MATERIAL SCIENCE

Crystal System & Bravais Lattice

Crystal System	Geometry		Bravais Lattices
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$	SC, BCC, FCC
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	ST, BCT
Orthogonal	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	SO, BCO, FCO, ECO
Rhombohedral	$a = b = c$	$\alpha = \beta = \gamma \neq 90^\circ$	SR
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90^\circ, \gamma = 120^\circ$	SH
Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90^\circ \neq \beta$	SM ECM
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$	STr

- X-Ray difraction is the technique used for determination of crystal structure.

Crystal structure characteristics

Characteristic ↓	BCC	FCC	HCP
a to r relation	$\sqrt{3}a = 4r$	$\sqrt{2}a = 4r$	$a = 2r$
Avg no. of Atoms (N_{av})	2	4	6
co-ordination no.	8	12	12
Atomic Packing fraction	0.68	0.74	0.74
Examples	iron (except 910-1400°C) Tungeston (W) Chromium (Cr) Vanadium (V) Malbydinum (Mo) Tantalum (Ta)	iron (910-1400°C) Aluminium (Al) copper (Cu) Nickel (Ni) Gold (Au) Silver (Ag) Platinum (Pt) lead (Pb)	magnesium (Mg) Zinc (Zn) Zirconium (Zr) Titanium (Ti) Cobalte (Co) Cadmium (Cd) Berilium (Be)

Properties:	• Hard & Brittle • Grain refiners, control grain growth. • Added to cutting tools.	• Strong & Ductile	• Easy shear, So used as solid lubricants
Stacking Sequence	ABABA ---- ∞	ABCABCA.....∞	ABABA ---∞

- Atomic packing factor (APF)

$$APF = \frac{N_{av.} \times \frac{4}{3}\pi r^3}{\text{Vol. of unit cell } (a^3)}$$

- Allotropy:- It is the tendency of an element to exist in different crystalline structure at diff. temp^r and pressure.

- millar indices of plane (hkl)

- rationalised reciprocals of intercept are known as millar indices of plane.
- when a plane is parallel to a axis, its millar indices is zero along it.
- two parallel planes will have quantitatively same miller indices, Ecept for Algebric sign of non zero index.
- Angle b/w two planes $(h_1 k_1 l_1)$ & $(h_2 k_2 l_2)$

$$\cos\theta = \frac{h_1h_2 + k_1k_2 + l_1l_2}{\sqrt{l_1^2 + k_1^2 + h_1^2} \cdot \sqrt{h_2^2 + k_2^2 + l_2^2}}$$

$$h_1h_2 + k_1k_2 + l_1l_2 = 0 \quad \text{for } \theta = 90^\circ$$

- Planes having low indices are far away from origin

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$; d = interplannar distance

a = edge length of unit cell

Miller indices of dir^n [u v w]

- rationalised components of a given direction vector.
- when a direction is ⊥ar to an axis, its miller index on that axis is zero.
- two parallel dir^n will have quantitatively same indices
- angle b/w two dir^n $[u_1 v_1 w_1]$ & $[u_2 v_2 w_2]$

$$\cos\theta = \frac{u_1u_2 + v_1v_2 + w_1w_2}{\sqrt{u_1^2+v_1^2+w_1^2}\cdot\sqrt{u_2^2+v_2^2+w_2^2}}$$

$$u_1u_2 + v_1v_2 + w_1w_2 = 0 \quad \text{for } \theta = 90°$$

- a dir^n vector & plane having same indices will be ⊥ar to each other.

Density of crystal structure

volume density (ρ_v)

Plannar density (ρ_p)

linear density (ρ_l)

$$\underset{gm/cm^3}{\rho_v} = \frac{\overset{atoms}{\boxed{N_{av}}}\cdot\boxed{A} \rightarrow gm/mole}{\underset{atoms/mole}{\boxed{6.023\times10^{23}}}\times\boxed{a^3} \rightarrow cm^3}$$

$$\rho_p = \frac{\text{no. of atoms}}{\text{Ar. of plane}}$$

$$\rho_l = \frac{\text{no. of atoms}}{\text{length of dir}^n}$$

- no. of atoms in planar density is the effective no. of circles enclosed in given plane.
- no. of atoms in linear density is the no. of atoms whose centers are intersected.
- <u>no. of slip system</u> = no. of closed packed plane × no. of closed packed dir^n

⇒ FCC more ductile than HCP bcz FCC have more no. of slip system

⇒ BCC is brittle compared to FCC (although BCC have more no. of slip system) bcz of ramdomness in closed packed planes.

Ductility to Brittle transition conditions

- Low tempr
- High strain rate
- presence of surface notches

→ main reasons

- residual stress due to cold working
- Sudden quenching
- Presence of interstitial carbide or nitride
- Low Atomic packing factor or high void space.

→ Secondary reasons

CHAPTER-2 STRUCTURAL IMPERFECTIONS

- **Point defects** (0-D)
  - Vaccancy
  - Self interstitial
  - Impurity
    - Interstitial
    - Substitutional
  - frankel defect [vaccancy & self interstialcy side by side]
  - Shotkey defect [Pair of vaccancies due to cation & anion]
- **Line defects** (1-D)
  - edge dislocation [$\vec{B}$ ⊥ar to dislocation line]
  - Screw dislocation [$\vec{b}$ ∥ to dislocation line]
- **Vol. Defects** (3-D)
  - Casting defects
  - forming defects
  - welding defects
- **Surface defects** (2-D)
  - grain Boundaries
  - Low angle boundaries
  - Twin boundaries
  - stacking defect

- Let n_v = no. of vacancies in metal

n_t = total no. of lattice sites

$\frac{n_v}{n_t}$ = vaccancy concentration or fraction of vaccancy.

$$\frac{n_v}{n_t} = e^{\left(-E/KT\right)}$$

here, K = Baltzman const.

T = absolute tempr (K)

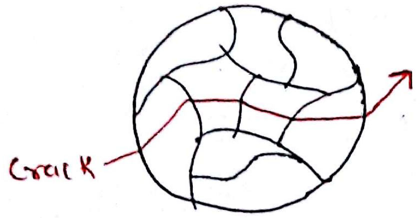
E = enthalpy of formation of vaccancy.

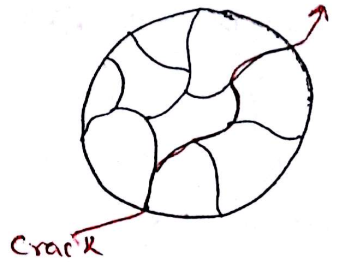
- Grain Boundary characteristics

- region of orientation mismatch
- region of high energy.
- Low melting point region
- Region of heavy impurity concentration.

- grains ⟺ Dendrite ⟺ crystal

Equi- cohesive tempr (Te) = it is tempr at which grain strength is equal to GB strength.





	Low tempr $(T < T_e)$		High tempr $T > T_e$
Grain	weaker	Grain	Stronger
GB	Stronger	GB	weaker

CHAPTER-3. STRENGTHENING MECHANISMS

A) Grain size refinement [Hall Petch effect]

$$\sigma_y = \sigma_i + K d^{-1/2}$$

σ_y = yield strength of polycrystalline material

σ_i = yield strength of material at infinite grain size

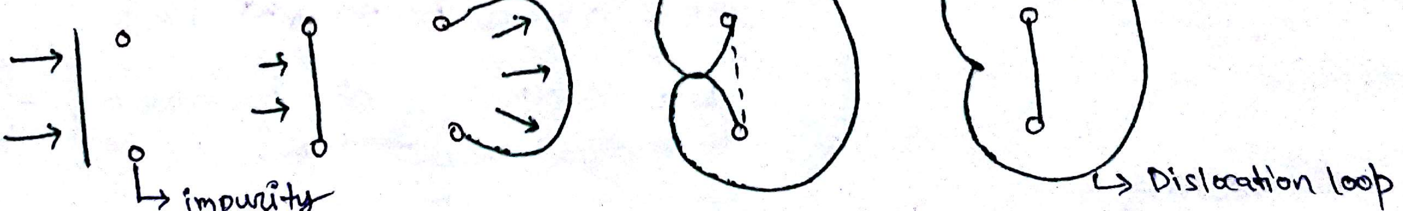
K = Hall Petch const.

d = avg grain dia.

methods :- 1. Heat treatment
2. Adding Alloying element
3. Hot working.

B) Cold working [Frank - Reed source mechanism]

$$\tau = \tau_0 + A\sqrt{\rho}$$



c) Solid Solution strengthening
- Interstitial solid solu^{n}
- Substitutional solid solu^{n}

- reason for strengthening is lattice distortion due to impurity particle.

Solid solu^{n}	Compounds
- made on wt % bases	- made on molar vol. basis
- Do not have formula	- have fixed formula
- They have freezing range	- They . Solidifies at a particular temp^{n}.
- named as "minor in major".	- names as "major & minor".
ex :- α - Ferrite solid solu^{n} of carbon in iron.	ex ! Fe_3C interstitial compound of iron and carbon

Hume-Rothery's rule : [for extensive solid solubility]
- Crystal structure of two elements should be same.
- Diff. in atomic radii < 15%.
- There should be less chemical affinity.
- Solvent should have lower valency.

- Alloy is a substance having metallic character & composed of two or more elements out of which atleast one is a metal.
- Composites are composed of two or more elements, all of them can be non- metal. no mutual desolution, no atomic bonding, can be transparent or translucent.
- Phase is defined as microstructurally distinct, chemically Homogenous and mechanically seperable part of system.

- **Gibb's Phase rule :**

$$P + F = C + N$$

N = variable available in alloy manufacturing process. normaly it is taken 1:

F = 0 → invariant reaction

F = 1 → univariant reaction

F = 2 → bivariant reaction

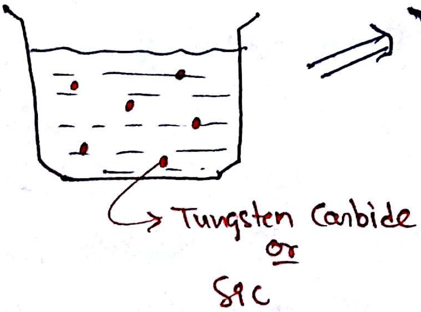
Classification of Binary alloys

- Homogenous (single phase)
  - Solid solu^n
  - Compounds
- Mixtures (multi phase Alloys)
  - 2 or more solid solu^n
  - 2 or more compound
  - Solid solu^n + compound

CHAPTER - 4 COMPOSITES

- Always two phase materials
  - matrix (continous)
  - Reinforcement (Discontinous)

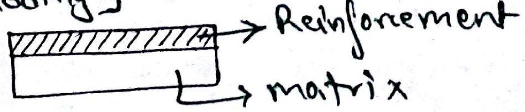
A) **Particulate composites**



⟹ Dispersion strengthening

Hard Particles are dispersed in soft molten metal like Al or Cu.

B) **Laminated composites**
[cladding]

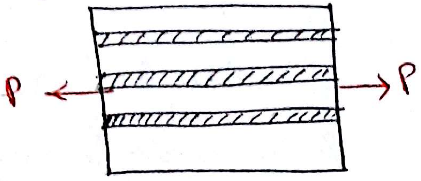


- improve corrosion & wear strengt
- improve creep & fatigue strength
- improve magnetic & elec. Property.
- uniform heat Distribution

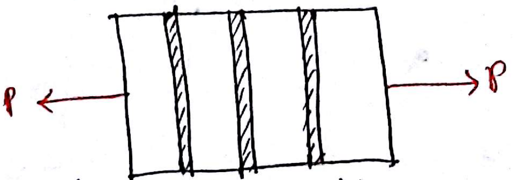
ex:- Al-clad, Cu-clad-Al, Cu-clad-steel

c) Fibre reinforced composite

Longitudinal loading
(isostrain condition)



Transverse loading
(iso-stress condition)



$$\frac{1}{E_c} = \frac{V_F}{E_F} + \frac{V_m}{E_m}$$

$$E_c = E_m V_m + E_f V_f$$

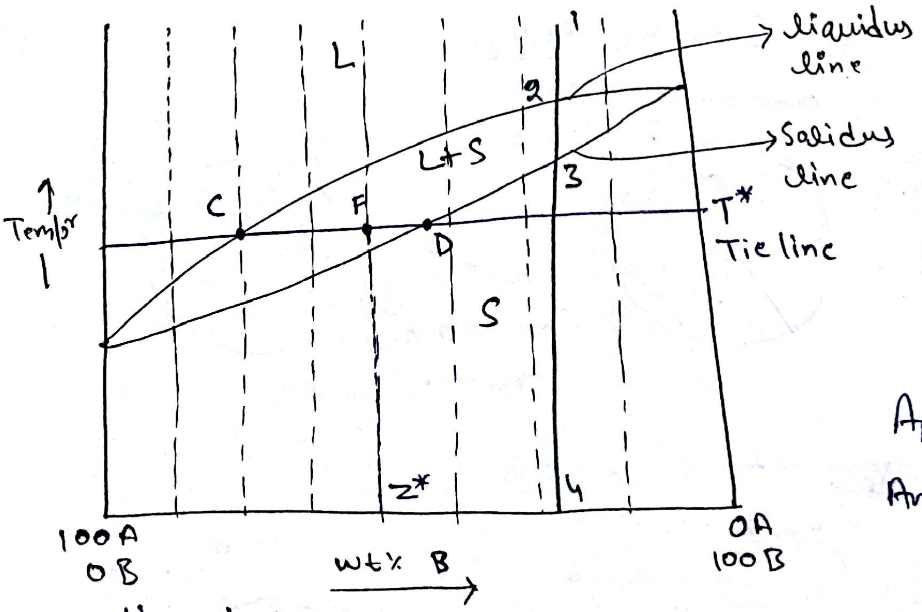
E_c = Young's modulus of composite
E_m = Young's modulus of matrix
E_F = Young's modulus of fibre
V_F = Vol. fraction of fibre
V_m = Vol. fraction of matrix

$[\therefore E_F >> E_m]$

CHAPTER – 5 PHASE DIAGRAMS

- A) Isomorphous System
- B) Eutectic system
- C) Partial Eutectic system
- D) Layer system

A) Isomorphous system

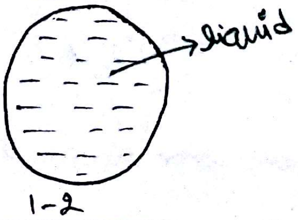


- two elements have complete solubility in solid as well as liquid
- ex - Cu-Ni, Au-Ag, Au-Cu, Mo-W
- Lever rule

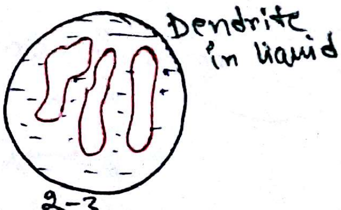
Amount of Liquid = $\frac{FD}{CD} \times 100$

Amount of Solid = $\frac{CF}{CD} \times 100$

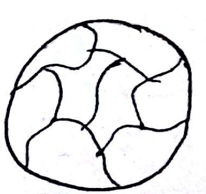
cooling behaviour of the mixture



1-2



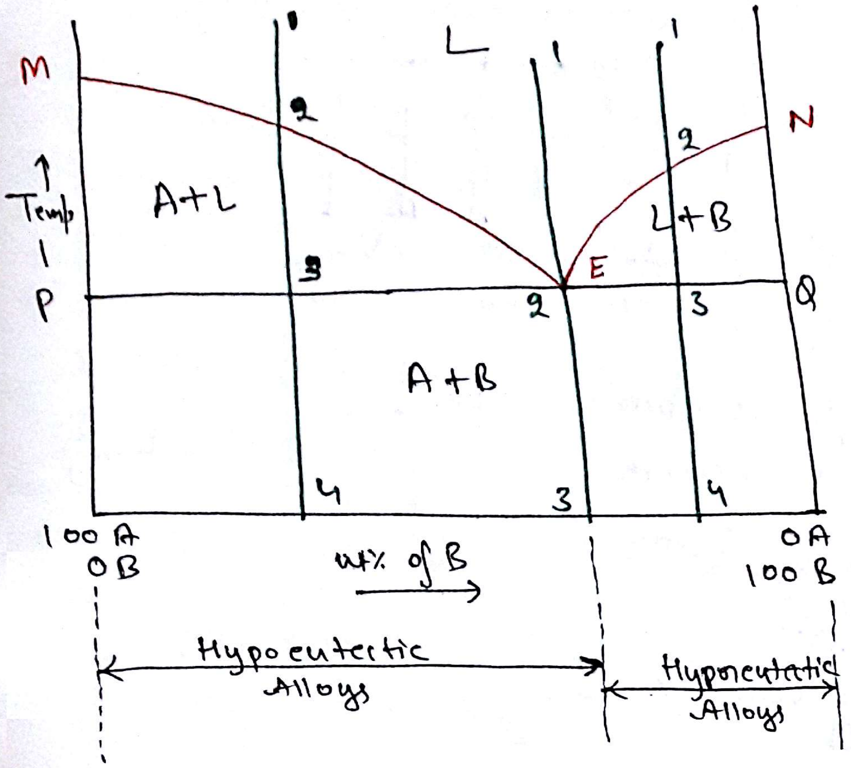
2-3



3-4

grains or Dendrite and grain boundaries

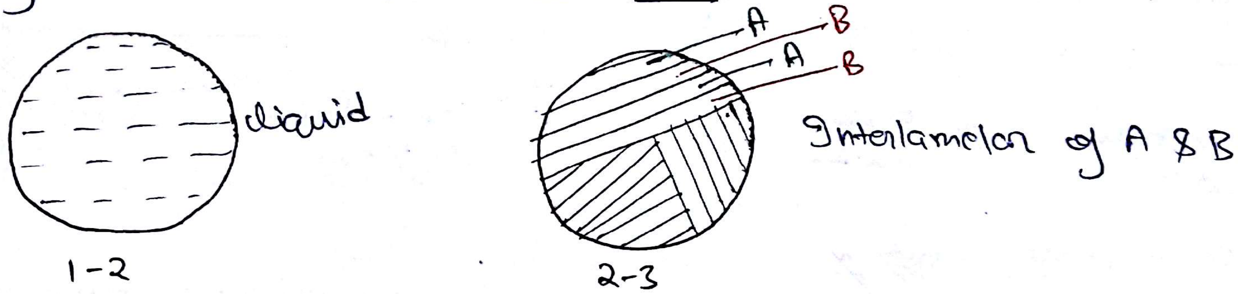
B) Eutectic System



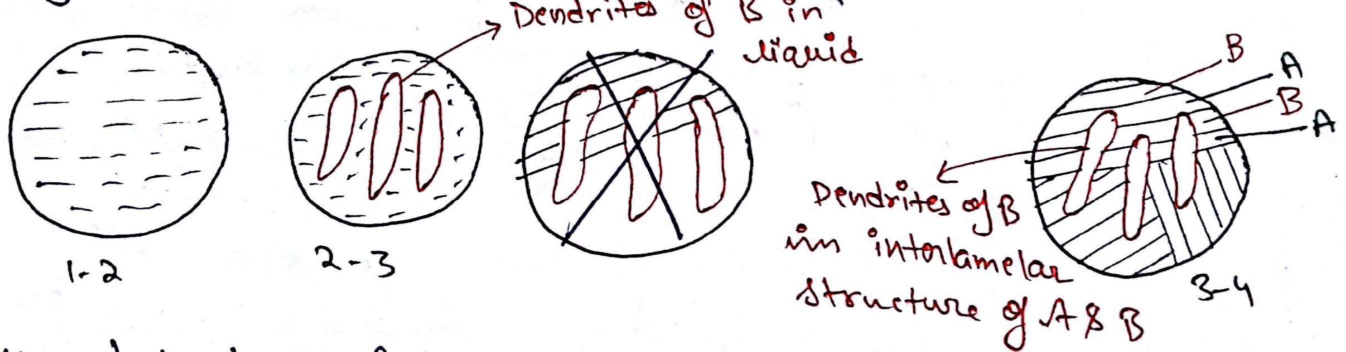
- two elements added will have complete solubility in liquid & insoluble in solids state.
- ex - Pb-As, Bi-cd, Au-Si

M = melting Point of A
N = melting Point of B
E = Eutectic point.
MEN = liquidus
MPEQN = Solidus

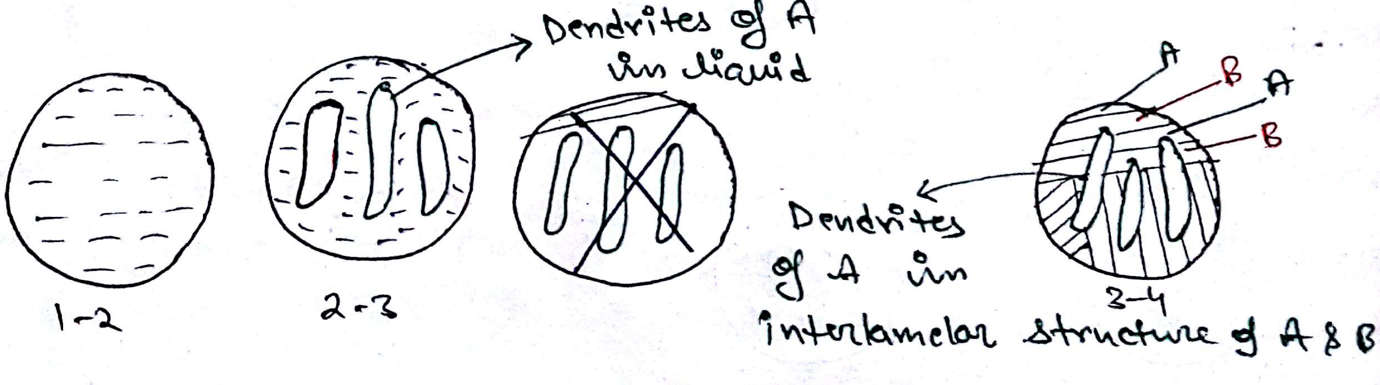
Cooling behaviour of Eutectic Alloys:



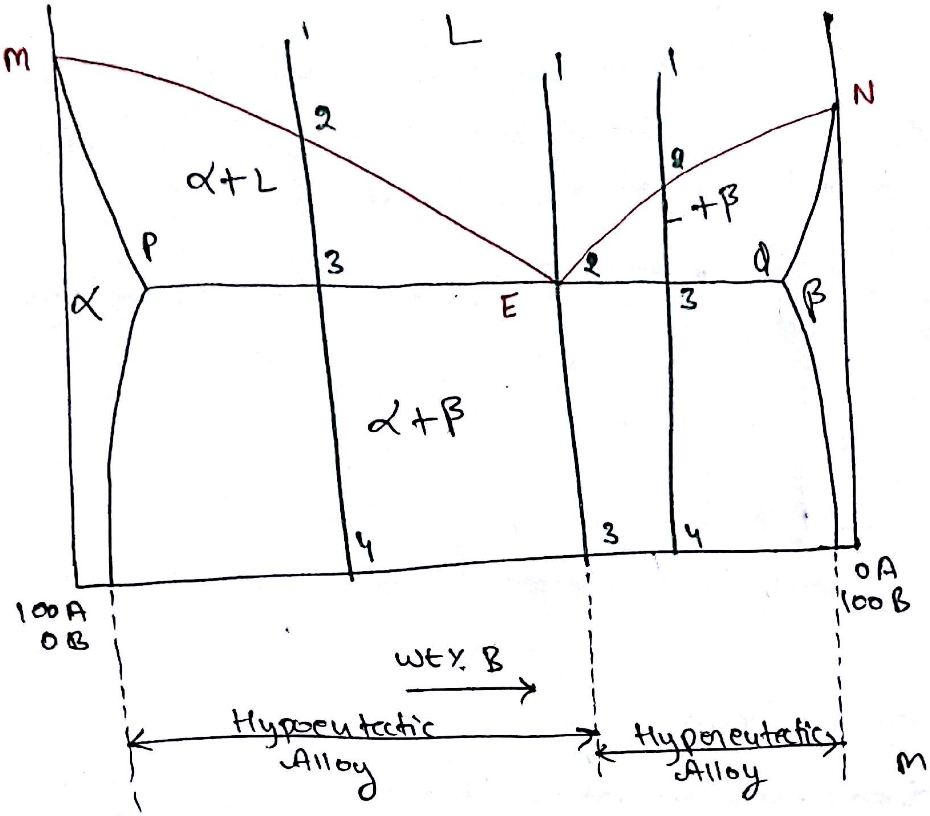
Cooling behaviour of hyper-Eutectic Alloys



Cooling behaviour of hypo-eutectic Alloys



c) Partial Eutectic System



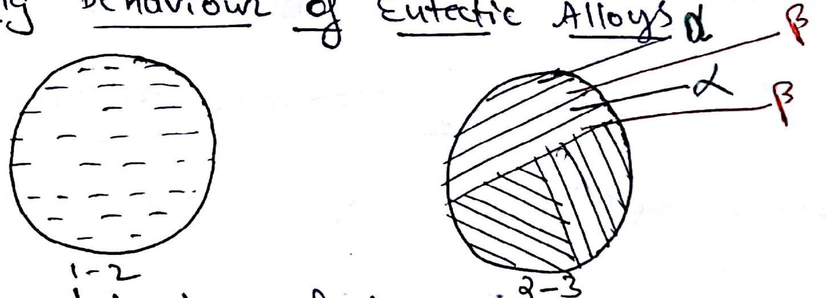
- two elements added will have complete solubility in liquid & partial solubility in solid state.
- ex - Ag-Cu , Pb-Sn , Sn-Bi , Pb-Sb

Sn → Tin
Sb → Antimony

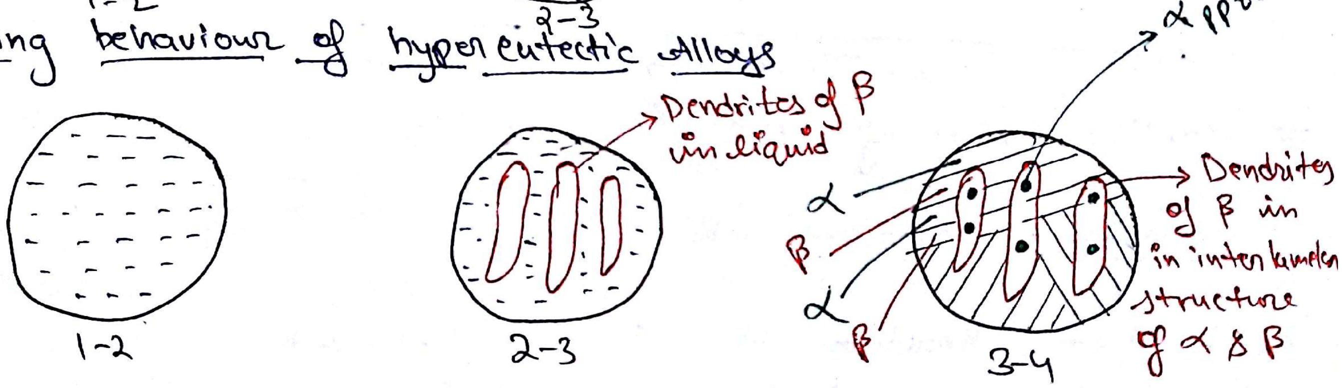
M = melting point of A
N = melting point of B
E = Eutectic Point
M PEQ N = Solidus
MEN = liquidus

α = Solid solnⁿ of B in A
β = Solid solnⁿ of A in B

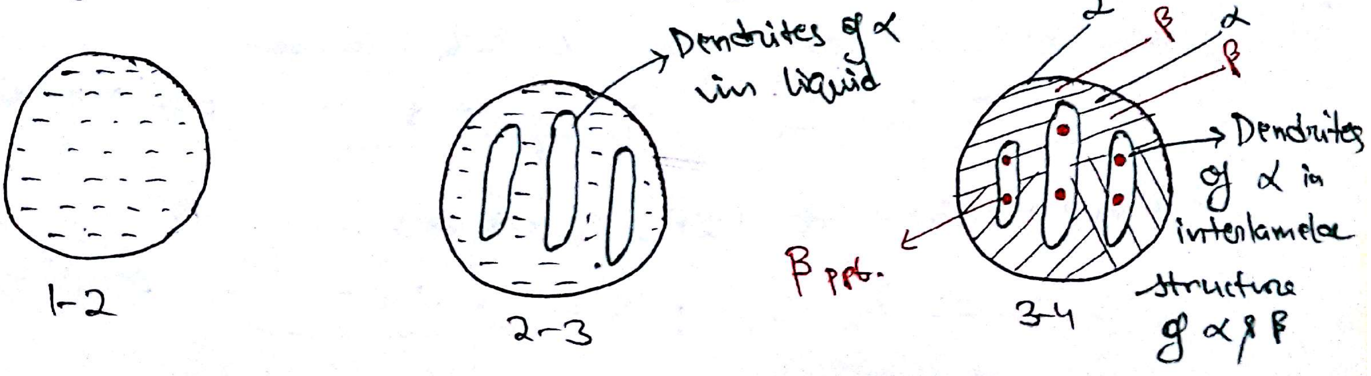
Cooling behaviour of Eutectic Alloys



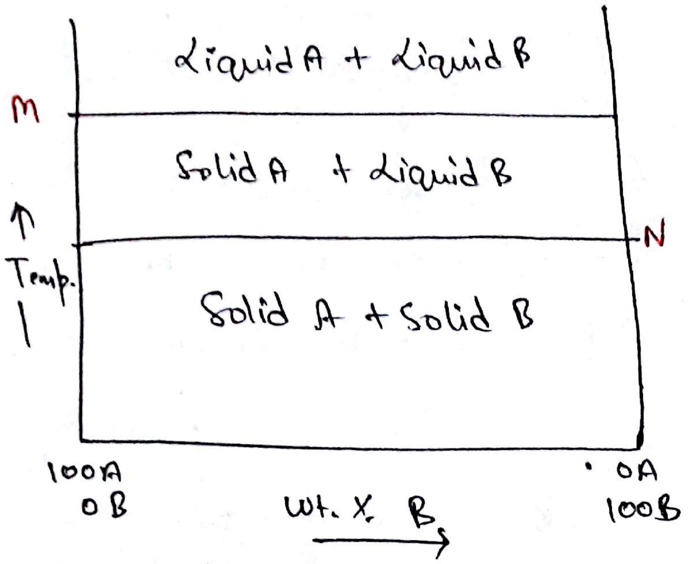
Cooling behaviour of hypereutectic Alloys



Cooling behaviour of hypoeutectic Alloys

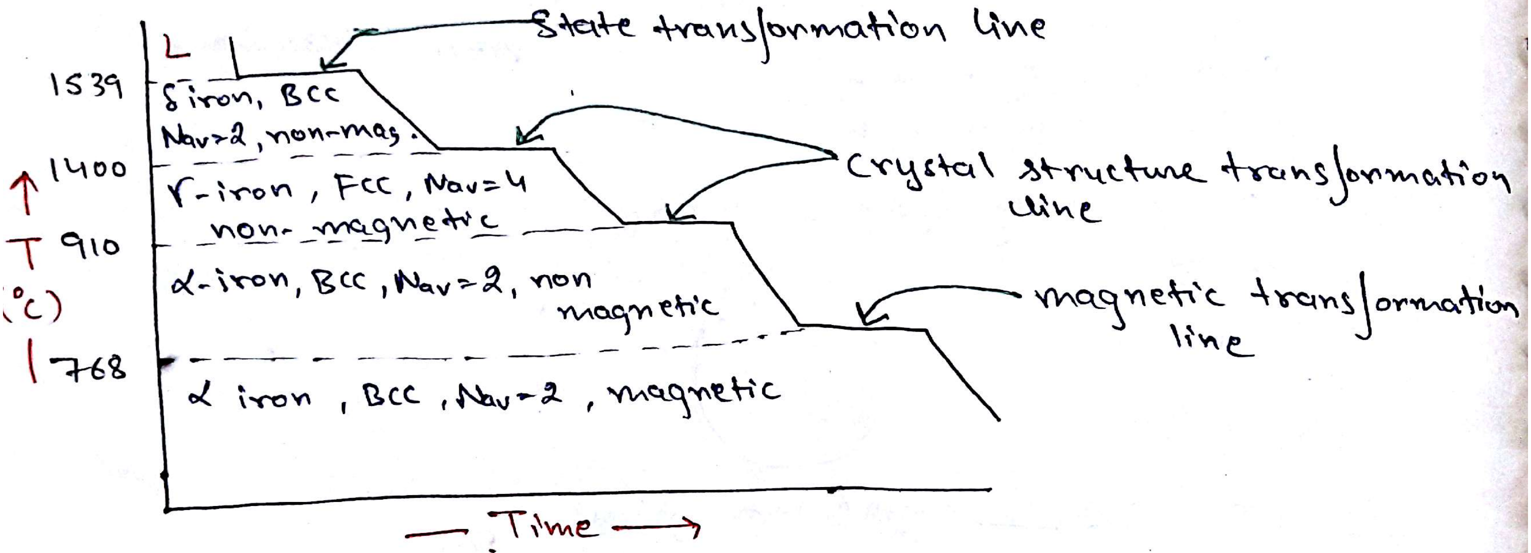


D) Layer System



- two elements added are completely insoluble in liquid as well as solid state.
- eg:- Cu-Mo, Cu-W, Ag-W, Ag-Fe

Cooling Curve of Pure iron



Cooling Curve of Iron-Iron Carbide

Invariant Reactions (F=0)

1. Peritectic Reaction at 1492°c & 0.18 wt% C

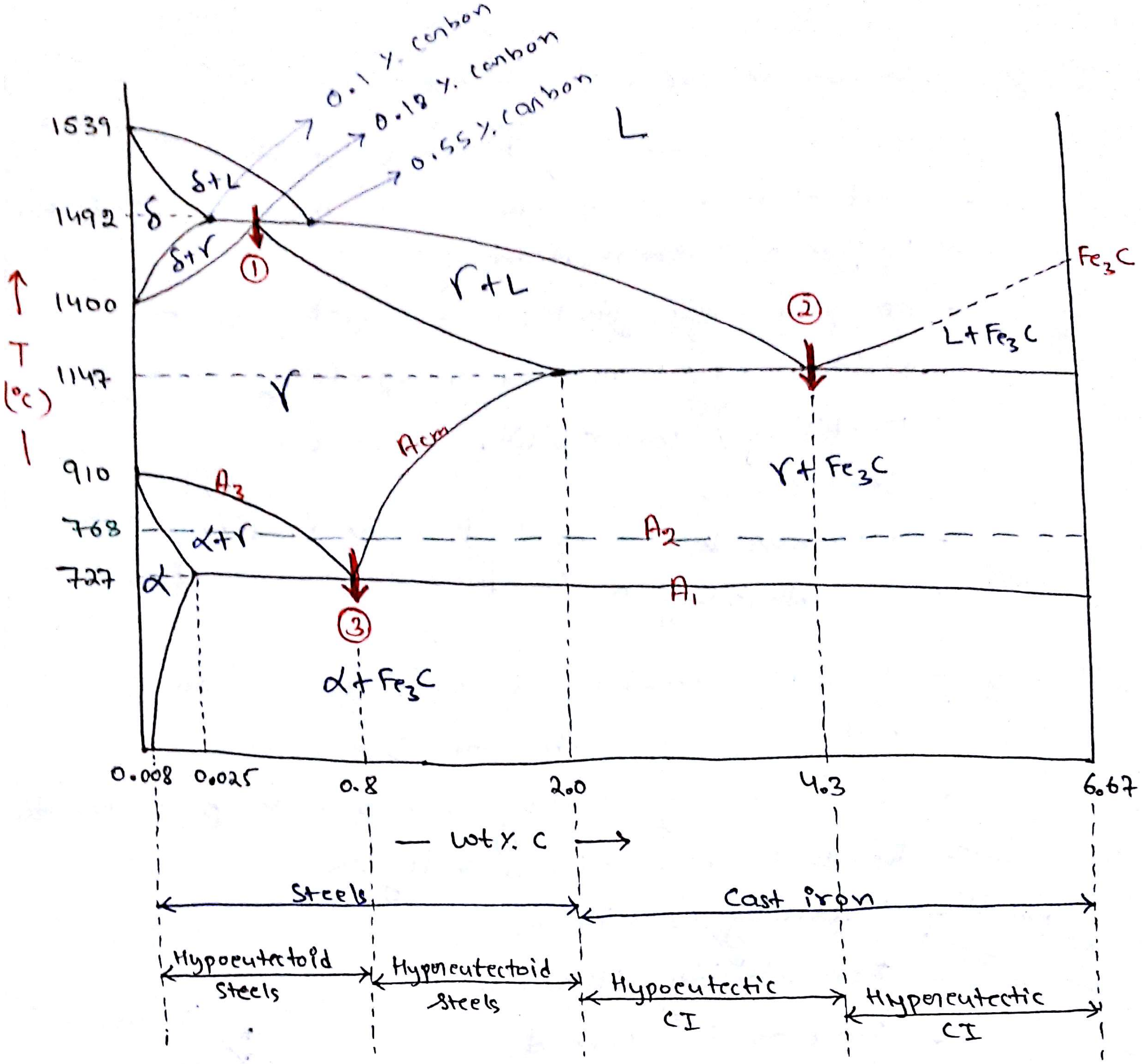
$$S_1 + L \rightleftharpoons S_2 \quad ; \quad \delta + L \rightleftharpoons \gamma$$

2. Eutectic Reaction at 1147°c & 4.3 % Carbon

$$L \rightleftharpoons S_2 + S_3 \quad ; \quad L \rightleftharpoons \boxed{\gamma + Fe_3C} \Rightarrow \text{ledeburite}$$

3. Eutectoid Reaction at 727°c & 0.8 wt% C

$$S_2 \rightleftharpoons S_3 + S_4 \quad ; \quad \gamma \rightleftharpoons \boxed{\alpha + Fe_3C} \Rightarrow \text{Pearlite}$$



CHAPTER-6 HEAT TREATMENT

Classic Heat treatment

- Annealing
- Normalising

→ medium C- Steel

- Hardening → High C - Steel
- Case (surface) Hardening
  - carburizing
  - Nitriding
  - Cyaniding

  → Low carbon steel

  - Induction hardening
  - flame hardening

  → High C Steel

1. <u>Annealing</u>
- cooling in furnace [takes 8-9 hrs]
- Heated to completely γ range (+ 50-100°c)
- Held at that temp. for 30-60 min for complete uniform austenisation.
- Recovery - Recrystallisation - Grain growth
- Residual stress relieved completely
- Ductility & formability increases
- Strength ↓
- Hardness ↓
- machinability ↑

$\boxed{\gamma \longrightarrow \text{Coarse Pearlite}}$

2. <u>Normalising</u>
- Heated to complete γ range + (50-100°c)
- Held at that temp. for 30-60 min
- followed by cooling to room temp. in open Air [2-3 hrs]
- Residual stress relieved partly
- Ductility will be less
- Formability will be less
- Fine grain formed
- Strength & Hardness is more
- machinability less

Compared to annealing

$\boxed{\gamma \rightarrow \text{Fine Pearlite}}$

3. <u>Hardening</u> - High carbon steel is heated to about 1000°c followed by sudden Quenching in water.

<u>Consequences</u>

Structural changes

$\gamma \longrightarrow$ Martensite

FCC $\longrightarrow$ BCT

⇓

Hardness = R_c 65

Hardest known phase in iron- iron carbide

Problems
- Corrosion
- Quench crack formation
- Distorsion of shape
- Retained Austenite (γ_{RA})
- Residual formation.

methods to eleminate retained Austenite (γ_{RA})

- Sub zero cooling $\gamma_{RA} \longrightarrow M$
- Permanent deformation $\gamma_{RA} \longrightarrow M$
- High tempr tempering $\gamma_{RA} \longrightarrow$ Bainite [stable at room temp]

$$\Downarrow$$

BCC = R_c55 ($\alpha + Fe_3C$)

- Carburising : Carburising (72 hrs) + Quenching ⇒ 800 VHN
- Nitriding : nitriding ⇒ 1000 VHN (no quenching)
- Cyaniding : cyaniding (15-20 mins) + Quenching ⇒ 900 VHN

Effects of Alloying elements

Ni ⇒ Increase Toughness, Do not effect Ductility
Cr ⇒ Increase corrosion resistance
Silicon ⇒ Increase hardenability, it is strong deoxidiser
Phosphorus ⇒ Increase hardenability, butt result in cold cracking tendency in steels
Sulphur ⇒ Increase hardenability but result in Hot cracking tendency in steels.
Manganese ⇒ Increase abrasive resistance
Tungsten ⇒ Increase hot hardness
molebedinum ⇒ Increase creep strength
cobalt ⇒ Increase toughness
Venedium ⇒ Increase endurance strength

Carbon % age	Applications
Low carbon steels	Screw, wires, nails, Boiler plates, structural works
Medium Carbon steels	Crank shaft, connecting rod, Gears
High carbon steels	Hammers, cutting tools, ball bearings.

Cast Iron

1. **White CI** : made under fast cooling rates
   - made with low Silicon content
   - Fe_3C needles present in Pearlite matrix
   - Hard Brittle & wear resistant.
2. **Grey CI** : made under slow cooling rates
   - made with high Silicon content.
   - $Fe_3C \longrightarrow$ graphite flakes
   - long graphite flakes disturbs continuity of lattice & hence decrease strength & hardness.
3. **Mechanite CI** : Originally grey CI
   - Added with CaSi to refine flakes
   - CaSi brakes flakes & Distribute uniformly
   - Composite type strength is observed.
4. **Chilled CI** : Produced in chilled moulds
   - outer layer - fast cooling
   - inner layer - slow cooling

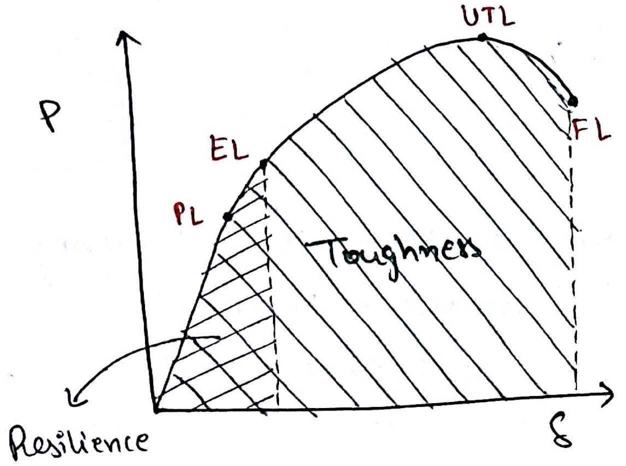
   $\Big\}$ Due to this transforms in flakes
5. **Spheriodal CI** or **Nodular CI** : originally grey CI
   - Li/Na/K/Ba are added as alloying elements
   - Graphite flakes are spherical in shape
   - machinability ↑

<table>
<tr><th colspan="2">Ceramics</th></tr>
<tr><th>Properties</th><th>Application</th></tr>
<tr><td>- non-metallic organic compounds like oxides, nitrides, carbides etc.
- usually crystalline but can be amorphous.
- thermal & electrical insulator
- Conduct electricity at high temp.
- good in Compression, weak in tension</td><td>- Semiconductor material in memory loops.
- Bricks, cements
- POP, lime
- Refractory lining of furnace
- floor tiles, wall tiles</td></tr>
</table>

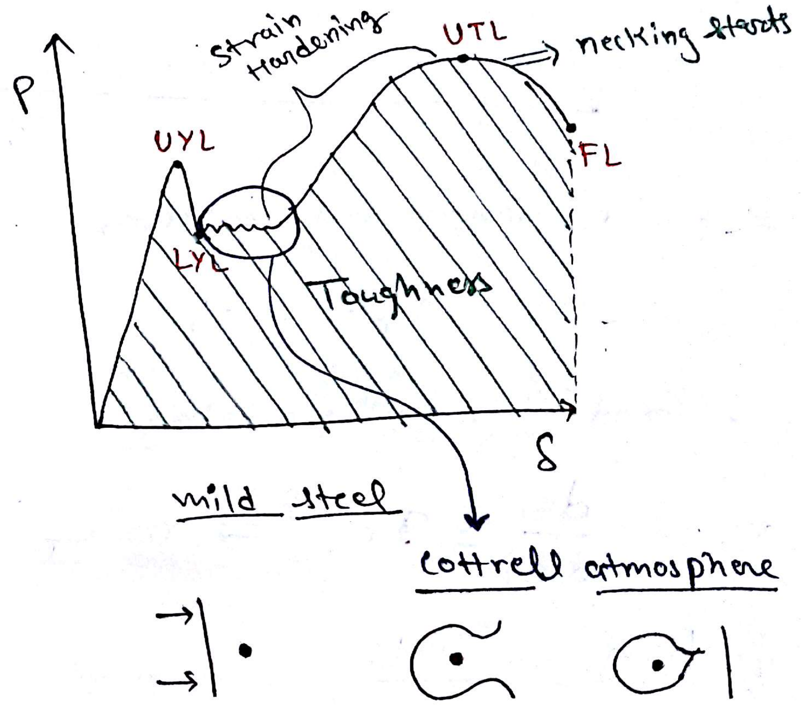
Polymers	Applications
Acrobutadiene Styrene (ABS)	Rafrigerator lining
Acrylics / Perspex	lenses, Aircraft windows.
Teflon	Anticorrosive seal, pipes, values, Bearings
Polystyrene	Battery cases
PVC	floor ~~coring~~ covering, electric insulation
Epoxies	Protective Coatings
Silicons	high temp. Insulations.

CHAPTER-7 MECHANICAL PROPERTIES (Testing & evaluations)

A) Tension test



Aluminium



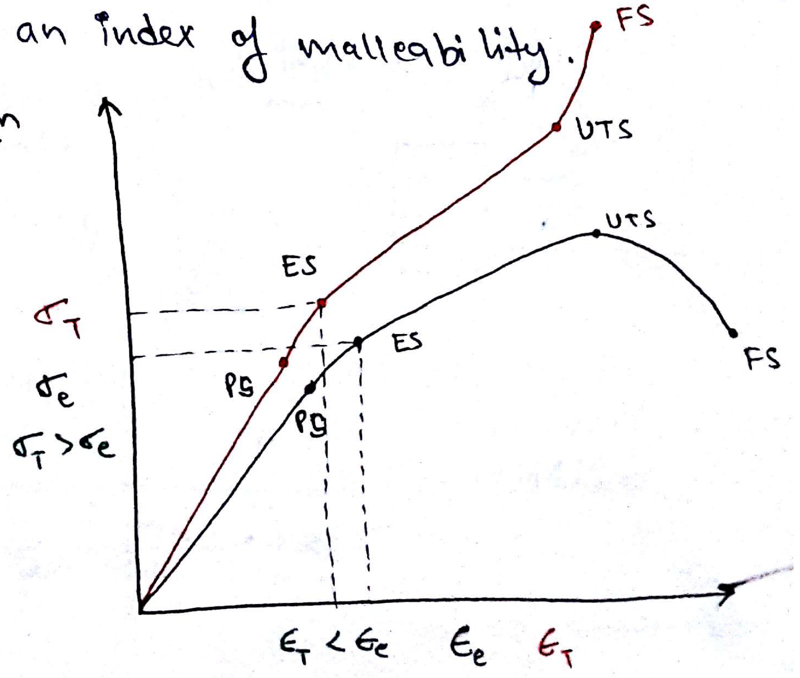
- % age elongation in length is taken as an index of Ductility
- % age reduction in Area is an index of malleability.

True stress & True strain

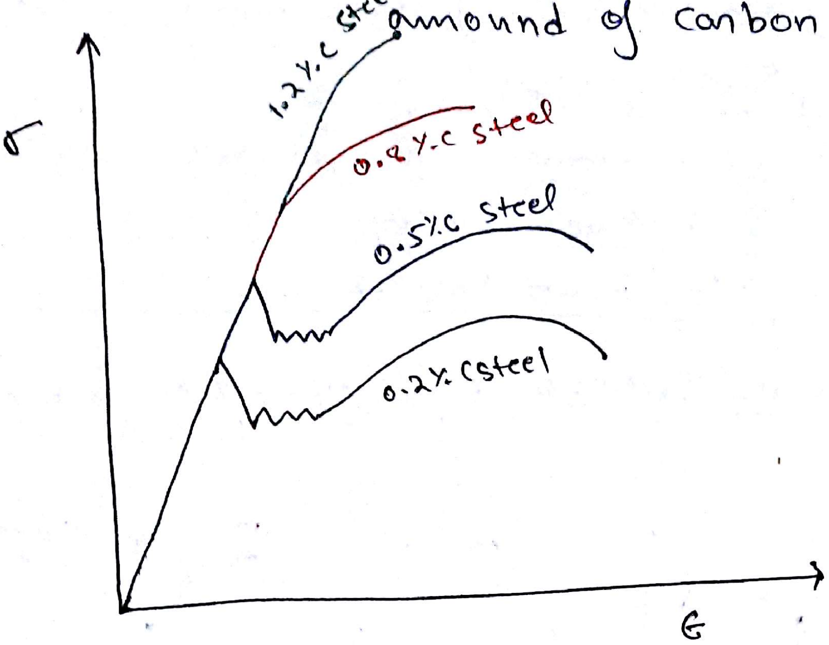
(σ_T) (ϵ_T)

$$\sigma_T = \sigma_e (1 + \epsilon_e)$$

$$\epsilon_T = \ln (1 + \epsilon_e)$$



Young's modulus: it is an index of stiffness of material. Young's modulus is structure insensitive property. Also, it does not depend on amound of carbon added to steels.



- Slope is same i.e. Youg's modulus is same for all carbon content.

\# For permanent deformations

$$\sigma_T = K \epsilon_T^n$$

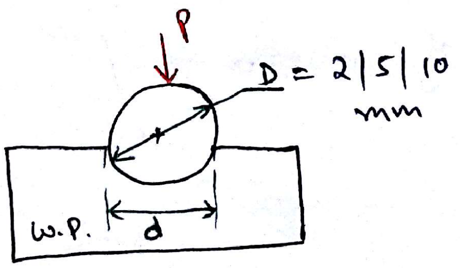
here, K = strength coefficient
n = work hardening Exponent.

- Condition for necking.

$$\frac{d\sigma_T}{d\epsilon_T} = \sigma_T \Rightarrow n = \epsilon_T$$

B) Hardness Tests

a) Brinnell's hardness test



Indentor = Hardened steel ball
or
Tungsten Carbide

Time of load = 10 - 30 seconds

P = 3000 Kg for Fe alloys
= 500 Kg for non-Fe alloy [for 10mm D]

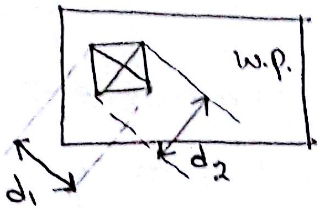
$$BHN = \frac{2P}{\pi D\left(D - \sqrt{D^2 - d^2}\right)} \quad ; \quad \frac{P}{D^2} = 30 \text{ Fe-alloys}$$

$= 5$ non-Fe alloys

|| 400 for indentor

$\boxed{\sigma_{ut} = 3.5\ BHN}$

b) Vicker's Hardness test

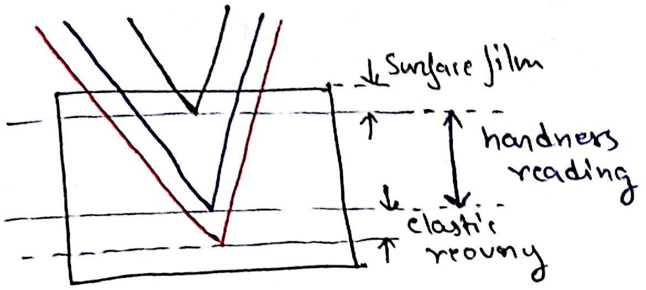


- Square base diamond pyramid as indentor
- included angle = 136°
- load = 1 to 120 Kg
- Time = 10 - 30 sec.

$$VHN = \frac{1.8544\,P}{d^2} \quad ; \text{ here } d = \frac{d_1 + d_2}{2}$$

- it cannot be used for powder metallurgy materials.

c) Rockwell hardness test

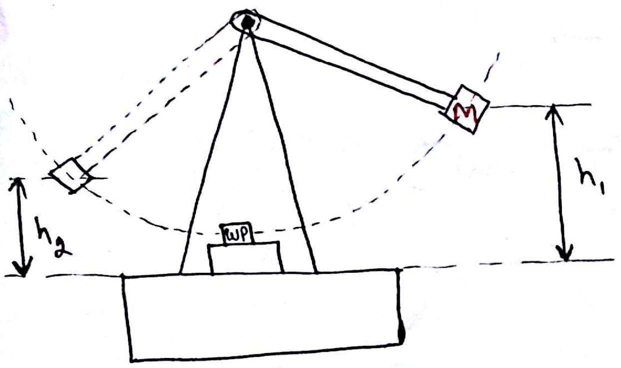


- Readings are found directly on reader, no formula.
- Uses brale indentor

$\Downarrow$

conical black diamond.

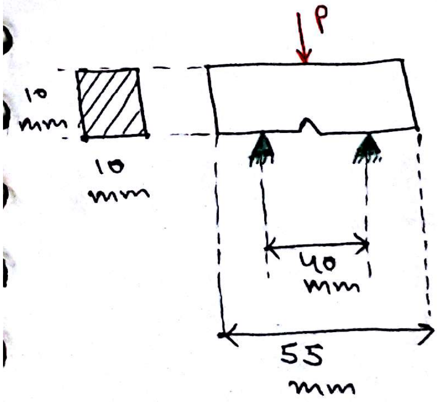
c) Impact test



- To find out dynamic toughness and notch sensitivity.
- To study ductile to brittle transition in metal.

$$\text{Dynamic Toughness} = Mg\,(h_1 - h_2)$$

Charpy test



Izod test