

* 1. Crystal Structure *

Space lattice:

The structure of metals greatly influence their behaviour and properties. The changing microstructure can change in a metallurgical frame. ductile to predict.

Based on the arrangements of atoms solids are classified as

(1) Amorphous solids

(2) Crystalline solids.

(1) Amorphous solids:

The solids are orderly arrangement of atoms lack is called non crystalline solids.

(2) Crystalline solids:

In crystalline solids atoms are arranged in a orderly configuration most metals are crystalline solids.

Crystal structures

When metals solidify from a molten state the atoms arrange themselves into various orderly configuration within the crystals.

Packing Factor:

Packing Factor (or) packing density is defined as ratio of total volume of atoms in a unit cell to the volume of unit cell.

$$\text{Packing Factor} = \frac{\text{Total volume of atoms in a unit cell}}{\text{Volume of unit cell}}$$

$$\text{For cubic structure PF} = n \cdot \frac{\frac{4}{3} \pi r^3}{a^3}$$

where r = radius of atoms

n = effective number of atoms per unit cell

a = lattice constant.

cooordinate number: (CN)

The cooordinate number in a crystal structure is defined as the number of nearest atoms directly surrounding a given atom is called cooordinate number.

cooordinate number indicates how tightly atoms are packed in a given crystal.

Density of crystal:

$$\text{Density} = \frac{\text{mass}}{\text{volume}}$$

$$\text{mass of unit cell} = \frac{A \cdot n}{N} \text{ gm}$$

where A = atomic mass, gm (numerically equals to atomic weight)

n = effective no of atoms

N = Avagadro's number

= 6.023×10^{23} per mole

$$\text{volume of unit cell} = a^3 \text{ cc}$$

where a = lattice constant, cm

$$\text{Density } \rho = \frac{A \cdot N}{N a^3} \text{ gm/cc}$$

also size of unit cell

$$a = \sqrt[3]{\frac{A \cdot n}{\rho \cdot N}}$$

crystal structure of metals:

most metals crystallise into three form of crystal systems.

- (1) Face centered cubic structure (FCC)
- (2) Body centered cubic structure (BCC)
- (3) Hexagonal closed packed structure (HCP)

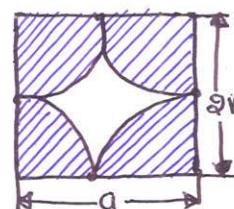
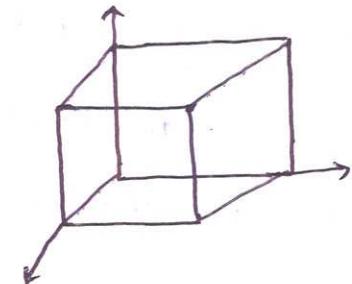
Simple cubic structure:

In simple cubic structure atoms take positions at the corners of the cube. Unit cell of simple cubic structure has 8 electrons and all corner atoms touch each other's actual in figure.

(P) Effective no of atoms: (n)

In each corner atom of a simple cubic structure is shaded by 8 unit cells. Thus each unit cell shades $\frac{1}{8}$ of the corner atom and there are 8 carbons in a simple cubic structure.

$$n = 8 \times \frac{1}{8} = 1 \text{ atom}$$



$$a = 2r$$

Packing Factor: (PF)

$$\text{P.F.} = \frac{n \cdot \frac{4}{3} \pi r^3}{a^3}$$

For simple cubic structure

$$n=1 \quad a=2r$$

$$\text{Packing Factor: P.F.} = \frac{1 \times \frac{4}{3} \pi r^3}{(2r)^3}$$

$$\boxed{\text{P.F.} = 0.52}$$

Packing Factor of simple cubic structure = 0.52.

Co-ordination number:

In simple cubic structure every carbon atom is directly surrounded with six other atoms along x, y, z directions.

Hence coordination number for simple cubic structure is "6"

Face centred cubic structures (FCC)

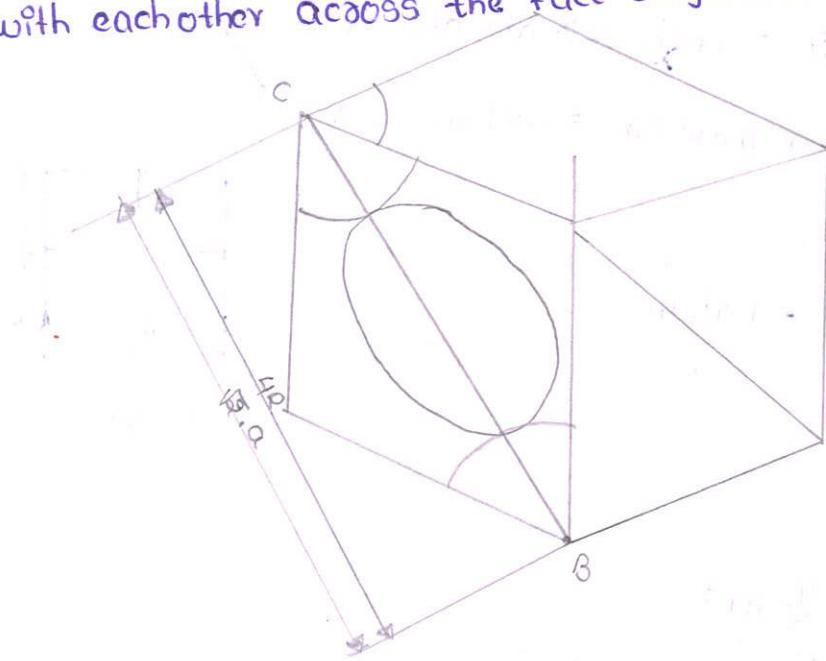
A unit cell of FCC structure consist of atoms located at each corner of a cube as well as at the centers of each face arranged such that the

atoms touch one another along the diagonals of face

Example of metals that crystalline in the FCC structure or aluminium copper, lead, gold, nickel, platinum and silver.

relation between A and R:

The corner atoms in FCC unit cell don't touch each other but contact with each other across the face diagonals.



consider the triangle ABC

$$\begin{aligned}BC^2 &= AB^2 + BC^2 \\&= a^2 + a^2 \\&= 2a^2\end{aligned}$$

$$BC = \sqrt{2}a$$

$$a = \frac{4Y}{\sqrt{2}}$$

Effective number of atoms:

In FCC structure effective no of corner atoms / is $\frac{1}{8} \times 8 = 1$

→ each face centred atom is shared by 2 unit cells and there are six faces in a unit cell of cubic structure.

∴ The effective number of face centred atoms = $\frac{1}{2} \times 6 = 3$

Thus effective no of atoms in FCC unit cell

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

$$n = 1 + 3$$

$$\boxed{n = 4}$$

Packing Factor:

$$\begin{aligned}\text{Packing Factor (P.F)} &= n \cdot \frac{\frac{4}{3} \pi r^3}{a^3} \\ &= 4 \cdot \frac{\frac{4}{3} \pi r^3}{\left(\frac{4r}{\sqrt{2}}\right)^3}\end{aligned}$$

$$\boxed{P.F = 0.74}$$

coordination number:

In FCC unit cell each atom is in contact with 12 adjacent atoms.

i.e directly surrounded by 12 equal distance nearest atoms.

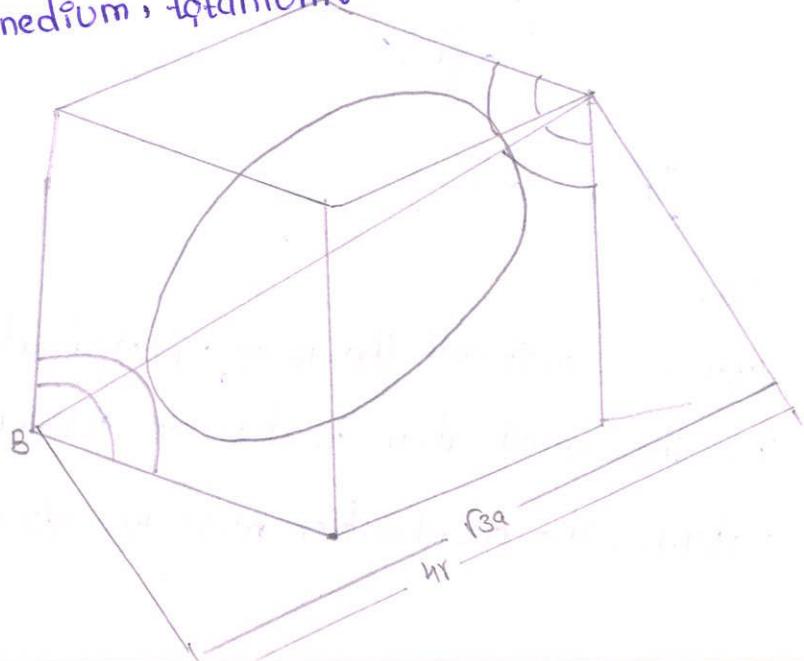
∴ Its coordination number is '12'

Body centered cubic structure (BCC):

→ In BCC structure unit cell consist of one atom. in 8 corners and one atom at the center of the cube all the touches all 8 corner atoms

examples of metals that crystallize in the BCC structure are cobodium, iron [α], molybdenum, potassium, sodium

tungsten and vanadium, titanium.



Relation between A and R:

The corner atoms in BCC unit cell do not touch each other but contact each other across the body diagonal as shown in the figure

considering the triangle ABC

$$BC^2 = AB^2 + AC^2$$

$$= 8a^2 + a^2$$

$$= 9a^2$$

$$BC = \sqrt{3}a$$

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

Effective number of atoms:

In BCC structure effective no of corner atoms is $\frac{1}{8} \times 8 = 1$
one central atom is not shared by any other unit cell

thus effective no of atoms in BCC unit cell.

$$n = \frac{1}{8} \times 8 + 1$$

$$n = 1 + 1$$

$$\boxed{n = 2}$$

Packing Factor:

$$\text{Packing Factor (P.F)} = \frac{n \cdot \frac{4}{3} \pi r^3}{a^3}$$

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

$$\boxed{(P.F) = 0.68}$$

coordination number:

In BCC structure unit cell the body centred atom is connect with 8 corner atoms i.e. the central atom is directly surrounded by 8 equal distance by nearest atoms. The coordination no. of BCC structure is "8"

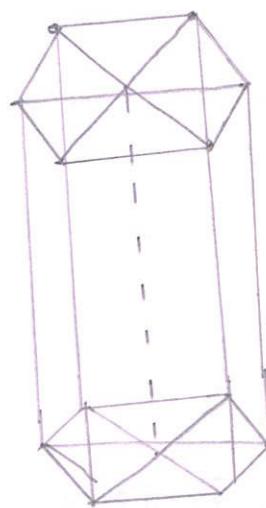
Hexagonal closed packed structure:

In HCP structure the atoms are placed as tightly as possible

The arrangement of atoms in HCP unit cell is shown in figure. The true unit cell of Hexagonal lattice is only the portion shown by thick lines. If these unit cells are packed together with the axis parallel to one another as shown space lattice. a Hexagonal prism may be carried out of them.

Examples of HCP:

Cadmium, Zinc, Mg, Cobalt, Zirconium, Titanium, and Berillium.



Relation Between A and R:

The atoms in HCP unit cell touch each other

$$a = 2r$$

Effective no of atom:

These are 6 corner atoms on both top and bottom layers.

and each carbon atom accounts for $\frac{1}{6}$ atom.

The contribution from the corner atom is $= 2 \left(\frac{1}{6} \times 6 \right)$

$$= 2$$

also there are 3 atoms in the middle layer which are not shaded by any other unit cell. the atoms at the center of top and bottom layers contribute 1 atom $(\frac{1}{6} \times 2) = 1$

$$\text{contribute 1 atom } (\frac{1}{6} \times 2) = 1$$

Thus effective no of atoms in HCP unit cell

$$n = 2\left(\frac{1}{6} \times 6\right) + \left(\frac{1}{2} \times 2\right) + 3$$

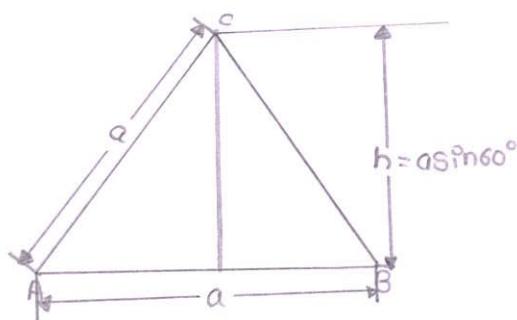
$$n = 2 + 1 + 3$$

$$\boxed{n = 6}$$

Packing Factor:

Packing Factor, $p.o.F = \frac{\text{volume of atoms in a unit cell}}{\text{volume of unit cell.}}$

Volume of unit cell:



base consists of 6 equilateral triangles

$$\begin{aligned}\text{Area of base} &= 6 \times \text{area of triangle} \\ &= 6 \times \frac{1}{2} \times a \times a \sin 60^\circ \\ &= 3a^2 \sin 60^\circ\end{aligned}$$

Volume of HCP unit cell = area at the base \times height

$$= 3a^2 \sin 60^\circ \times c$$

$$\frac{c}{a} = 1.633$$

$$\begin{aligned}\text{Volume of HCP unit cell} &= 3a^2 \sin 60^\circ \times c \\ &= 3a^2 \sin 60^\circ \times 1.633a \\ &= 4.2426a^3 \\ &= 4.2426(2r)^3\end{aligned}$$

$$\text{Packing factor} = \frac{\text{No. } \frac{4}{3} \pi r^3}{a^3}$$

$$= \frac{6 \cdot \frac{4}{3} \pi r^3}{4 \cdot 8426 (2r)^3}$$

$$\boxed{P.F. = 0.74}$$

Crystal defects:

Crystals are rarely perfect. They contain large no of imperfections (defects) which influence the behaviour of metals. Because of these defects the actual strength of metal is much less than the theoretical strength.

~~Crystal defects affect the actual strength of metal~~

Crystal defects are classified as

(1) point defect:

(2) Line defect:

(3) surface defect:

(4) volume defect:

(1) point defects:

Point defects are localised disruption of the lattice involving one or few atoms. They are regarded as dimensional defects.

→ Important defects are:

(i) vacancy:

Vacancy occurs as a result of atom missing from a normal site such defects are called due to imperfect packing during crystallisation or may be cause from thermal vibration of atom at elevated temperature. Vacancies increase the kinetics of diffusion and phase transformation. The concentration of vacancy is important in determining the amount of diffusion that occurs in solids. Vacancy concentration increases with increasing temperature and number of vacancies at any temperature is given by

$$n_v = n_t \cdot e^{-\left[\frac{E}{kT} \right]}$$

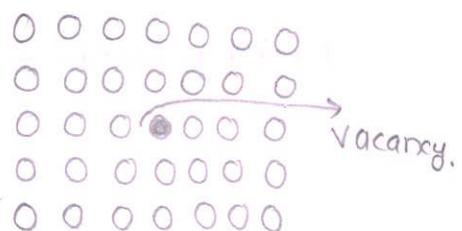
e = energy of formation of vacancy

k = Boltzmann constant $= 1.38 \times 10^{-24} \text{ J/K}$
(or)

$8.63 \times 10^5 \text{ ev/K}$

T = absolute temperature

n_t = total number of atomic sites for cubic meter or per mole.

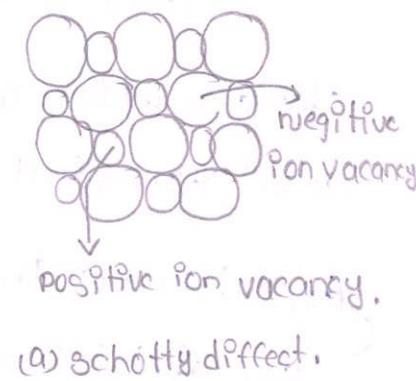


Schottky defects

Schottky defects are closely related to vacancy but are found in compounds which must maintain charged balance.

→ In Schottky defect the removal of positive ion must be counter balanced by the removal of negative ion in order to maintain neutrality

→ The pair of vacancies caused by removal of positive ion and negative ion is called Schottky defect.



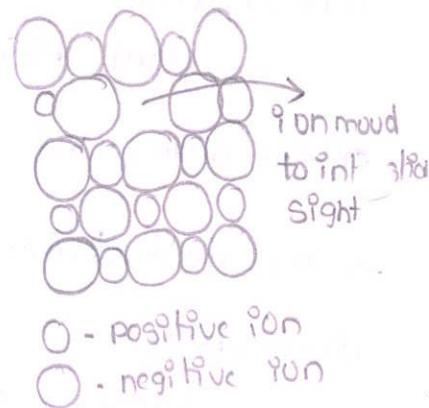
(a) Schottky defect.

Frenkel defect:

If an atom displaced from the normal lattice point to an interstitial sight then the defect is known as Frenkel defect:

Interstitial defects

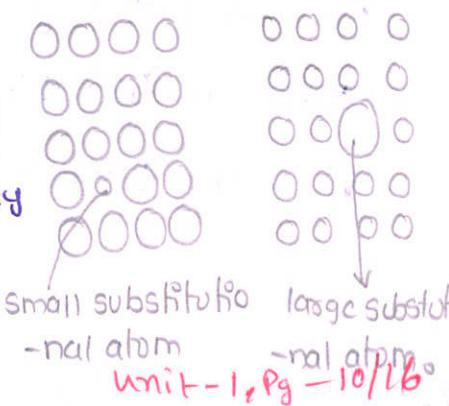
It is formed when an extra atom is inserted into the lattice at a normally unoccupied sight such atoms may be impure or deliberate alloying elements.



O - positive ion
○ - negative ion

Substitutional defects:

It occurs when one atom in a lattice is replaced substituted by other different atom which may be impurity or deliberate alloying element. Such substitutional atom may be smaller or larger than original atom.



Small substitutional atom
Large substitutional atom
Unit-1, Pg - 10/16

Line defects:

Line defects are one dimensional defects and extend along some direction. The most common type of line defect within a crystal is dislocation.

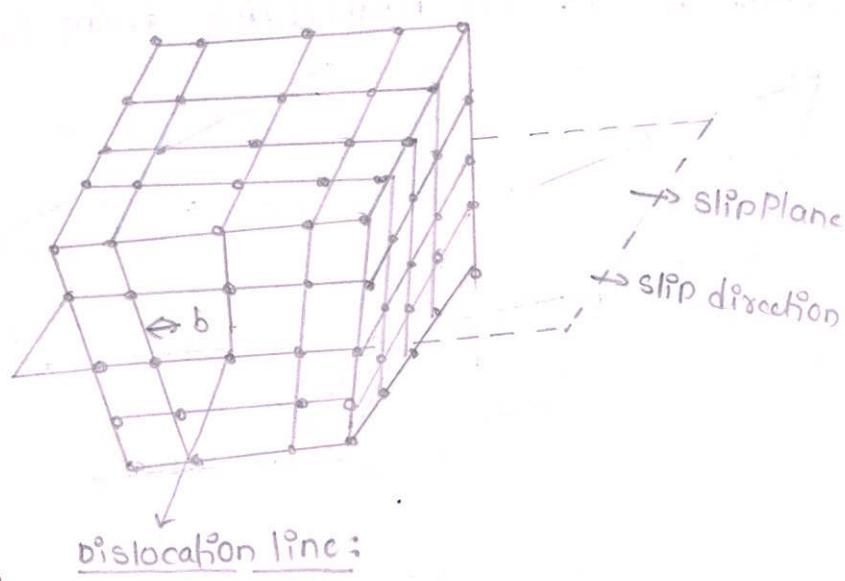
Dislocations may be produced during crystallisation. But more commonly, originate during deformation they are most significant defects which reduce the strength of metals. A slip plane containing dislocation requires less shear stress to allow slip than does a plane in a perfect lattice.

Dislocations are classified as

1) Edge dislocation:

→ It is may be described as lattice distortion at the edge of an extra plane of atoms within the crystal structure if an extra plane is above the slip plane the edge location called positive and represented by + it is below the slip plane then is called negative and represented by -.

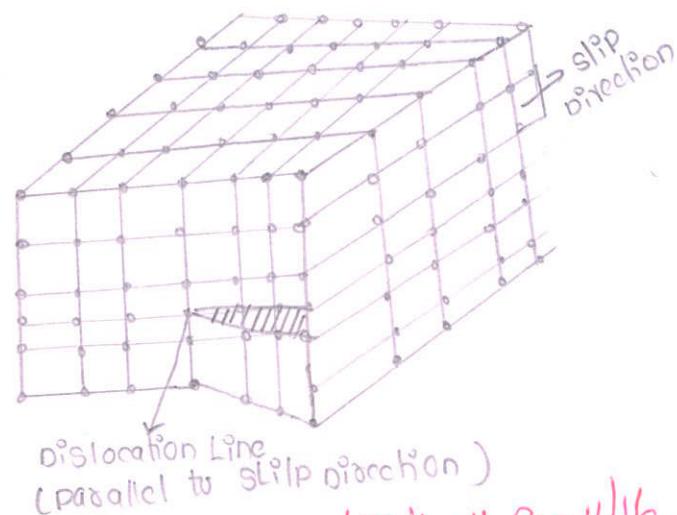
→ In case of edge dislocation Burgers vectors is refer to the dislocation line.



2) Screw dislocation:

In screw dislocations the atoms are displaced in two separate planes refer to each other.

The lattice points trace a helical path around the dislocation therefore it is called as screw dislocation.



Surface defects:

surface defects or imperfections or two dimensional defects, and are the region of disturbance of few atomic diameters important surface imperfections are

1) stacking fault

2) grain boundaries

3) twinned boundaries.

1) stacking faults

stacking fault results due to breaking the stacking sequence of atomic planes thus if fault is created there is a missing of atomic plane from the normal sequence.

2) grain boundaries

it is a narrow region between two grains of about two few atomic diameters in width and it is the region of atomic mismatch between adjacent grains.

→ If the orientation between two neighbouring grains is less than 10° then it is called low angle boundary tilted boundary. If the mismatch i.e. orientation difference b/w two grains is more than 10° to 15° the grain boundary is known as high angle grain boundary.

(3) twinned boundaries

→ surface imperfections which separate two orientations that are mirror images of one another is called twinned boundary.

→ Twinned boundaries constitute a pair and the region between them is the twinned plane.

volume effects:

(7)

volume effects originate during solidification or processing of metal and include gas cores and cracks. These effects are of large dimensions and affects the property of metal.

* strengthening mechanisms:

→ material can be increased by hindering dislocation, which is responsible for plastic deformation.

→ different ways to hinder dislocation motion / strengthening mechanisms:

in single - phase materials:

→ grain size reduction

→ solid solution strengthening

→ strain hardening.

in multi phase materials:

- precipitation strengthening

- dispersion strengthening

- fiber strengthening

- martensite strengthening.

→ Impure foreign atoms in a single phase material produces lattice strains which can anchor the dislocations.

→ effectiveness of this strengthening depends on two factors - size difference and volume fraction of solute.

→ solute atoms interact with dislocations in many ways.

- elastic interaction.

- modulus interaction

- stacking-fault interaction

- electrical interaction

- short range order interaction

- long range order interaction.

→ Elastic modulus and long-range order interactions are of long-range i.e they are relatively insensitive to temperature and continue to act about $0.6 T_m$.

Strengthening by Grain Size Reduction:

→ It is based on the fact that dislocations will experience hindrances while trying to move from a grain into the next because of abrupt change in orientation of planes.

→ Hindrances can be two types : forcible change of slip direction, and discontinuous slip plane.

→ Smaller the grain size often a dislocations encounters a hindrance. Yield strength of material will be increased

→ yield strength is related to grain size (diameter d) as Hall-Petch relation

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

→ Grain size can be tailored by controlled cooling or by plastic deformation followed by appropriate heat treatment.

→ Grain size reduction improves not only strength but also the toughness of many alloys

→ If d is average grain diameter & S_V is grain boundary area per unit volume N_L is mean number of intercepts of grain boundaries per unit length of test line, N_A is number of grains per unit area on polished surface

$$S_V = 2N_L \quad d = \frac{3}{S_V} = \frac{3}{2N_L} \quad d = \sqrt{\frac{6}{\pi N_A}}$$

→ grain size can also be measured by comparing the grains at a fixed magnification with standard grain size charts.

→ Other method: use of ASTM grain size number (Z). It is related to grain diameter D (in mm) as follows

$$D = \frac{1}{100} \sqrt{\frac{645}{Z^{G-1}}} \text{ unit - I - Pg - 14/16}$$

Martensite strengthening:

- This strengthening method is based on formation of martensitic phase from the retained high temperature phase at temperatures lower than the equilibrium invariant transformation temperature.
- martensite forms as a result of shearing of lattices.
- martensites platelets assumes characteristic lenticular shape that minimizes shear elastic distortion in the matrix. These plates divide and subdivide the grain of the parent phase
- Martensite formation occurs in many systems.
E.g : Fe-C, Fe-Ni, Fe-Ni-C, Cu-Zn, Au-Cd, and even in pure metals like Li, Zr and Co.
- High strength of martensite is attributed to its characteristic twin structure and to high dislocation density.

Fiber strengthening:

- second phase can be introduced into matrix in fiber form too.
- Requisite for fiber strengthening
 - fibers material - high strength and high modulus.
 - matrix material - ductile and non reactive with fibers material.

Eg's Fiber material - Al_2O_3 , boron, graphite, metal, glass etc.
- mechanism of strengthening is different from other methods.
- strengthening analysis involves application of continuum, not dislocation concept as in other methods of strengthening.

→ To achieve any benefit from presence of fibers, critical fiber volume which must be exceeded for fiber strengthening to occur.

$$f_{\text{critical}} = \frac{\sigma_{mu} - \sigma_m'}{\sigma_{fu} - \sigma_m'}$$

→ minimum volume fraction of fiber which must be exceeded to have real reinforcement

$$f_{\min} = \frac{\sigma_{mu} - \sigma_m'}{\sigma_{fu} + \sigma_{mu} - \sigma_m'}$$