Materials and their structures

2.1 Introduction:

The ability of materials to undergo forming by different techniques is dependent on their structure and properties. Behavior of materials depends on their structure-atomic structure, crystal structure and grain structure.

Materials are generally classified into metals/alloys and non-metals such as plastics, ceramics, composites. Metals are further classified into ferrous and nonferrous metals. Further, materials can be classified into crystalline and amorphous materials.
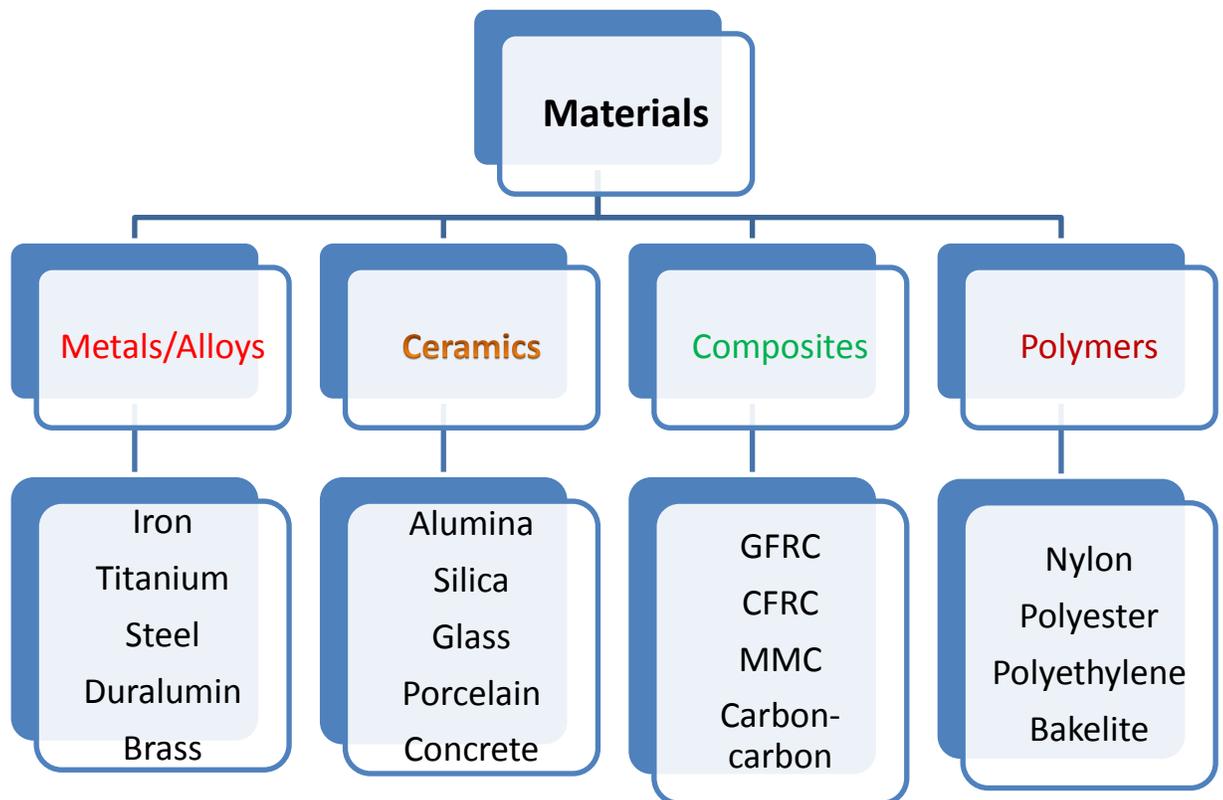
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                              Materials

   Metals/Alloys      Ceramics      Composites      Polymers

   Iron               Alumina       GFRC            Nylon
   Titanium           Silica        CFRC            Polyester
   Steel              Glass         MMC             Polyethylene
   Duralumin          Porcelain     Carbon-         Bakelite
   Brass              Concrete      carbon
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Fig. 2.1.1: Classification of materials

2.2 Crystalline arrangement:

Crystalline materials have atoms arranged symmetrically in long range order. In amorphous materials there is short range order, the orderly arrangement of atoms being discontinuous.

Crystalline solids have their atoms arranged in three dimensional space in basic forms called lattices – Bravais lattices.

There are basically 7 lattice systems, namely, Cubic, hexagonal, tetragonal, orthorhombic, rhombohedral, monoclinic, triclinic.

Crystal structures of commonly used engineering metals and alloys can be grouped into three types, namely, body centered cubic [BCC], face centered cubic [FCC] and hexagonal closed pack [HCP]. The smallest group of stacked atoms which repeats itself in three dimensional space and hence fixes the lattice structure can be defined as unit cell.

Physical and mechanical characteristics of crystalline solids are dependent on the effective number of atoms in a unit cell, density and orientation of packing of atoms within the unit cell.

Unit cells are represented by hard-ball models. The effective number of atoms in a unit cell represents the extent of packing of atoms and void space within the unit cell.
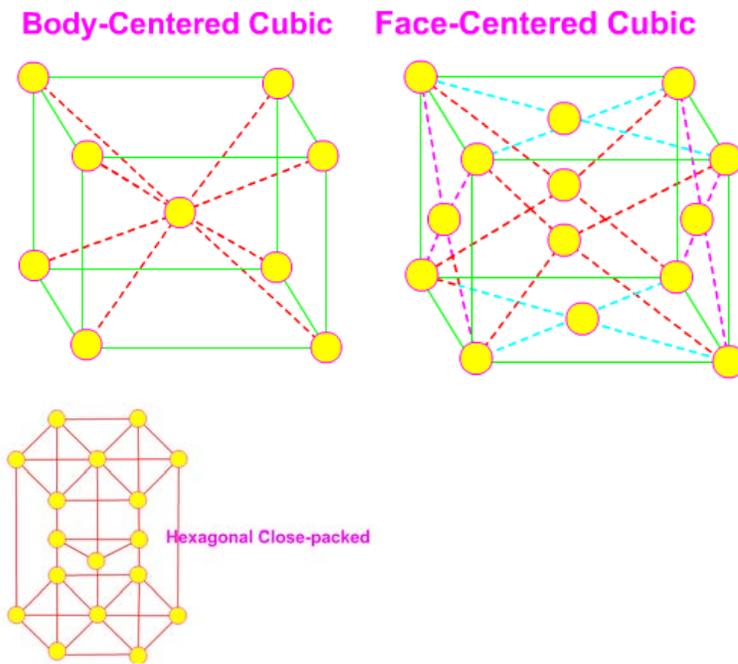
Fig. 2.2.1: Unit cell structures of Cubic and HCP lattices

BCC: Metals like alpha iron, chromium, molybdenum, tungsten, vanadium exhibit BCC structure. The packing efficiency which is the ration of the volume of effective number of atoms per unit cell to the volume of the unit cell for BCC is found to be 58%.

Number of neighboring atoms in a BCC unit cell is 8 – called coordination number.

FCC: Metals like nickel, copper, aluminium, silver, gold, platinum have fcc structure with a packing efficiency of 74%. And coordination number of 12.

HCP: For hcp metals such as zinc, magnesium, alpha titanium, cobalt, cadmium the packing efficiency is 74% and coordination number is 12.

FCC and HCP have more densely arrangement of atoms within, than BCC.

2.3 Planar and direction indices

Mechanical properties of crystalline materials such as ductility, strength etc are also dependent on the directions and planes of close packing of atoms. Atomic planes and atomic directions in unit cells are represented by Miller indices and Miller Bravais indices, respectively.

Closely packed directions and planes determine the nature of deformation in crystalline objects.Miller indices are represented as <abc> and Bravais indices are represented as {xyz}. Miller indices are the reciprocal of the intercepts of the atomic plane with the three coordinate axes, rounded off to nearest whole number. Miller indices of direction are the intercepts of atomic direction with the three coordinate axes.
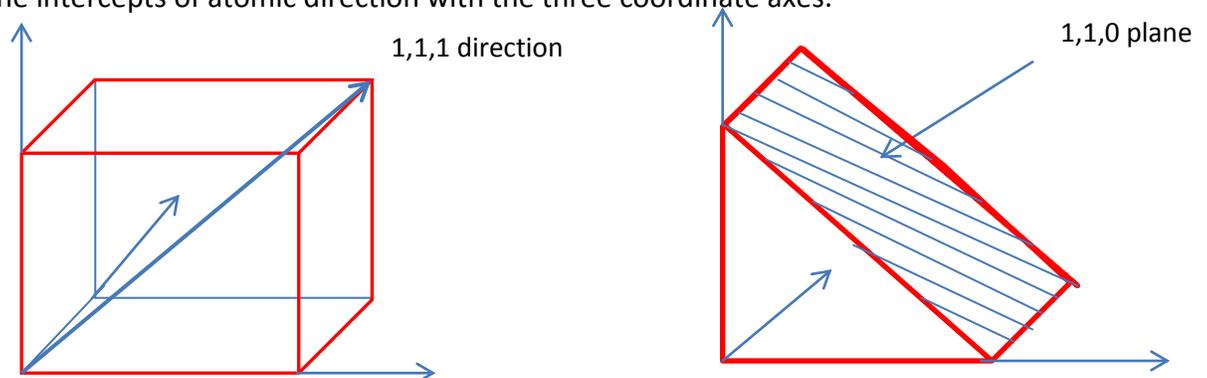

Fig. 2.3.1:Miller indices of direction and plane

Miller indices of atomic directions are obtained as the difference between the intercepts of the end point of the direction and origin of the direction with the respective reference axes.

Difference in crystal structures of metals is due to the difference in energy required for the formation of the structures among different atoms. Some metals can exist in different crystal structures under different conditions of temperature. Iron exists as BCC at room temperature, but when heated to 1185 K it becomes FCC. This property is called polymorphism or allotropism.

Adding another element to a pure metal forms an alloy. For example carbon added to iron forms steel which has different properties compared to iron.

Alloying generally improvesstrength and hardness of pure metals. Pure metals as such have limited engineering applications in view of their limited strength, hardness, wear resistance, fatigue and creep resistance.
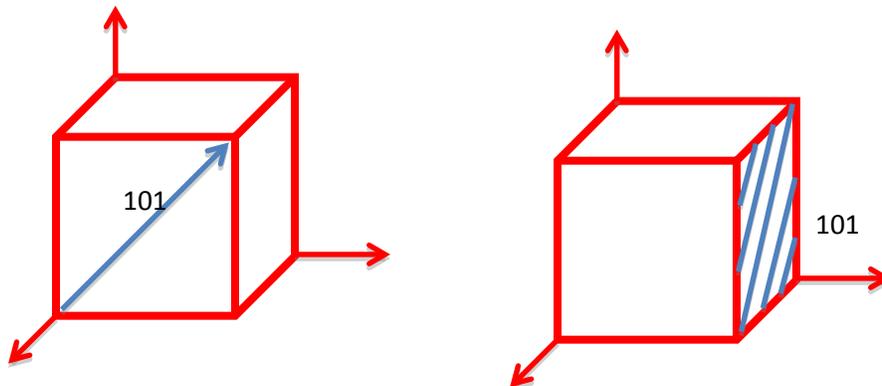
Fig. 2.3.2: 101 direction and 101 plane in cubic lattice

2.4 Crystal imperfections:

Crystal structures are never perfect – there are defects in the arrangements of atoms in crystalline materials. Imperfections arise during solidification of crystalline materials, or they may occur during processing of materials like mechanical deformation. Adding alloying element is a deliberately introduced imperfection.

There are generally three kinds of defects, namely, point defects, line defects and surface defects.

Vacancy – missing of an atom from the lattice position. It can happen due to nuclear irradiation of a material.

Interstitialcy – presence of an additional atom in the interstitial space.

Frenkel defect – Ion removed from its regular position and moved to interstitial position.

Schottky defect – missing pair of ions of opposite charge.
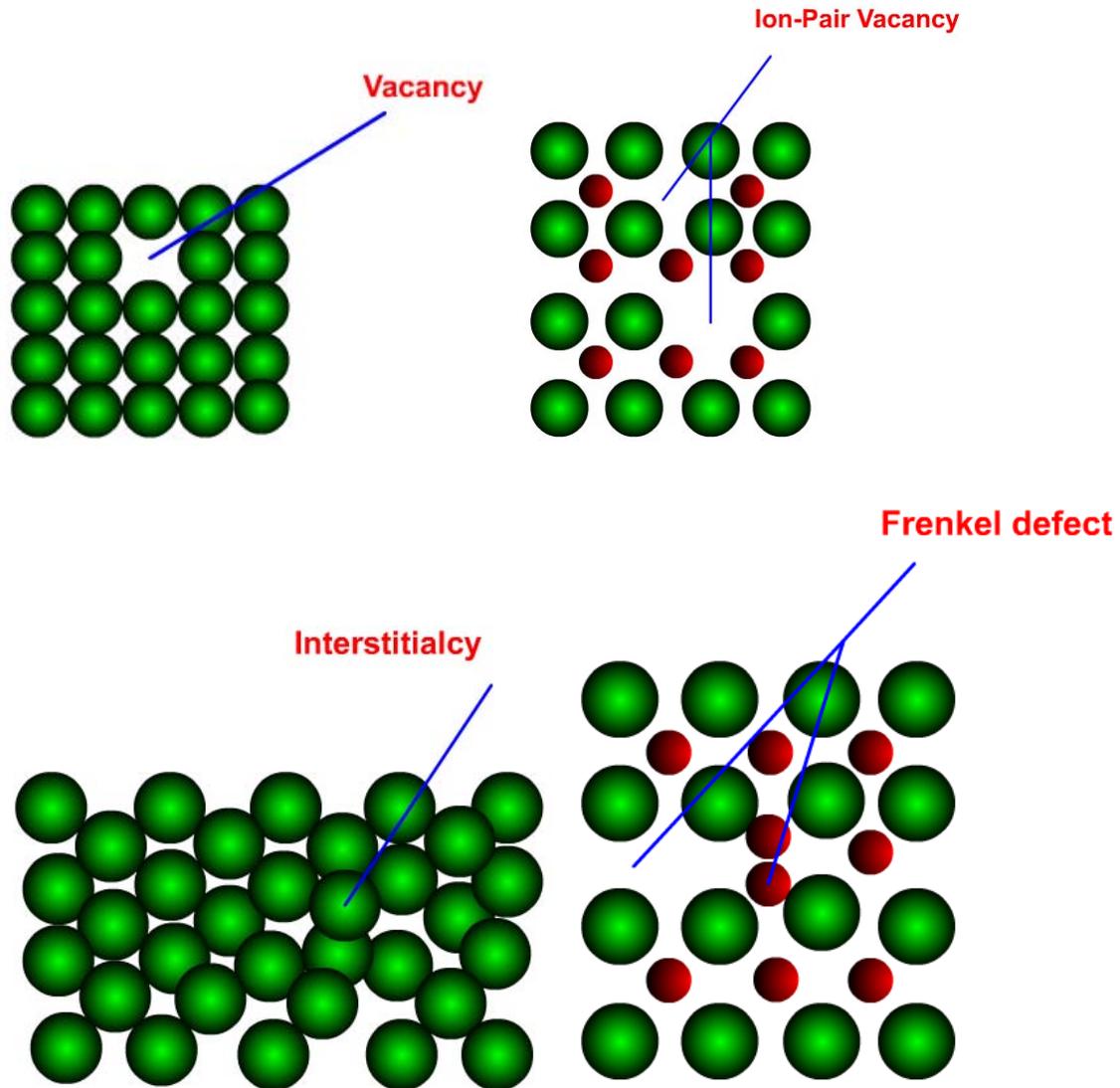
**Fig. 2.4.1: Point imperfections**

Line defects – these are collection of point defects. There are two types of line defects – edge and screw dislocations.

Edge dislocation – extra plane of atoms present within the crystal – giving raise to distortion of the structure.

Screw dislocation – It is a kind of distortion in the arrangement of atoms produced by a shear between two halves of a crystal – the upper front part moved by one atomic distance with reference to lower front.

Unit displacement of atoms in dislocations is represented by the Burgers vector.

Dislocations play active role during plastic deformation of crystalline solids.
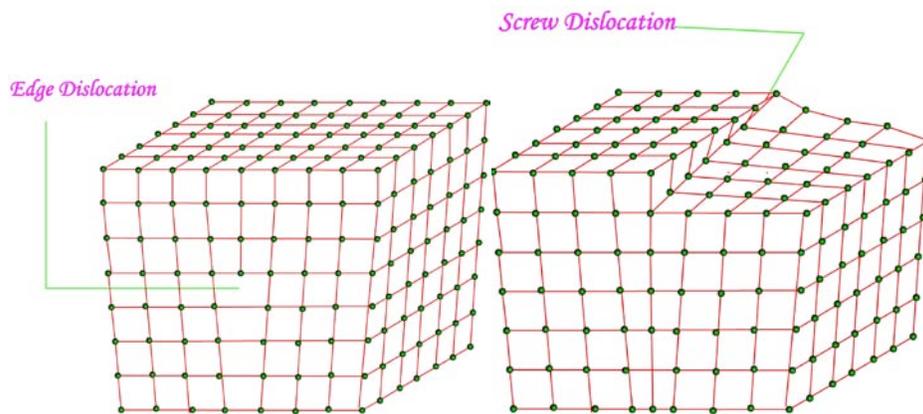
Fig. 2.4.2: Line defects-dislocations

Surface defects – grain boundaries in polycrystalline materials – which are orientation mismatch between adjacent grains. Grain boundaries are high energy regions and are amorphous. For large grains, the interfacial energy is lower due to lower interfacial area compared to small grains. At elevated temperatures, grains become larger in order to reduce the interfacial energy.

In single crystals there are no grain boundaries – therefore single crystals are stronger.

2.5 Deformation of crystalline solids:

2.5.1 Single crystals:

Application of external force on a crystalline solid results in distortion of the lattice structure. If the applied force is small, the distortion called elastic deformation can take place. At the removal of the force, the crystal structure comes to original shape.

If the applied force exceeds a certain limit, the deformation undergone by the solid is called plastic deformation – as the deformation remains even after removal of load or force.

Permanent deformation is called plastic deformation.

Maximum theoretical shear strength of a perfect crystal – stress causing plastic deformation – is given to be:

$\tau = G/2\pi$

where G is shear yield strength of the material.

Similarly, it can be shown that the maximum theoretical tensile strength of a perfect crystalline solid is given by:

$\sigma = E/10$

where E is elastic modulus. Theoretical strength is of the order of GPa.

However, actual shear strength and tensile strength of crystals is much less than that predicted by the above expressions because of crystal defects discussed in sections above.

2.5.2 Polycrystalline materials

Polycrystalline materials have defects in the crystal structure, which considerably reduce their strength.

Basic mechanisms causing plastic deformation in crystalline solids are slip and twinning.

Slip is sliding of one plane of atoms over another plane due to application of force-shear force. It is similar to the sliding of playing cards. A minimum shear stress called critical resolved shear stress is required to cause slip in single crystals. Slip specifically happens only along specific planes called slip planes and along specific directions called slip directions. Family of slip planes and slip directions together form slip systems.
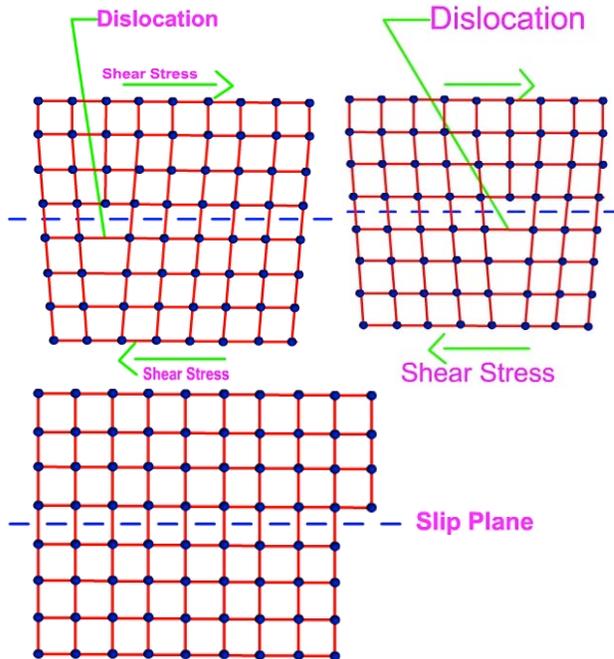
Fig. 2.5.2.1: Dislocation motion by slip

Different crystals have different slip systems. For example, for FCC structured metals, there are 12 slip systems, and for BCC metals there are 48 slip systems. However, out of 48 slip systems only some are active. BCC metals have higher strength than FCC metals generally.

Slip always happens along planes of maximum atomic density.

Less number of slip systems in HCP – only three – makes materials with HCP more brittle.

Slip is also caused by the movement of edge and screw dislocations in materials. Movement of an edge dislocation can be analogous to the motion of a caterpillar.

In single crystals, the magnitude of slip produced is dependent on the magnitude of shear stress induced by the external stress acting on the material. Slip begins when the shear stress reaches a critical value called critical resolver shear stress (CRSS). This principle is called Schmid's law. It is shown that this stress, CRSS is equal to:

CRSS = **σ cosθcosΦ**

Where σ is the tensile stress applied on the crystal, θ is angle between normal to slip plane and axis of the tensile stress, Φ is angle between slip direction and the tensile axis.
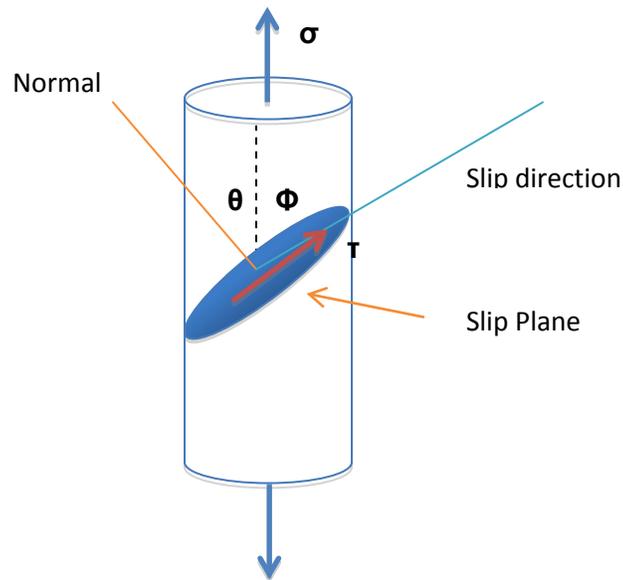
Fig. 2.5.2.2: Critical resolved shear stress

CRSS is a material property which depends on the type of structure and temperature.

For iron, the CRSS value is given at room temperature as 27.5 MPa, for nickel it is 5.7 MPa, for zinc it is 0.18. As seen here, Zn being hcp, has low CRSS. Alloying can increase the critical resolved shear stress. If there are more dislocations, impurities, solutes, the CRSS value of the metal increases, due to increased resistance to dislocation movement.

Twinning is the other mechanism of plastic deformation. Twinned structure is a mirror image of atoms across a plane of twinning. In HCP and bcc materials twinning may take place causing cracking sound during failure.

Plastic deformation of crystalline solids causes an increase in dislocation population. Dislocation density – defined as total length of dislocation per unit volume in cold-worked materials can be as high as 10^{12}.

Dislocation entanglements and obstruction to slip movement of dislocations during deformation can cause increase in strength of a metal. This is called strain hardening or work hardening.

Deformation in polycrystalline materials – grains of almost equal size are called equiaxed grains. Finer grains are formed during rapid cooling of molten metal. Higher the cooling rate finer the grain size.

Finer grains prevent easy motion of dislocations thereby increasing the strength of crystalline materials.

Single crystal has anisotropic properties, whereas polycrystalline materials have isotropic properties. Isotropy refers to uniform properties along all directions in the crystal.

Grain size has profound effect on strength and hardness of metals. Large grains produce smaller strength. Yield strength dependence on grain size is given by Hall-Petch relation:

$$Y = Y_i + kd^{-1/2}$$

where Y_i is resistance to dislocation motion, d is grain size, k is a constant indicating dislocation pileup.

Grain size is given by ASTM grain size number, n.

$N = 2^{n-1}$, where N is number of grains per square inch at a magnification of 100X and n is grain size number-varies between 0 and 10.

Source:
http://nptel.ac.in/courses/112106153/2