical properties :-

* Do not dissolve in water.
* cannot conduct electricity.
* soft and slippery.
* Brittle.
* low melting points.

chemical properties :-

* Fullerenes are stable but not totally un-reactive.

* The sp^2 hybridized carbon atoms, which are at their energy minimum in planar graphite, mus be bent to form the closed sphere or tube, which produces angle strain.

* The decrease in bond angles allows for bonds to bend less when closing the sphere or tube and thus the molecule become more stable.

* Fullerenes are sparing soluble in a solvents-aromatic such as toulene and carbon disulfide.

* These are the chemical properties of fullerene.

Write about the physical vapour deposition and chemical vapour deposition:

Physical vapour deposition :-

* It is called as (PVT) - physical vapour transport.

* It describes a variety of vaccum deposition methods which can be used to produce thin films and coatings.

* PVD is characterised by a process in which the material goes more a condensed phase to a vapour phase and then back to a film condensed phase.

* The most common PVD processes are sputtering and evaporation.

* PVD is the manufacture of items which require the thin films for mechanicals, optical, chemical or electronic functions.

* Examples include semiconductor devices such as,
  - thin film solar panels
  - PET film
  - balloons
  - titanium
  - nitrited coating cutting tools for metal working.

Source
(solid / liquid)

↓ Evaporation

Gas phase

↓ Transport & Deposition

solid phase

* Examples are cardiac arc deposition, Electron beam physical vapour deposition etc.,

chemical vapour deposition:

* Chemical vapour deposition (CVD) is a chemical process used to produce high purity, high performance solid materials.

* In typical CVD process, the substrate is exposed to one or more volatile precursors which react and decompose on the substrate surface to produce a desired deposit.

* During this process, volatile by-products are also produced, which are removed by gas flow through the reaction chamber.

Steps Involved in chemical vapour deposition:

(Transport of reactants by forced convection to the deposition region.)

↓

(Transport of reactants by diffusion from the main gas stream to the substrate surface.)

↓

(Adsorption of reactants in the wafer (substrate) surface.)

↓

(chemical decomposition and other surface reactions take place.)

↓

(~~Tran~~ Desorption of by-products from the surface.)

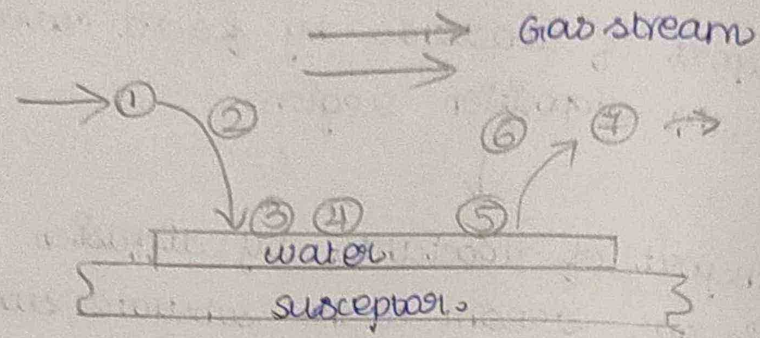
↓

(Transport of by products by forced convection away from the deposition region.)

These are the steps which are involved in the chemical vapour deposition.

* The CVD are of types are it is represented as;

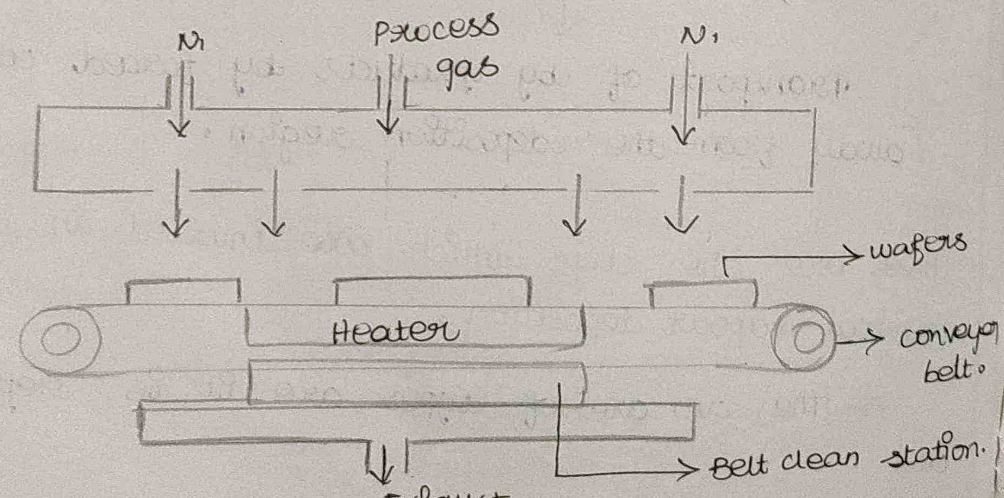
Schematic Diagram - steps Involved in CVD,



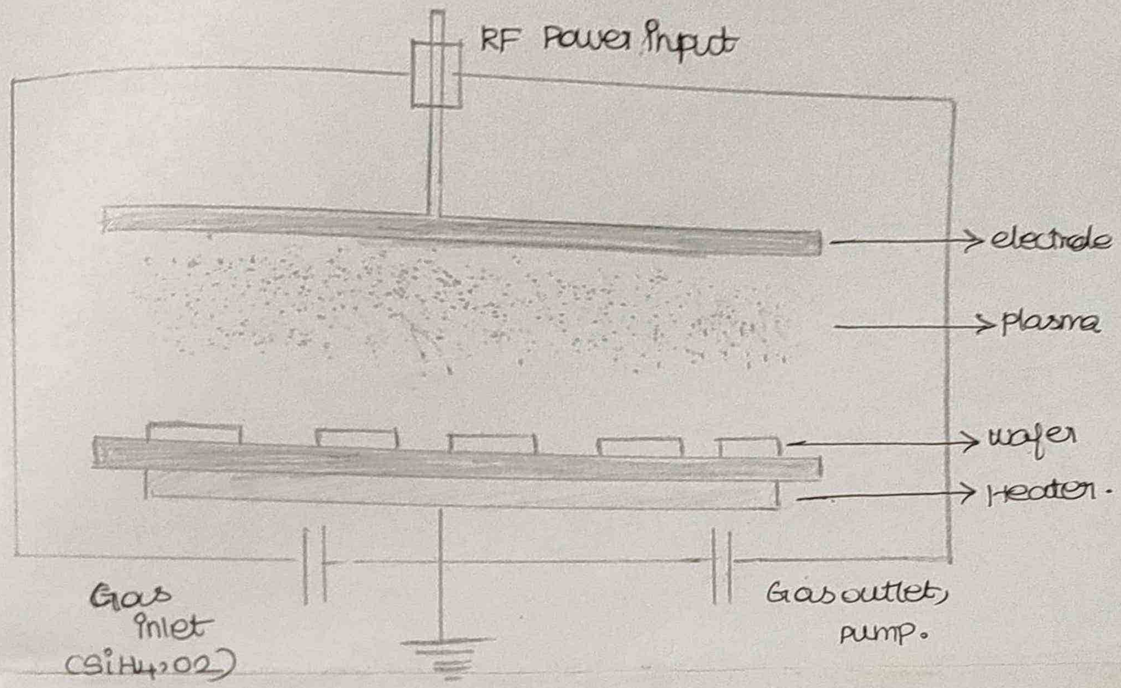
The types are,

1) Atmospheric pressure CVD
2) Low pressure LCVD
- Plasma enhanced CVD
- Photochemical vapour Deposition
- Thermal CVD.

Diagram of APCVD and PECVD and About the Advantages:-



PECVD :-



Advantages of CVD :-

- Variable shaped surfaces given reasonable access to the coating powders of gases, such as screw threads, blind holes or channels or recesses, can be coated evenly without blind up on edges.
- High purity can be obtained
- High density - nearly 100% of theoretical value.
- Material formation below the melting point.

'TWO MARKS' Unit-4

1) What are metallic glases?

* metallic glases are the newly developed engineering materials.

* Metallic glasses share the properties of both metals and alloys.

* Most metals and alloys are crystalline, ie their atoms arranged in some regular pattern that extends over a long distance.

* In contrast glass is an amorphous, brittle and transparent solids.

* Thus, metallic glasses are metal alloys that are amorphous that is, they do not have a long range atomic order.

* The major advantages of such glasses are that they are generally homogeneous in composition and after strong and superior corrosion resistance.

* They also have good magnetic properties and corrosion resistance.

* Eg: Ni-Nb and Fe, Co, Ni with B, Si, C, P.

2) What are ceramics?

* An inorganic compound consisting of a metal and are more nonmetals.

* Important examples,

* Silica - silicon dioxide (SiO_2) the main ingredient in most glass products.

* High hardness, electrical and thermal insulating, chemical stability and high melting temperatures.

* ceramics can be processed in molten ceramics and particulate ceramics.

3) Write SAW materials?

* A surface acoustic wave (SAW) is an acoustic wave travelling along the surface of a material exhibiting elasticity, with amplitude that typically depths exponentially with depth into the substrate.

* The velocity of acoustic waves is typically 3000 m/s, which is lower than the velocity of the electromagnetic waves

* A basic SAW device consist of two IDTs on a piezoelectric substrate such as quartz. The input IDT launches and the output IDT receives the waves.

4) What do you mean by SMART Materials ?

* Smart or Intelligent materials that have to respond to stimuli and enviornmental changes and to activate their functions according to these changes.

* The stimuli like temperature, pressure, electric flow, magnetic flow, light, mechanical etc, can originate internally or externally.

* They are divided to Active & Passive :

1) Stress 2) Electric field	Piezo electric Material	1) Electric charge 2) Mechanical strain
Heat	Shape Memory Alloy	original memorized shape
Electric field	Electro - rheological fluid	change in viscos (internal dampi
Temperature, Pressure mechanical strain	optical fibre	change in opto electronic signa
Magnetic field	Magneto - strictive Material.	Mechanical strain.

FIVE MARKS

Write about ceramics :

* An inorganic compound consisting of a metal and one or more nonmetals.

* Important examples,

• Silica - silicon dioxide (SiO_2), the main ingredient in most glass products.

• Alumina - aluminium oxide (Al_2O_3) used in various applications from abrasives to artificial bones.

Properties :

* High hardness, electrical and thermal insulating chemical stability and high melting temperatures.

* Brittle, virtually no ductility - can cause problems in both processing and performance of ceramic products.

* Some ceramics products are translucent, window glass being the clearest example.

Products from ceramics :

* Glass - bottles, glasses, lenses, window pane and light bulbs.

- Glass fibres – thermal insulating wool, reinforced plastics, and fibre optics communications lines.
- Abrasives – aluminium oxide and silicon carbide.
- cutting tool materials – tungsten carbide, aluminium oxide and cubic boron nitride.
- ceramic insulator – application include electrical transmission components, spark plugs and micro-electronic chip substrates.
- Bioceramics – artificial teeth and bones.

Methods to strengthen ceramic Materials :-

* Make starting more uniform.
* Decrease grain size in polycrystalline ceramic products.
* Minimize porosity.
* Introduce compressive surface stresses.
* use fiber reinforcement
* Heat treat.

Physical properties of ceramics :-

* Density – In general, ceramics are lighter than metals and heavier than polymers.
* Melting temperatures – higher than for most metals.
* some ceramics decompose rather than melt.
* Electrical and thermal conductives – lower than for metals, but the range of values is greater, so some ceramics are insulators while others are conductors.
* Thermal expansion – somewhat less than for metals, but effect are more damaging because of brittleness.

Applications :-

- Industrial sectors.
- tappet heads for use in automotive engines
- oil free bearings
- aerospace turbine blades
- nuclear fuel rods
- light weight armour
- cutting tools
- thermal barriers
- ceramic substrates for electronic devices
- abrasives
- furnace / kiln furniture.

2) **Explain optical materials with eg :-**

* Materials used for optical components

* Various kinds of materials are used for making optical elements.

* optical materials are usually understood to be transparent materials.

* ie, materials with good light transmission in some spectral ranges, exhibiting little absorptio[n] and scattering of light.

* However, absorption can be utilized for optical filters, and even light scattering is used in some application.

* Further more, some materials are useful for making optical components which do not transm[it] light.

* For example, some materials with full transparency can be used as substrates for mirrors.

* In which,
  - crystalline Materials
  - semiconductors
  - Polycrystalline ceramics.

Crystalline Materials :-

* Most crystalline optical materials are monocrystaline, since light scattering at interfaces between grain boundaries could be detrimental.

* optical crystals are basically always artificially grown materials. The growth velocity is usually very small because otherwise one would not obtain a single crystal.

* Therefore, crystalline optical materials tend to be more expensive than glasses or cermics.

* This is particularly so in the mid and far infrared, where there is a limited choice of materials with good transparency.

* In some cases, optical anisotropy is required for example in the form of birefringence, which is obtained for crystal symmetry.

* optical crystal particularly those without special dopants, are highly pure materials with very consistent optical properties.

* In contrast to glasses, where the exact composition of the used raw materials may

somewhat vary.

* And there are certain fluctuations of the local chemical composition.

Semiconductors :-

* Semiconductors are not transparent in the visible spectral region, because their band gap energy is smaller than the photon energy of visible light.

* However, they exhibit good transparency in the infrared.

* For example, silicon, germanium and gallium arsenide are used for infrared optics. The refractive index is usually rather high.

* Semiconductor materials are used for infrared optical windows.

* For example, there are nonlinear frequency conversion devices with quasi-phase-matched gallium arsenide.

* There is also the whole research area of silicon photonics, involving integrated optics on the basis of silicon.

Polycrystalline ceramics :-

* Polycrystalline materials have been found some applications in optics.

* Their basic challenge is the light scattering at grain boundaries.

* However, like certain transparent ceramic materials like alumina (Al_2O_3) and yttrium aluminium garnet (YAG = $Y_3Al_5O_{12}$) have been developed with good optical quality including low scattering losses.

* This can be achieved if the used materials are very pure and the raw material have small dimensions, so that the grain also becomes rapidly stronger at shorter wavelengths.

* The optical properties of ceramics can be similar to those of glasses.

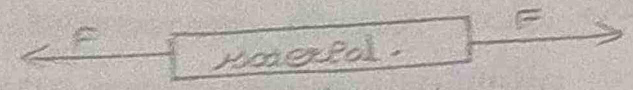
* Therefore, ceramic materials can be used for many typical of optical components such as, lenses, prism, optical windows etc..

* An advantage of ceramics over single crystals is that they can be made with very large dimensions without a time consuming crystal growth.

3) **Factors affecting mechanical properties of materials**

Tensile strength:

* This is the ability of a material to withstand tensile (stretching) loads without rupture occurring. The material is in tension.



F = applied load

Compressive strength:

* This is the ability of material to withstand compressive (squeezing) loads without being crushed or broken. The materials is in compression.

Shear strength:

These are some of the mechanical properties.

The factor that affect these properties are,

- Grain size
- Heat treatment
- Atmospheric exposure
- Low and high temperature.

Effect of grain size :-

* The metals are composed of crystals (or) grains. If the grain size of a metal is small it is called a fine grained metal on the other hand, when the grain size is comparatively large then it is called a coarse grained metal.

* A fine grained metal has a greater tensile and fatigue strength. It can be easily work harded.

* A coarse grain causes the surface of roughness.

* coarse grain metal is difficult to polish.

Effect of Heat treatment :-

* To refine the grain and improve mechinability.

* To relieve the internal stress induced in the metals during cold and hot working of the metals.

* To improve resistance to corrosion.

* To modify the structure, either coarse grained or fine grained.

* To improve chemical, magnetic, electrical and thermal properties.

Effect of atmospheric exposure :-

* characteristics properties of the metal.
* value of the protective film on its surface.
* presence of certain reducing agents.
* Local cells formed due to development of cracks and discontinuity on the protective film surf

Effect of low temperature :

* Decrease in temperature there is an increase in the tensile strength and yeld strength of all metals.
* Alloys of nickle, copper and aluminium reta most of their ductility and toughness at low tempera
* For Below -100°c non ferrous metals show bette properties than ferro metals.

Effect of high temperature :-

* Field stress and ultimate tensile strength decrease with rise in temperature.
* At high temperature, the toughness of steel is reduced.
* At high temperature, creep takes place and the material fails even at very small stress.

Fibre reinforced metals :-

* Fibre reinforced are made of metals, ceramics, glasses or polymers, Boron, carbon, Al_2O_3, SiO_2.

* The most common form in which fibre reinforced composites are used in structural applications called laminate.

Properties :-

- Low coefficient of expansion
- High dimensional stability
- High tensile strength
- High heat stability.
- Better abrasion and wear resistance.
- Better toughness
- Impact strength
- Low density
- Good shear properties
- High stiffness.

Advantages :-

* A higher performance for a given weight leads and fuel savings.

* Excellent strength to weight and stiffness to weight ratios can be achieved by composite materials.

* Production of cost is reduced.

* composites may be made by a wide range of process.

* composite offer excellent resistance to corrosion, chemical attack and outdoor weatheri

Disadvantages :-

* composites are more brittle than wrought metals and thus are more easily damaged.

* Hot curing is necessary in many cases requiring special equipment.

* Repair at the original cure temperature it requiring tool and pressure.

Application :-

- Body components.
- chassis components.
- engine components.

TEN MARK

Explain in detail about Bio-materials :

Biomaterials :

* Biomaterial is used to make devices to replace a part or a function of the body in a safe, reliable, economic and physiologically acceptable manner [Hench and Ethridge 1982].

Materials of synthetic as well as of natural origin in contact with tissue, blood and biological fluids and intended for use for prosthetic, diagnostic, therapeutic and storage applications without adversely affecting the living organism and its components [Bruck-1980].

Late early 1960, 1970's biomaterial field solidified. In 1975 society for Biomaterials formed.

Characteristics of Bio-materials :

Physical Requirements :

* Hard materials.
* Flexible materials.

Chemical Requirements :

* Must not react with any tissue in the body.
* must be non-toxic to the body.
* Long term replacement must not be biodegradable.

Main Features for medical Applications :-

Biofunctionality :-
* playing a specific function in physical and the mechanical terms.

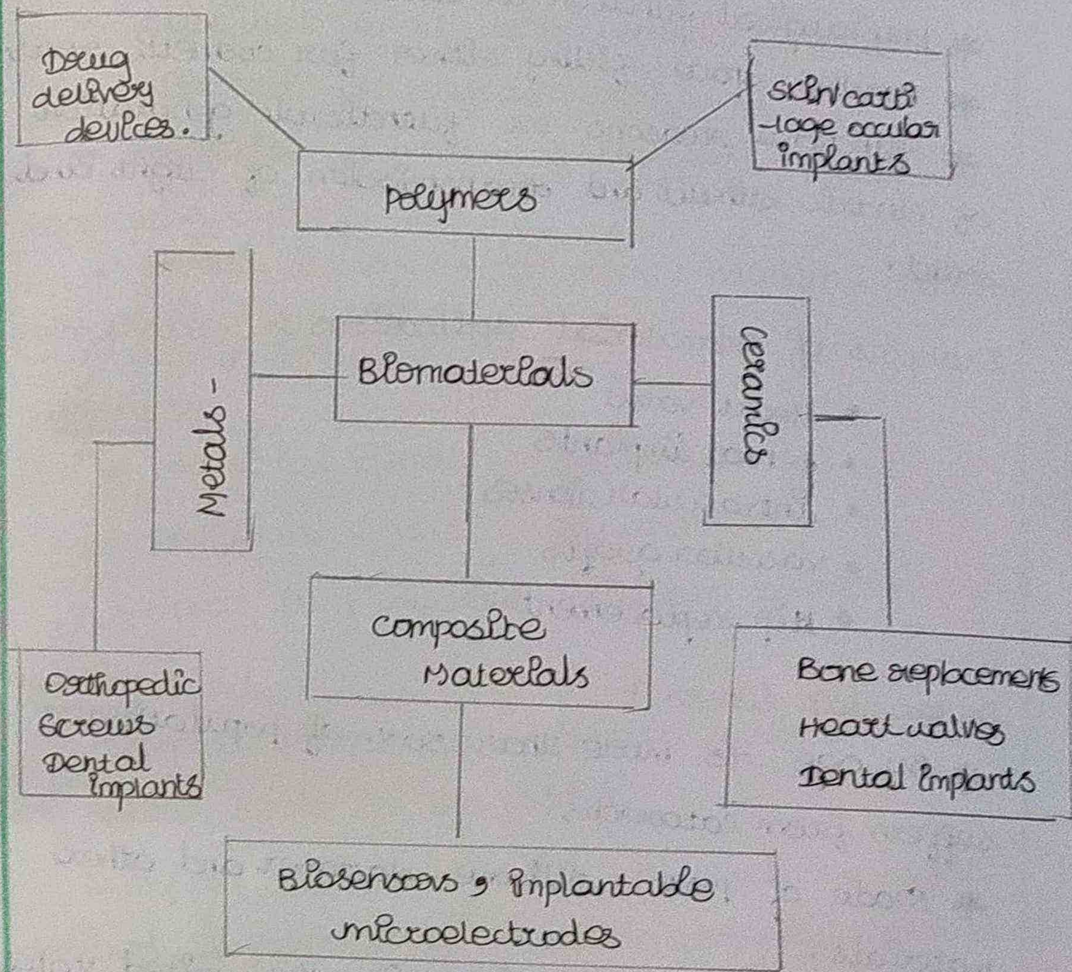
Bio-compatibility :-
* That refers to a set of properties that a material must have to used.
* safely in a biological organism.

Biocompatible Material features :-
* Absence of carcinogenicity (the ability or tendency to produce cancer).

Absence of Immunogenicity (absence of recognition of an external factor which could create rejection).

Absence of teratogenicity (ability to cause birth defects).

Absence of toxicity.



Function of Biomaterials :-
* The functions of implants fall in one of the categories.

* Load bearing or transmission
* The control of fluid flow in order to stimulate normal.
physiological function or situation.
* Passive space filling either for cosmetic reaso
* functional reasons or functional generation of electric stimuli and transmission of light and sound.

Examples of Biomaterial Applications :

- Heart valve
- Dental implants
- Intraocular lenses
- vascular grafts
- Hip replacement.

Intraocular lenses :

* By age 75 more than 50% of population suffers from cataracts.
* Made of PMM, silicone, elastomer and other materials.
* 1.4 million implantation in the united states yearly.
* Good vision is generally resorted almost immediately after lens is inserted.

Heart Value :-

- Fabricated from carbons, metals, elastomers, fabrics and natural values.
- Must not react with chemicals in body.
- Attached by polyester mesh.
- Artificial tendon and ligament - teflon and Dacron.
- Dental implants - titanium, alumina, calcium-phosphate.

Organs :-

- Artificial kidney - cellulose.
- Artificial heart - polyurethane.
- Heart lung machine - sillicone rubber.

Healing :-

- special process are invoked when a material or device heals in the body.
- Injury to tissue will stimulate the well-defined inflammatory reaction sequence that leads to healing.
- when a foreign body (eg. an implant) is present in the wound site (surgical incision) the reaction sequence is reffered to as the foreign

body reaction.

- Furthermore, this reaction will differ in intensity and duration upon the anatomical site involved.

Mechanical and performance

- Biomaterials that have a mechanical operation must perform to certain standards are be able to cope with pressures.

- It is therefore essentials to that all biomaterials are well designed and tested.

- Biomaterials that are used with a mechanical application such as hip implants are usually designed using CAD.

Steps involved in development :-

- Identifying a need, device design, Material synthesis, Material testing, fabrication, sterilizing and packaging, device testing and clinical use.

- These are the applications of Bio-materials. They are closely replicate complex tissue, architecture and arrangement in vitro.

Write about Nuclear engineering materials :-

Nuclear Material :-

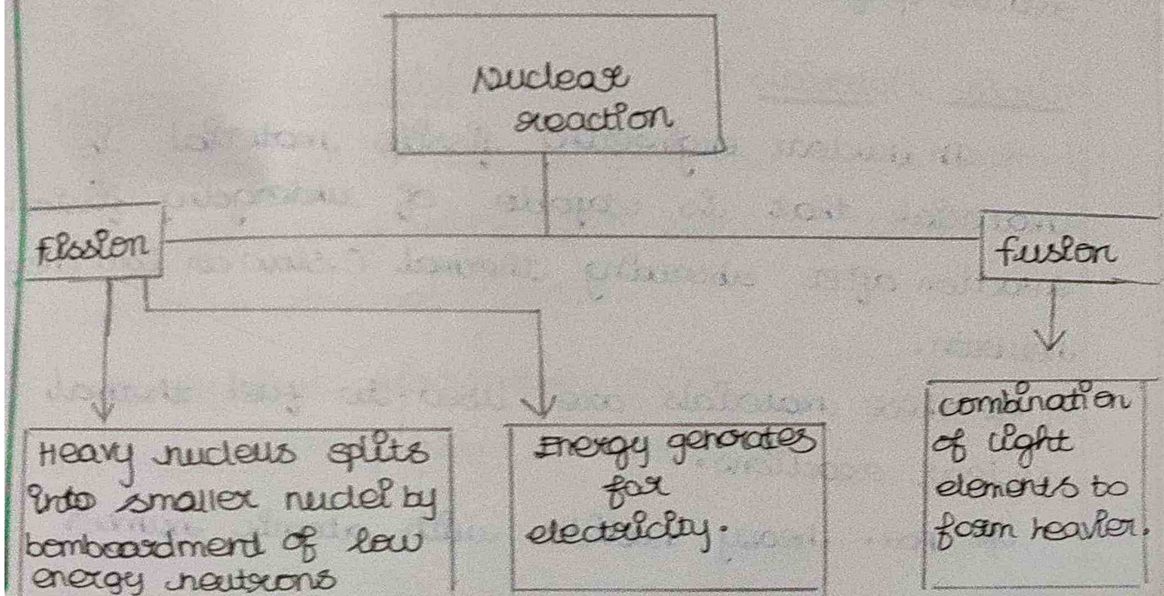
* A material that possess radioactive properties.

- Nuclear material such as uranium 233 and 235 are used to produce nuclear energy.

- Nuclear materials commonly refers to fissile materials that are capable of sustaining a chain reaction in a process that release energy called nuclear fission.

- The nuclear include isotopes of uranium, thorium and plutonium.

Nuclear Energy :-



Nuclear Heat :-

- Nuclear power generates heat from fission heavy isotopes.
    - uranium 233, 235 (258).
    - plutonium 239.
- Multiple options exist for the coolant, light water, heavy water, CO_2, helium, fluoride salts lead, sodium, organic fluids etc.
- In a thermal reactor, the coolant also slows down neutrons.
- Thermal or fast reactors
- Reactors are designed to be stable systems.
- If you increase the power or temperature, the reactor physics will try to reduce power.

Fissile Materials :-

* In nuclear engineering fissile material is material that is capable of undergoing fission reaction after absorbing thermal (slow or low ene[rgy]) neutron.

* These materials are used to fuel thermal nuclear reactions.

* For, heavy nuclides with atomic number

of higher more than 90 most of fissile isotopes meet the fissile rule.

Isotopes of fissile materials :-

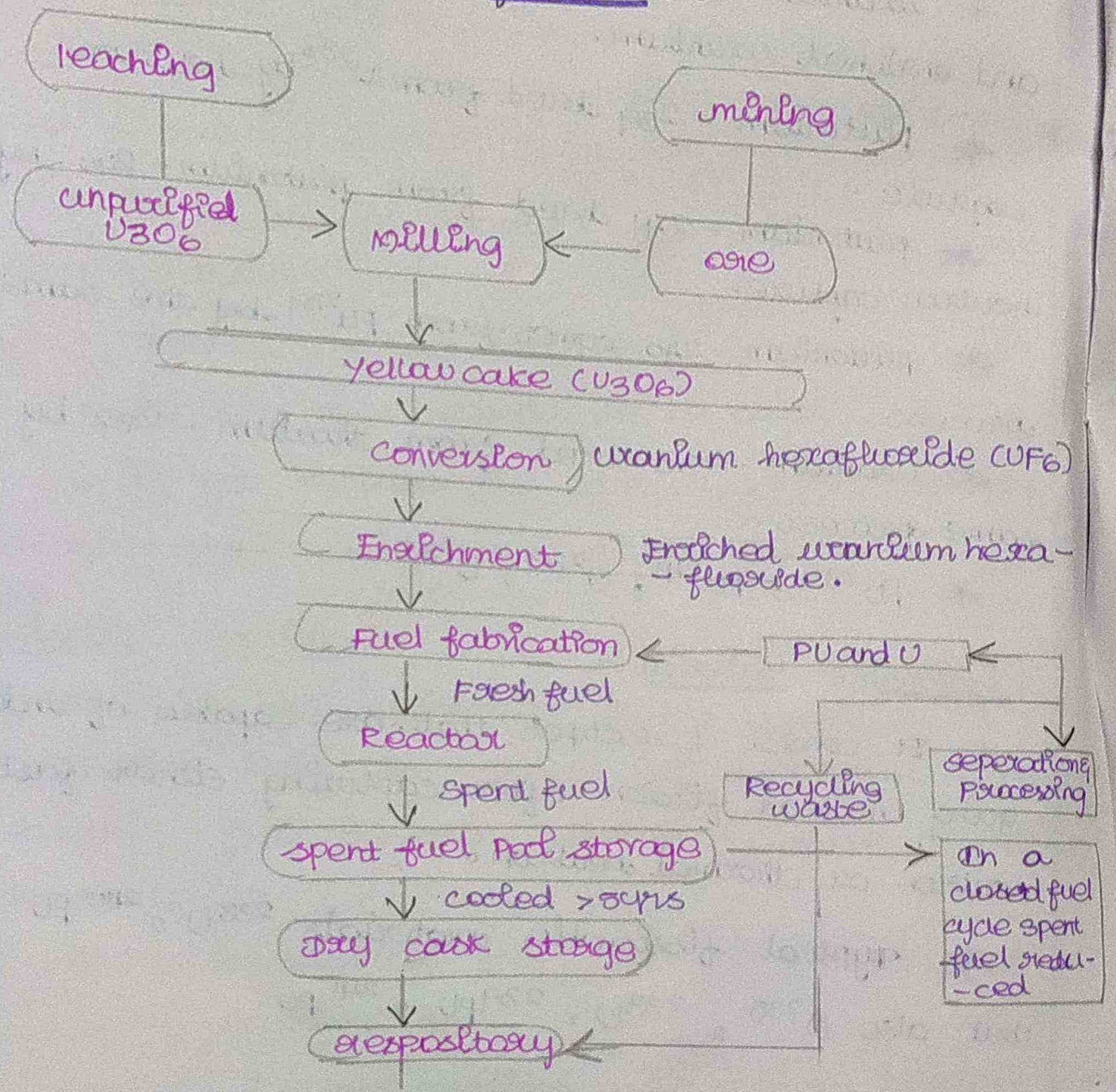
* uranium - 235 which occurs in natural uranium and enriched uranium.
* plutonium - 239 bred from U^{238} by neutron capture.
* plutonium - 241 bred from plutonium - 240 by neutron capture.
* plutonium - 240 comes from Pu^{239} by the same process.
* Uranium - 233 bred from thorium - 232 by same process.
* Pu^{239}, Pu^{241}, U^{233}, U^{235}

Fissionable Material :-

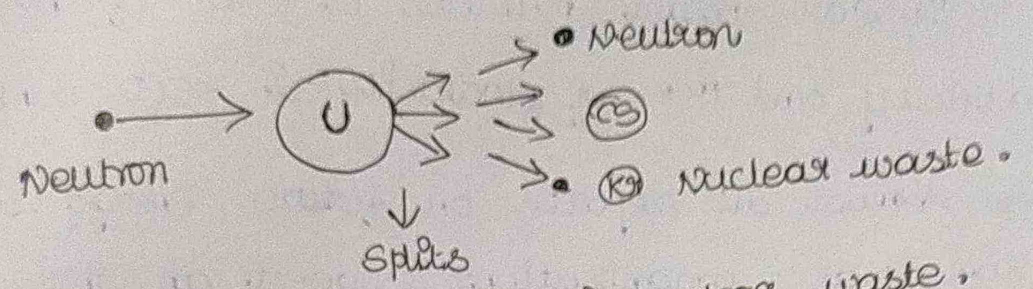
* It consist of isotopes that are capable of under-going nuclear fission after capturing either fast neutron or thermal neutron.
* Typical fissionable materials ^{238}U, ^{240}Pu but also U^{235}, ^{233}U, ^{239}Pu, ^{241}Pu.

- The fissile material consist of fissionable istopes that are capable of undergoing nuclear fission only after capturing a thermal neutron.

Nuclear fuel cycle - flowchart :

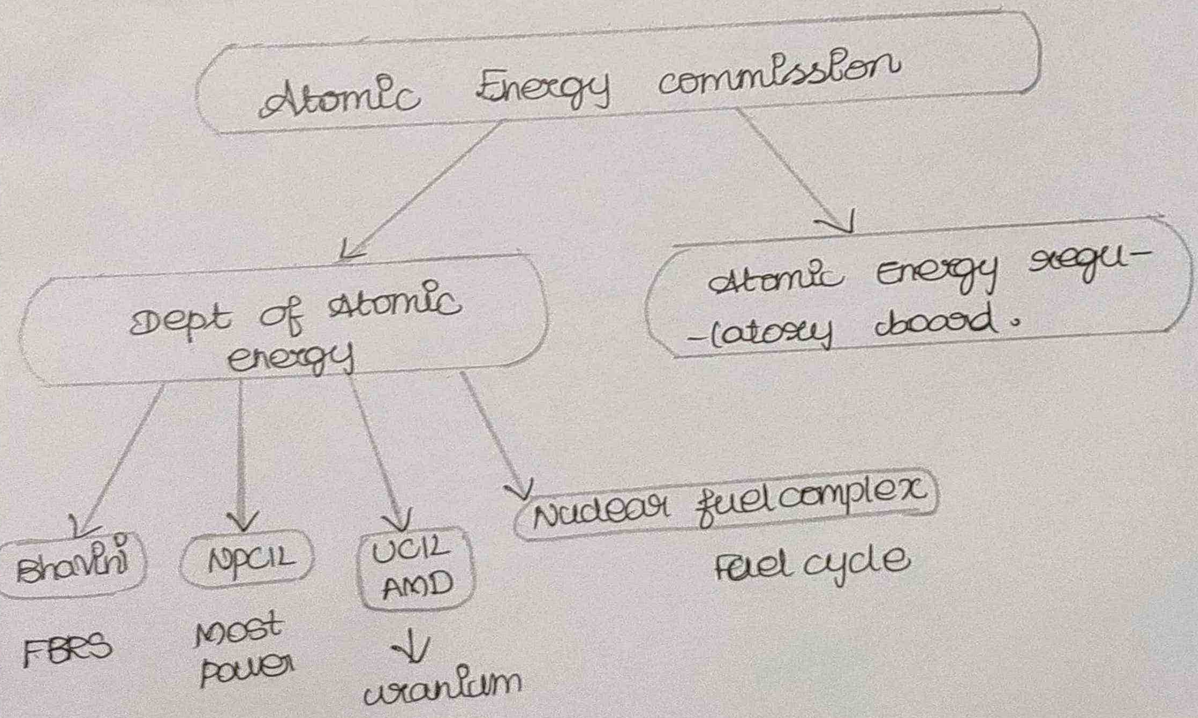


This is how the nuclear fuel is processed.



The splitting make up high nuclear waste.

Nuclear power in India.



Nuclear power in Future :

* Nuclear power provides over 10% of the world's electricity and 18% of electricity in OECD countries.

* Almost all reports on future energy supply from major organisations suggest an increasing role of nuclear power as an environmentally begning way of producing reliable electricity on a large scale.

UNIT-V

"MECHANICAL BEHAVIOUR OF MATERIALS"

TWO MARK QUESTIONS :-

1) Define creep :-

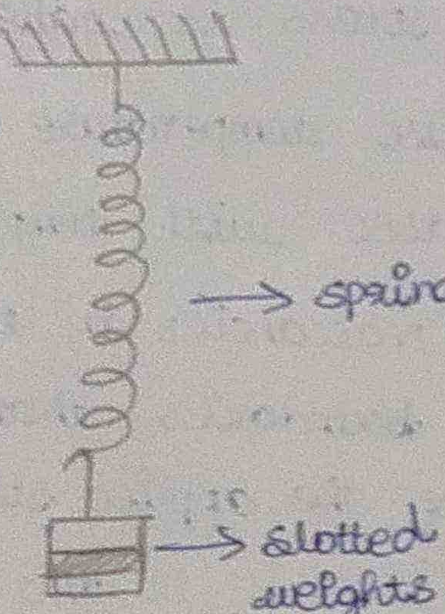
- Creep is a time-dependent process where a material under an applied stress exhibits a dimensional change at high temperature.
- High temperature progressive deformation of a material at constant stress is called creep.
- The process is also temperature-dependent
- creep always increases with temperature.
- creep occurs when vaccancies in the material migrate toward grain boundaries that are oriented normal to the direction of the applied stress.
- Threshold for creep will be the critical temperature for creep is 40% of the melting temperature.
- If $T > 0.40 T_M$ → creep is likely
- where T_M = melting temperature.
- Creep can be occur due to different mechanisms.

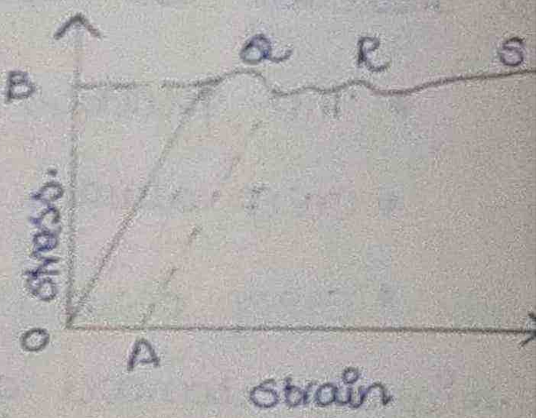
2) State Hooke's law :

- According to Hooke's law, strain produ[ced] in a body is directly proportional to the stre[ss] that produces it.

- stress ∝ strain

- $\frac{\text{stress}}{\text{strain}}$ = a constant known as a modulus of elasticity.





- The unit is Nm^{-2}.
- It's dimension is $ML^{-1}T^{-2}$.

what is hot working treatment?

- when the processing temperature of the mechanical deformation of is above the recrystallization temperature the process is termed as hot working.

- Large deformation can be successively repeated as the metal remain soft and ductile.

- The hardness of the material cannot be controlled after hot working cooling).

- Hot working does not produce strain hardening.

- Hence, yield strength will decrease with in temperature and the ductility will improve.

- Example: Hot rolled steel, surface finish and tolerances are inferior to cold working process because of surface reaction oxidation scale etc),

- Deformation process (forces) are low.

4) Give example for ductility?

- Ductility is the measure of plastic deformation that has been sustained future.
- A material that suffers very little plastic deformation is brittle.
- Ductility may be expressed as either percent reduction in area.
- Examples are gold, silver, copper, and Nonmetals.

5) How can you find hardness of the material?

- The hardness of material can be found using Rockwell / Brinell } Hardness test.
- Indentation hardness using for steel as opposed to scratch or rebound hardness.
- It is indicative of ultimate tensile strength
- Atoms move out of the way to create the indentation.

what is deformation?

- Deformation is change in shape due to applied force.
- This can be a result of tensile (pulling), forces, compressive (punching), shear bending or twisting.
- Elastic deformation – This type of deformation is reversible, once the forces are no longer applied, the object returns to its original shape.
- plastic deformation – This type of deformation is not reversible. However an object in the plastic deformation range will first have undergone elastic deformation, which is reversible, so the object will return part way to its original shape.

'Part-B'

1) What are the factors affecting mechanical properties of materials :-

- The mechanical properties of materials are,
  - Tensile strength.
  - compressive strength.
  - shear strength
  - Toughness : Impact resistance
  - Elasticity
  - plasticity
  - Ductility
  - Malleability and
  - Hardness.

The factor which affect the above mechanical properties are,

- Grain size
- Heat treatment
- Atmospheric exposure
- Low and high temperature.

Effect of Grain size :

- The metals are composed of crystals (or) grains.
- If the grain size of a metal is small, it is called a fine grained metal.
- On the otherhand, when the grain size is comparatively large, then it is called a coarse grained metal.
- A fine grained metal has a greater tensile and fatigue strength. It can be easily work hardened.
- A coarse grain causes surface roughness.
- coarse grain metal is difficult to polish.
- coarse grained metal is less tough and has a greater tendency to cause distortion than the fine grained metal.
- coarse grained metal has a better workability, hardenability and forgeability.
- At room temperature the grain boundary is more or fine grained metals. Therefore, it has a higher strength and hardness than the coarse grained metal.
- At high temperature coarse grained materials have better creep resistance than the coarse grained metal (ones).

Effect of Heat treatment :-

- Heat treatment is generally done for the following purposes.
- To refine the grain and improve machinability.
- To relieve the internal stresses induced in the metals during cold and hot working of the metals.
- To improve resistance to corrosion.
- To modify the structure, either coarse grained or fine grained.
- To improve chemical, magnetic, electrical and thermal properties.

Effect of Atmospheric Exposure :-

- Most of the metals get oxidized when exposed to the atmospheric. Due to oxidation, of metal surface, a film is formed. The presence of moisture, sulphur dioxide, hydrogen sulphide and other corrosive conditions decrease the electrical resistivity of metals.
- The atmospheric effect on the metal depends on the following.
- characteristics properties of the metal.

- value of the protective film on its surface.
- Presence of certain reducing agents.
- Local cells formed due to development of cracks and discontinuity on the protective film surface.

Effect of low temperature :-

- Decrease in temperature there is an increase in the tensile strength and yield strength of all metals.
- Alloys of nickle, copper and aluminium retain most of their ductility and toughness at low temperature.
- For mild steel, the elongation and reduction in cross - sectional area is satisfactory upto 130°C but after that it goes down to a large extent.
- Near absolute zero temperature many metals exhibit the phenomenon of superconductivity.
- Below -100°c non-ferrous metals show better properties than ferro metals.
- Low temperature causes low thermal vibrations and lattice parameters are stablized.

Effect of high temperature :-

- Yield stress and ultimate tensile strength decrease with rise in temperature.
- Stiffness and fracture stress of many metals also decrease with increasing temperature.
- At high temperature the toughness of steel is reduced.
- At high temperature creep takes place and the material fails even at a very small stress.
- Due to rise in temperature, there is a corresponding rise in thermal vibration of atoms causing changes in structural properties.

~~Write a report about ceramics:~~

2) Write about metal forming process :-

- Metal forming - Large set of manufacturing processes in which the material is deformed plastically to take the shape of the die geometry.
- The tools used for such deformation are called die, punch etc, depending on the type of process.
- Plastic deformation - stresses beyond yield strength of the workpiece material is required.

categories - Bulk metal forming, sheet metal forming.

Metal - forming

- Bulk deformation
  - Rolling processes
  - Forging processes
  - Extrusion processes
  - Wire and bar drawing
- Sheet deformation.
  - Bending operations
  - stretching.
  - Deep or cup drawing
  - shearing processes
  - Miscellaneous processes.

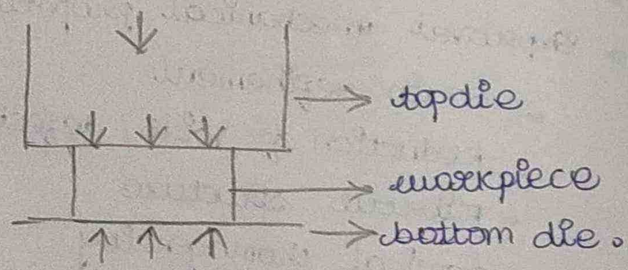
- Metal forming process are used for plastically deforming workpiece to desirable shape and obtaining optimum mechanical properties.
  - Desired shape
  - Improved mechanical properties.
    - Grain refinement
    - Reduction of voids / defects
    - Fibrous structure
    - chemical homogeneity
    - strain hardening.
- The metal forming process is also known as metal working process.

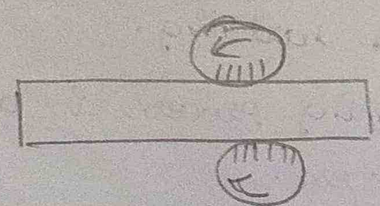
Classification of metal working process :-

- Based on type of forces applied.
- Direct compression - Type process ⇒ Forging and rolling.
- Indirect compression - Type process ⇒ wire and tube drawing, extrusion, Deep drawing.
- Tension type process ⇒ strech forming.
- Bending processes ⇒ Bending of sheets.
- Shearing process ⇒ In sheet metal forming applications.

Direction compression type process :-

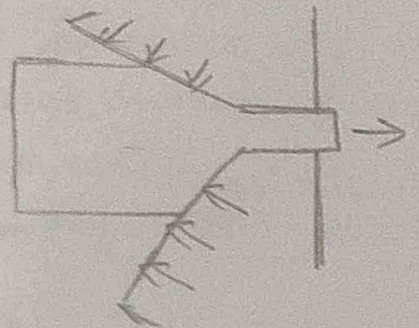
- Force is applied to surface of workpiece and metal flow takes place at right angles to direction of compression.

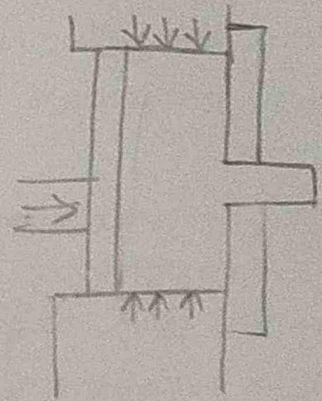


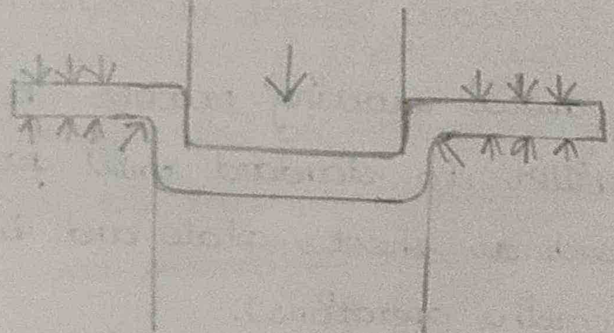


Indirect compression type process :-

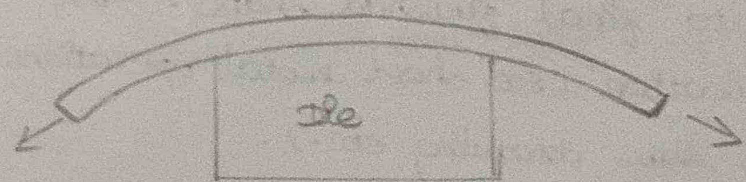
- Primary applied forces are frequently tensile but indirect compressive forces are developed because of the reaction of the workpiece with the die and reach very high values.

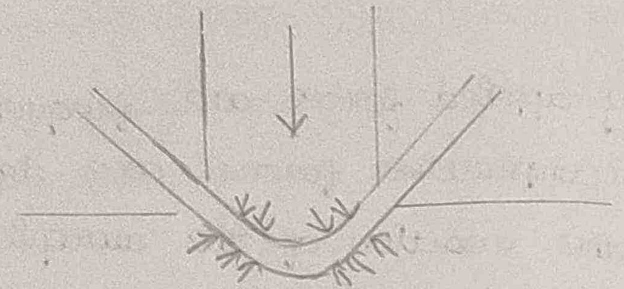


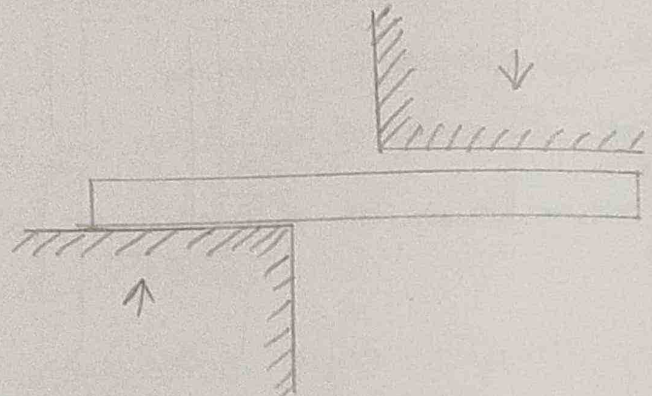




Tension type bending and shearing process.



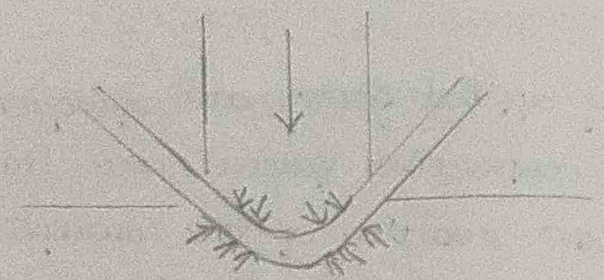


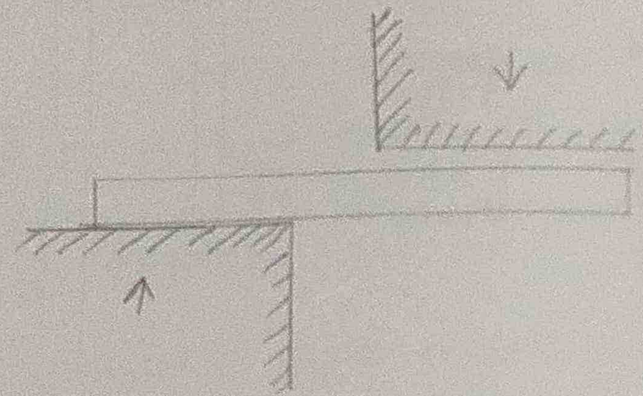


Primary and secondary metal working process :-

- Primary metal working process - Reduction of ingot or billet to standard mill product of simple shape such as sheet, plate and bar (also known as processing operations).

- Secondary metal working processes produ a part to final finished shape. Also known as fabrication (Ex. sheet metal operations, wire drawing, tube drawing etc.).





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Deformation process :-

Hot working process : Done at sufficiently high temperature such that continued deformation does not result in increased hardness.

- Example : Hot rolled steel, surface finish and tolerances are inferior to cold working process because of surface reactions (oxidation scale etc).
- Deformation forces are low.

Cold working process : strain hardening effects predominate over thermal recovery effects.

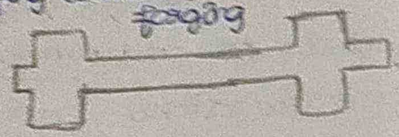
- With continued deformation the hardness and strength increase and the ductility decrease.
- It results in an elongated grain structure and can be used to harden metals and alloys that do not respond to heat treatment.
- Example : cold rolled sheet steel, Excellent surface finish and tolerances.
- Deformation forces are high.

Design sequence for a multiple stage forging process.

1) Blank

2) Fullering open die forging

3) Edging (double) open die forging



4) Blocking impression die forging

5) Finishing impression die forging

6) Forged product (after trimming flash)

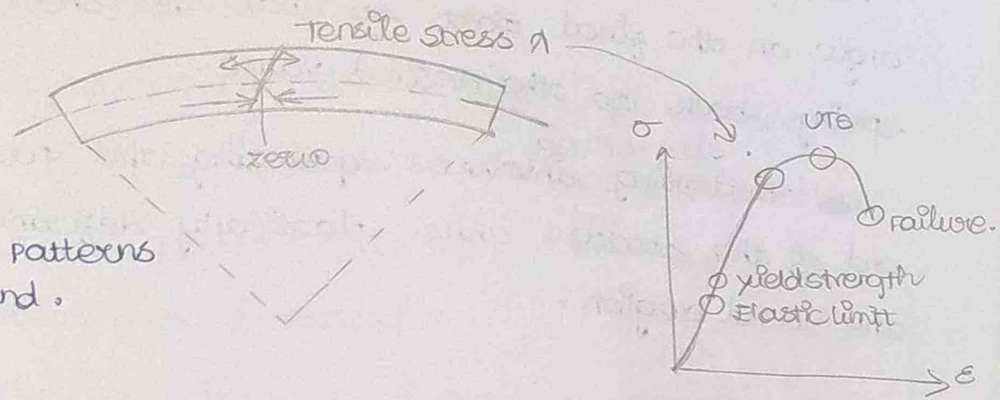
Types of forging process :-

- Hand forging
- Hammer forging
- Drop forging
- Press forging
- Machine forging or upset forging
- Roll forging.

Spring back :-

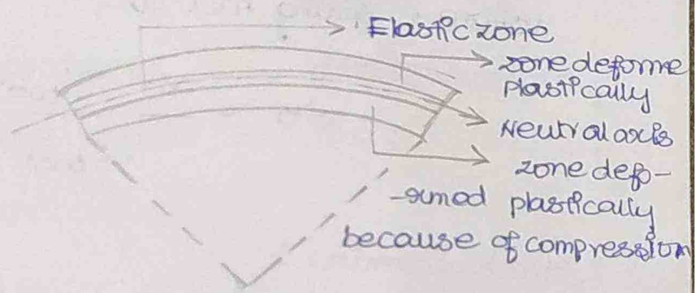
- Spring back occurs because of the variation in bending stresses across, the thickness. ie, from inner surface to neutral axis to outer surface.

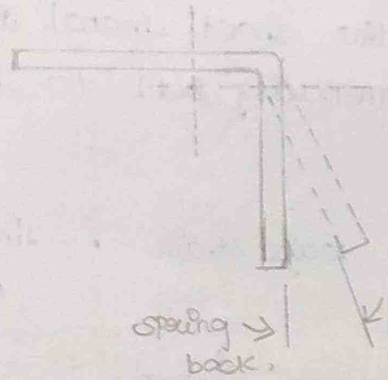
- The tensile stresses decrease and become zero at the neutral axis.



changing patterns in bend.

Elastic and plastic deformation during bending.





spring back can be minimized by overbending, bottoming and stretch forming.

- In overbending the punch angle and radius are made smaller than the specified angle on the final angle on the final part so that the sheet metal springs back to the desired value.

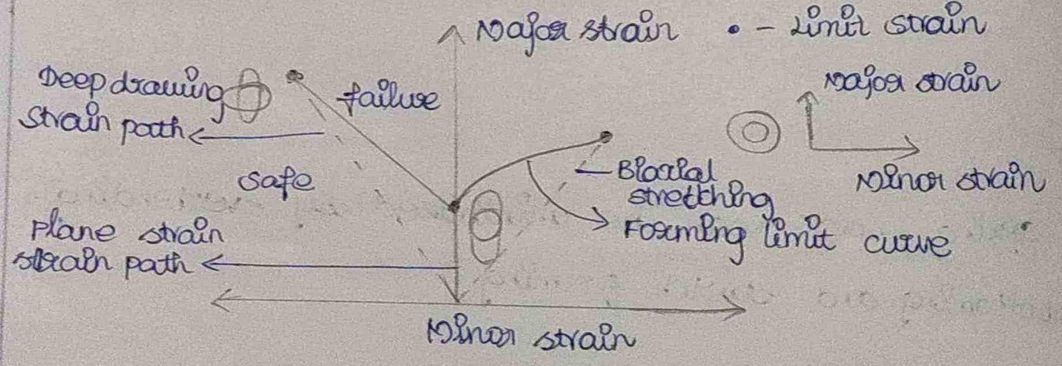
- Bottoming involves squeezing the part of the end of the stroke, thus plastically deforming it in the bend region.

where, spring back is

$$SB = \frac{\alpha - \alpha_{tool}}{\alpha_{tool}}.$$

Strech forming :

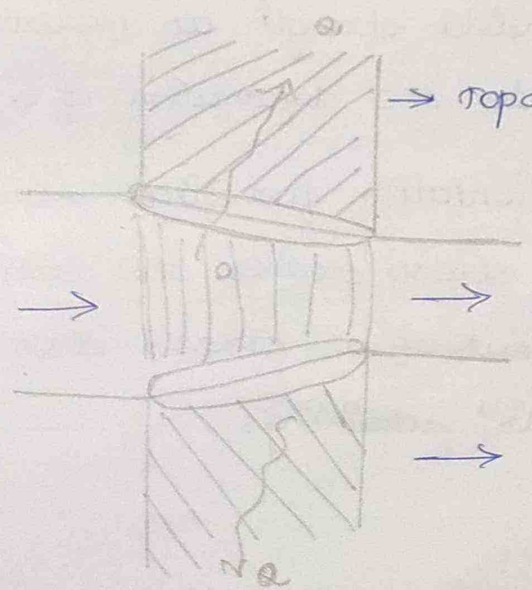
- streck forming is a sheet metal forming process in which the sheet metal is intentionally streched and simultaneously bent to have the shape change.



Write notes on deformation of metals :-

Deformation processing system :-

- Need to know distribution of stress strain practice particle velocities and overall pressure required to perform the operation. Following considerations are important.
- Yielding because of applied forces
- Mettalurgical phenomena like strain hardening, recrystallisation, fracture under strain.
- Friction and lubrication
- Heat transfer from workpiece to die.



Excessive elastic deformation.

- under condition of static equilibrium
- sudden deflection

yielding or excessive plastic deformation.

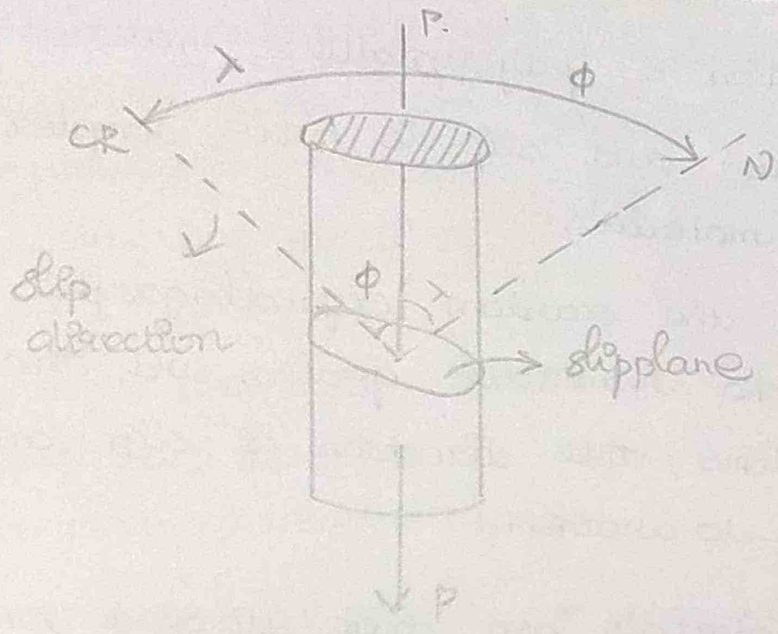
- change of shape, strain hardening and the effect of temperature.

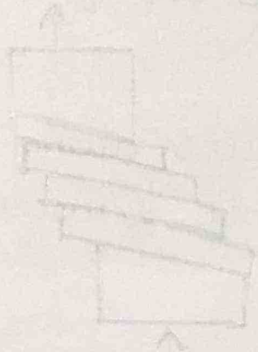
Fracture :-

- sudden brittle fracture, fatigue fracture or delayed fracture.

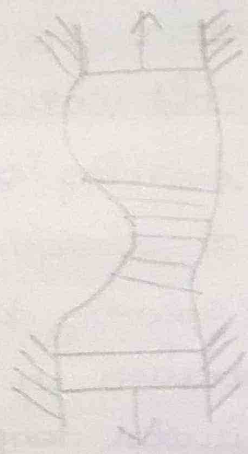
Single crystal deformation :-

- To make the connection between dislocation behaviour and yield strength as measured in tension, consider the deformation of a single crystal.
- Give an orientation for single slip. ie) the resolved shear stress reaches the critical value of one system a head of all others, then one obtains a 'pack of cards' straining.





→ Tensile deformation of single crystal without constrain



→ rotation of slip plane due to constrain.

Plastic deformation of polycrystalline materials

- Deformation and slip is more complex in polycrystalline materials.

- Due to the random crystallographic orientation of the numerous grains and the effe of neighbouring atoms, the direction of slip varies from one grain to another.

- These materials are made up of a number of small crystals or grains.

- For each crystal slip occurs along the slip system that has the most favourable orientation.

4) Difference between hot and cold working process:-

Hot working	Cold working.
• Hot working is the process of plastically deforming a metal above the metals recrystallization temperature.	• cold working is the process of strengthening a metal by plastic deformation at temperatures below the recrystallization temperature.

• Hot working is carried out above the recrystallization temperature and below the melting point.	• cold working is carried out below the recrystallization temperature.
• Hence the deformation of metal and recovery take place simultaneously.	• As such, there is no appreciable recovery.
• If hot metal working process is properly done, it does not affect tensile strength, hardness, corrosion strength, and fatigue resistance of the metal.	• cold working process improves ultimate tensile strength, yield and fatigue strength but reduces the corrosion resistance of the metal.
• Hot working is most refines metal grains resulting in the improved mechanical properties	• Most of the cold working processes decrease mechanical properties of metal like a elongation reduction of area and impact values.
• Hot working is most preffered where heavy deformation is required.	• cold working is preferred where work hardening is required.

• In hot working, no internal and residual stresses build up in the metal.	• In cold working, there is internal and residual stresses build up in the metal.
• Heavy oxidation requires less energy for plastic deformation therefore, pickling is required to remove oxide.	• Cold working does not require pickling because no oxidation of metal takes place
• Hot working requires less energy for plastic deformation because at higher temperature, metal becomes more ductile and soft.	• Cold working requires more energy for plastic deformation.
• Deformation of metal and its recovery happens in hot working.	• There is no appreciable metal recovery that happens in cold working.
• Due to higher deformation temperatures, the stress required for a deformation is much less.	• The stress required.

PART-C

VICKER'S HARDNESS TEST :-

- The vickers hardness test was developed in the early 1920's as an alternative method to measure the hardness of the materials.

Vickers tests has two versions :

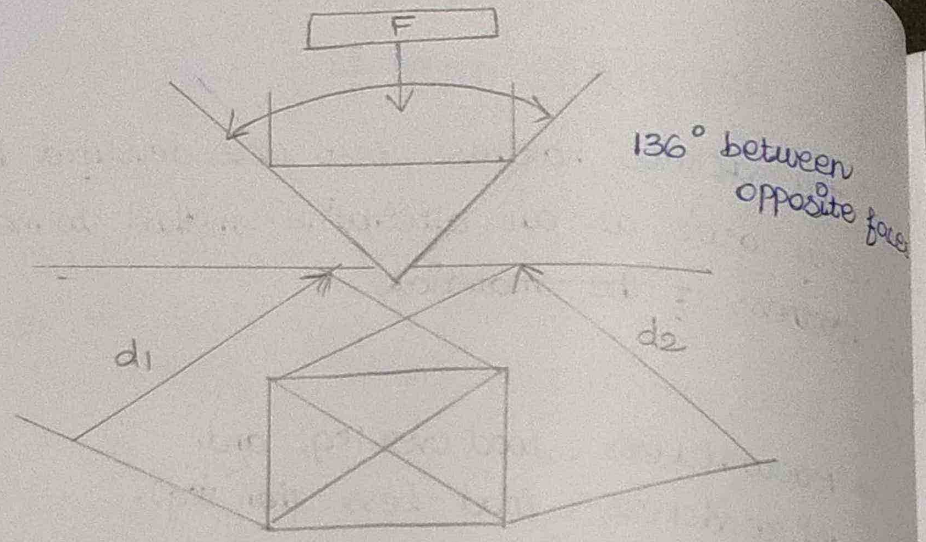
- Macro vickers (load over 1kg) and
- Micro vickers (load less than 1kg).

- The vickers macrotest is often easier to use than other hardness tests. Since the required calculations are independent of the size of the indenter, and the indenter can be used for all materials irrespective of hardness.

- However, vickers macrohardness test is not as widely used for all materials irrespective of hardness Brinell or Rockwell test.

- A diamond in the form of a right pyramid with a square base angle of 136° between on faces is forced into the in under a load.

- It is represented as,



The two diagonals d_1 and d_2 indentation left in the surface of the material after removing they are measured,

Vicker's hardness number :-

$$V.H.N = \frac{P}{A}$$

$$= \frac{2P(\sin\theta/2)}{d^2}$$

$$= 1.8544\frac{P}{d^2}$$

where,

P - applied load in kg

A - surface area of indentation in sq.mm

D - mean of diagonal impression mm

θ - angle between opposite faces of diamond pyramid (136°)

$$d = \frac{(d1+d2)}{2}$$

Diagonal Measurement in vicker's test :-

Diagonals of the indentation produced are approximately seven times larger than the depth of indentation, especially with high hardness metals it provides better accuracy than that could be obtained with the Brinell or Rockwell.

This is because of the fact by virtue of its indentation, higher measurement accuracy can be obtained even if the indentation depth is small, so this makes the vickers test especially suitable for hardness measurements in thin layers and very hard alloys.

Vickers hardness number is nearly independent of the test loads for homogenous materials due to the fact that the ratio between the diagonals of the impression remains constant under different test loads above 5kg.

At lower loads it may be load dependent.

The diagonal of the square indentation is measured to an accuracy of 0.001 mm.

Advantages:-

The Indentation always have the same shape whatever be the load. This makes the measurement independent of load.

Soft as well as hard metals may be tested.

Test may be conducted in low-load and m[illegible] range as well.

The vickers hardness apart from the micro and low range is independent of the testload applied (abo[illegible] 5kg).

The pyramidal Impression damages the work pieces only slightly.

This test is very useful for testing hardness of polished or nitrides surface due to small Impress[illegible] made on the test.

This test is accurate suitable for metals as thin as 0.15nm.

Hardness is decreased exponentially with absolute temperature of the material $H = Ae^{-BT}$. where A and B are constants.

Disadvantages:-

It takes more time for each measurement

when Irregularites are present then the measu-rement taken by vickers shows more deviation than those of Brinells test.

Write the technological properties of engineering materials :-

- Technological properties are those qualities which give information regarding the suitability of metals for various technological operations or processes such properties are highly desirable in shaping, forming and fabrication of materials.

The following technological properties will be discussed

- Machinability
- weldeability
- castability
- Formability
- Malleability.

Machinability :-

- It is defined as the with a given material can be cut permitting the removal of material with a satisfactory finish at lower cost. It is used to signify how well a material takes a good finish.

- It may also called finish ability.

- It have high cutting speed.
- It have low power consumption
- It have a good surface finish

Machinability Index:-

- The machinability of different metals to be machined may be compared by using the machinability index of each material which may be defined as follows.

$$\% = \frac{\text{cutting speed of metal investigated for 20min}}{\text{cutting speed of std. steel for 20min tool life.}}$$

A standard or steel has a carbon content of 0.13% max, manganese of 0.06 to 0.10% and sulphur of 0.80 to 0.03% and can be machined relatively easily its machinability index is arbitarily fixed as 100%.

Weldability:-

- It is defined as the capacity of a metal to be welded under the fabrication conditions imposed in a specific suitably designed structure,

- The weldability is affected by the following factors,
  - composition of metal
  - thermal properties
  - filler materials
  - flux material
  - welding technique

The following materials have good weldability in the ascending order.

- stainless steel
- low alloy steel
- cast iron
- carbon steel
- Iron.

castability.

- The ease with which a metal can be cast into form is known as castability of the metal.
- It is based on factors like solidification rate, gas porosity, segregation, shrinkage etc,

- The following factors are favourable to castability of metal.
    - fluidity of metal
    - Low rate of shrinkage (It is the reduction in the volume of a metal when it goes from a matter to a solid state).
    - Low or negligible segregation
    - Low gas porosity.

Formability:-

- It is the ability of metals of forming into different shapes.
- the various factors which given to a large content. The flow ability or ductility of the material are.
    - metal structure
    - grain size
    - Hot and cold working
    - Alloying elements
    - softening heat treatments (Annealing and normaling).

A small grain size is recomended for shallow drawing of metals whereas for heavy drawing relatively large grains are recommender

In softening heat treatments the annealing and normalising the ductility of metal is resolved,

The wraped and distorted crystal are reformed and consequently the force requested slippax is reduced.

Malleability:-

- It is the ease with which the material undergoes too much charge in shape under compressive stresses without repture.

The materials like soft steel, wrought iron, copper and aluminium have good malleability,

They can be hammered or rolled into the desired shape without rupture.