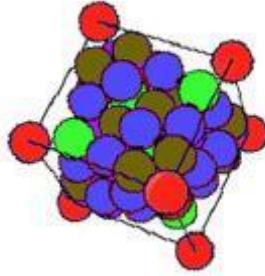


## Module-1

### Crystal Structure



#### OBJECTIVES:

To learn and understand the concepts of

- Crystal structures and its types
- Importance of coordination numbers
- Imperfection in crystals & types
- Diffusion process
- Ficks diffusion law
- Factors affecting diffusion.

#### OUT COMES

Based on different types of crystal structure, a student can understand why some of the materials are strong, and also the relation ship between structure and property,

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## Introduction

One of the ways to classify engineering materials is based on their nature. Such a type of classification is given below.

- i. Metals and alloys: - Cast irons, Steels, Al, Copper, Silver, Gold etc
- ii. Ceramics and Glasses: - MgO, ZnO, SiC, Silica, Concrete, Cement etc
- iii. Polymers: - Plastics-polyethylene, PVC, PTFE, Epoxy, Polyester etc

Each of the above group materials has their own sets of properties. Every engineering material is actually known by its properties. Some of the important properties of materials are

**Mechanical:** strength, hardness, ductility, malleability, toughness, resilience, creep, fatigue. **Physical:** shape, size, density, porosity, color.

**Chemical:** Acidity, alkalinity, composition, corrosion resistance, atomic number, molecular weight.

**Electrical:** Conductivity, resistivity, dielectric constant,

**Thermal:** Specific heat, thermal conductivity,

refractoriness **Aesthetic:** Feel, texture, appearance, lusture

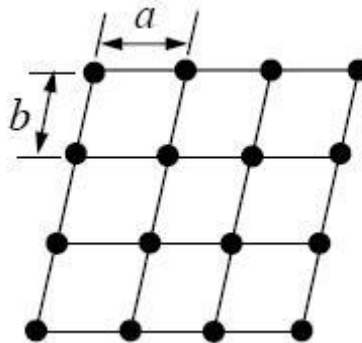
All the above properties are related structure of the material.

**Crystal structure** is one of the most important aspects of materials science and engineering as many properties of materials depend on their crystal structures. The basic

principles of many materials characterization techniques such as X-ray diffraction (XRD), Transmission electron microscopy (TEM) are based on crystallography. Therefore, understanding the basics of crystal structures is of paramount importance.

### Space lattice

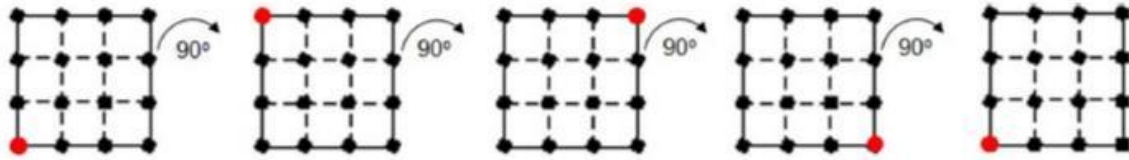
- A space lattice can be defined as a three dimensional array of points, each of which has identical surroundings.
- If the periodicity along a line is  $a$ , then position of any point along the line can be obtained by a simple translation,  $r_u = ua$ .
- Similarly  $r_{uv} = ua + vb$  will repeat the point along a 2D plane, where  $u$  and  $v$  are integers.



### Symmetry

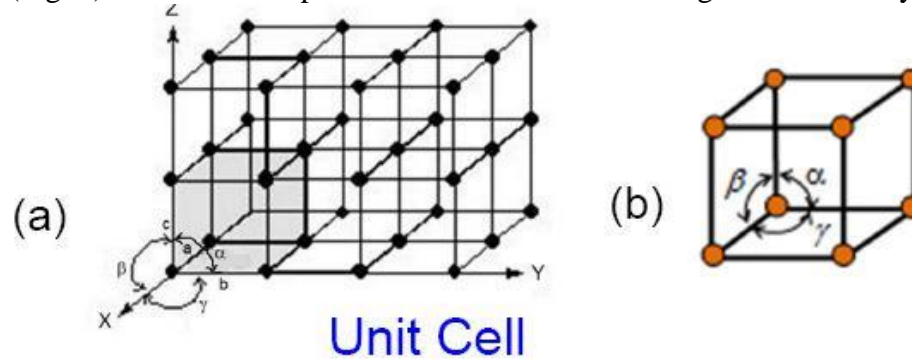
Symmetry refers to certain pattern or arrangement. A body is symmetrical when it is reproduced by certain operation.

In the picture below the plane looks identical after a 90° rotation. The plane has 4 fold rotation symmetry as it repeats itself 4 times (shown by the red dot) in a full 360° rotation.



## Crystal Systems

The space lattice points in a crystal are occupied by atoms. The position of any atom in the 3D lattice can be described by a vector  $r_{UVW} = ua + vb + wc$ , where  $u, v$  and  $w$  are integers. The three unit vectors,  $a, b, c$  can define a cell as shown by the shaded region in Fig.(a) This cell is known as unit cell (Fig. b) which when repeated in the three dimensions generates the crystal structure.



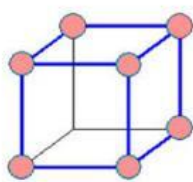
## Crystal Systems

### Bravais Lattice

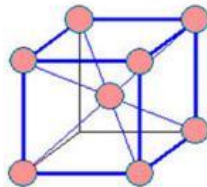
The unit vectors  $a, b$  and  $c$  are called lattice parameters. Based on their length equality or inequality and their orientation (the angles between them,  $\alpha, \beta$  and  $\gamma$ ) a total of 7 crystal systems can be defined. With the centering (face, base and body centering) added to these, 14 kinds of 3D lattices, known as **Bravais lattices**, can be generated.

## Crystal Systems

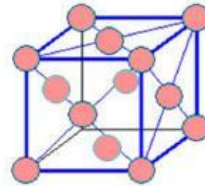
Cubic:  $a = b = c, \alpha = \beta = \gamma = 90^\circ$



Simple cubic

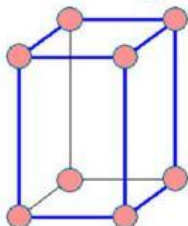


Body-centered cubic (BCC)

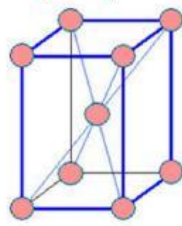


Face-centered cubic (FCC)

Tetragonal:  $a = b \neq c, \alpha = \beta = \gamma = 90^\circ$

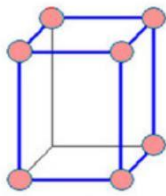


Simple Tetragonal

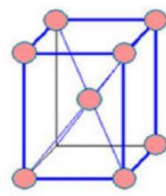


Body-centered Tetragonal (BCT)

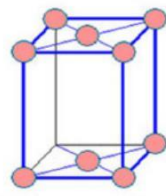
Orthorhombic:  $a \neq b \neq c, \alpha = \beta = \gamma = 90^\circ$



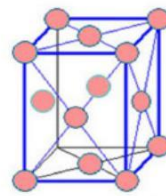
Simple



Body-centered

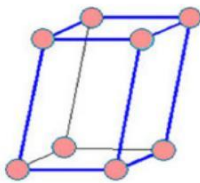


Base-centered

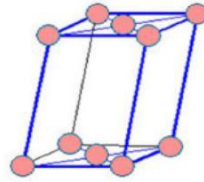


Face-centered

Monoclinic:  $a \neq b \neq c, \alpha = \gamma = 90^\circ \neq \beta$

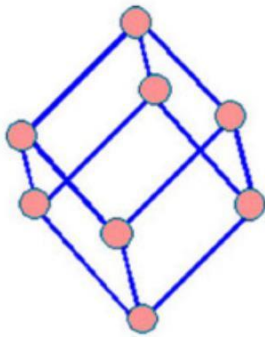


Simple monoclinic

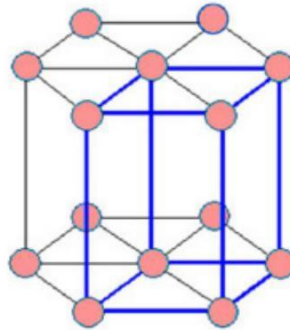


Base-centered monoclinic

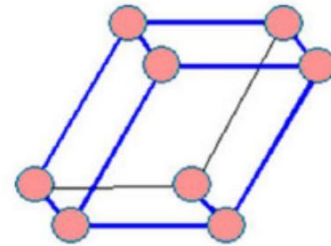
## Crystal Systems



Rhombic  
 $a = b = c$   
 $\alpha = \beta = \gamma \neq 90^\circ$



Hexagonal  
 $a = b \neq c$   
 $\alpha = \beta = 90^\circ \neq \gamma = 120^\circ$

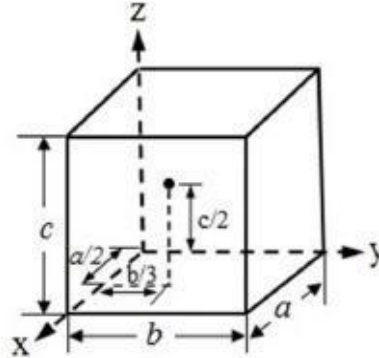


Triclinic  
 $a \neq b \neq c$   
 $\alpha \neq \beta \neq \gamma \neq 90^\circ$

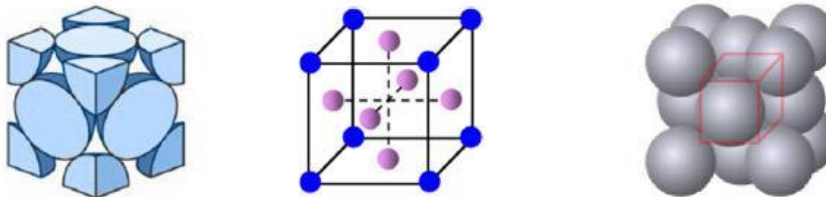
Crystal system	Example
Triclinic	$K_2S_2O_8, K_2Cr_2O_7$
Monoclinic	$As_4S_4, KNO_2, CaSO_4 \cdot 2H_2O, \beta-S$
Rhombic	$Hg, Sb, As, Bi, CaCO_3$
Hexagonal	$Zn, Co, Cd, Mg, Zr, NiAs$
Orthorhombic	$Ga, Fe_3C, \alpha-S$
Tetragonal	$In, TiO_2, \beta-Sn$
Cubic	$Au, Si, Al, Cu, Ag, Fe, NaCl$

### Point Coordinates

Position of any point in a unit cell is given by its coordinates or distances from the x, y and z axes in terms of the lattice vectors a, b and c. Thus the point located at  $a/2$  along x axis,  $b/3$  along y axis and  $c/2$  along z axis, as shown in the figure below, has the coordinates  $1/2 \ 1/3 \ 1/2$ .



**Coordination number** is the number of nearest neighbor to a particular atom in the crystal

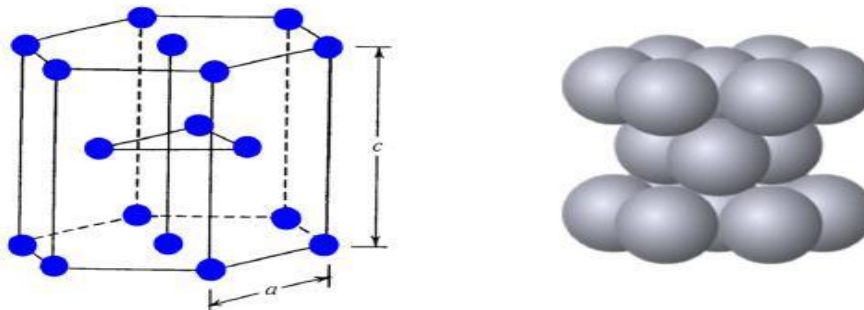


In the FCC lattice each atom is in contact with 12 neighbor atoms. FCC coordination number  $Z = 12$  Coordination number is the number of nearest neighbor to a particular atom in the crystal

For example, the face centered atom in the front face is in contact with four corner atoms and four other face-centered atoms behind it (two sides, top and bottom) and is also touching four face-centered atoms of the unit cell in front of it.

The coordination number of BCC crystal is 8. Coordination number the body centered atom is in contact with all the eight corner atoms. Each corner atom is shared by eight unit cells and hence, each of these atoms is in touch with eight body centered atoms.

**In Hexagonal lattice**  $Z = 12$ . The center atom of the top face is in touch with six corner atoms, three atoms of the mid layer and other three atoms of the mid layer of the unit cell above it.



**Atomic packing factor (APF) or packing efficiency** indicates how closely atoms are packed in a unit cell and is given by the ratio of volume of atoms in the unit cell and volume of the unit cell

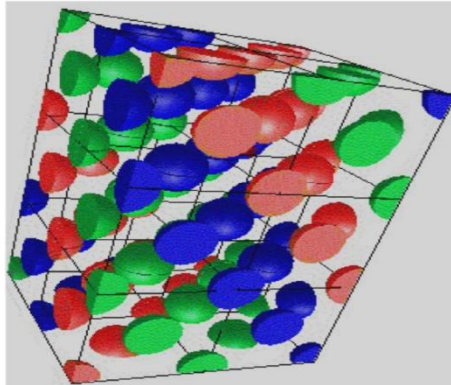
$$APF = \frac{\text{Volume of atoms}}{\text{Volume of unit cell}}$$

### Atomic packing factor

#### FCC lattice

In the FCC unit cell effective number of atoms = 8 corner atoms x (1/8) (each atom is shared by 8 unit cells) + 6 face centered atoms x 1/2 (each shared by two unit cells) = 4

The corner atom **C** is shared by unit cells 1, 2, 3, 4 and four more in front of each of them. The face-centered atom, **F** is shared between cells 1 and 2.



The corner atom **C** is shared by unit cells 1, 2, 3, 4 and four more in front of each of them. The face-centered atom, **F** is shared between cells 1 and 2.

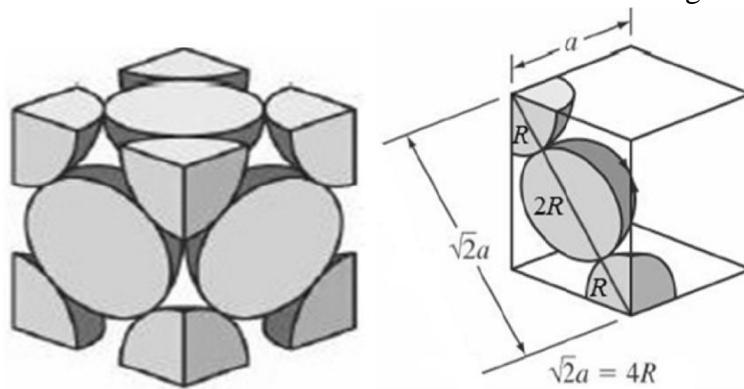
### Atomic packing factor

#### FCC lattice

Considering the atoms as hard spheres of radius  $R$

$$\text{Total volume of atoms} = 4 \times \frac{4}{3} \pi R^3$$

The relation between  $R$  and the FCC cell side  $a$  as shown in the figure below is  $\sqrt{2}a = 4R$



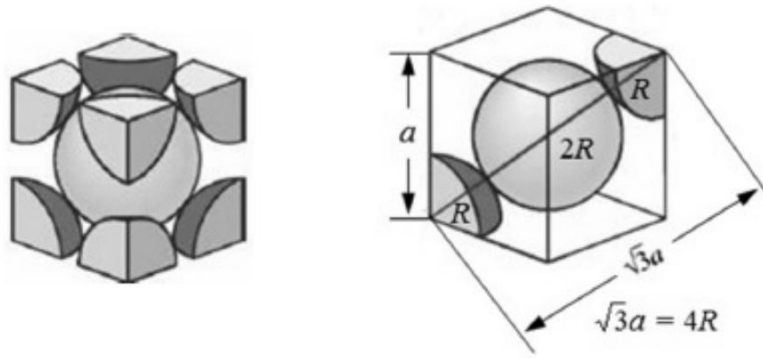
$$APF(FCC) = \frac{4 \times \frac{4}{3} \pi R^3}{a^3} = \frac{16 \times 2\sqrt{2} \pi a^3}{3 \times 64 a^3} = 0.74$$

#### BCC

For BCC crystals effective number of atoms per unit cell is  $8 \times 1/8 + 1 = 2$  and the relation between  $R$  and  $a$  is



$$\square 3a = 4R$$



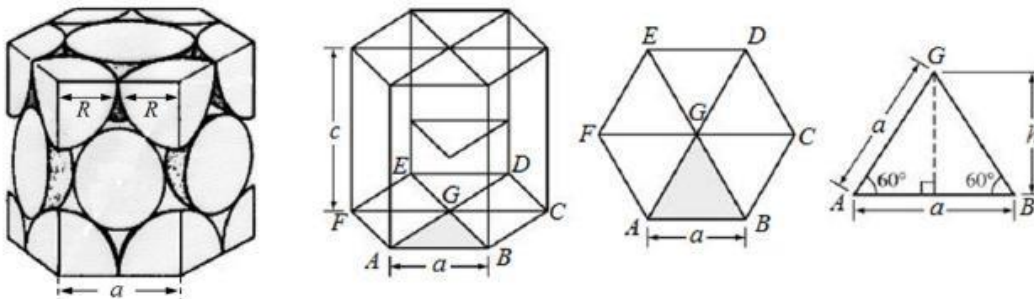
$$APF(BCC) = \frac{2 \times \frac{4}{3} \pi R^3}{a^3} = \frac{8 \times 3 \sqrt{3} \pi a^3}{3 \times 64 a^3} = 0.68$$

## Hexagonal lattice

In the Hexagonal unit cell, number of atoms = 12 corner atoms x 1/6 (shared by six unit cells) + Two face atoms x 1/2 + 3 interior = 6.

$$2R = a$$

Unit cell volume = (6 x 1/2 x a x h) x c = (3 x a x a sin60°) x c = 3a<sup>2</sup> c sin60°



## Types of lattice defects

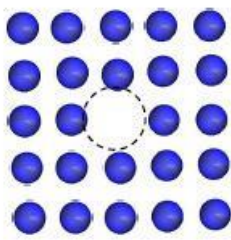
- Point defects
- Line defects
- Surface defects
- Volume defects

## Point defects

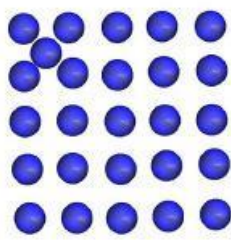
**Vacancy** – An atom missing from regular lattice position. Vacancies are present invariably in all materials.

**Interstitialcy** – An atom trapped in the interstitial point (a point intermediate between regular lattice points) is called an interstitialcy.

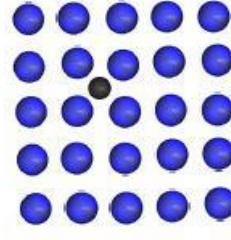
An impurity atom at the regular or interstitial position in the lattice is another type of point defect.



Vacancy



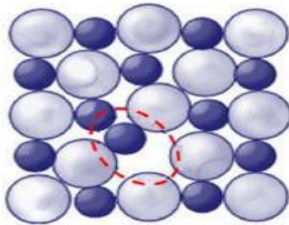
Interstitialcy



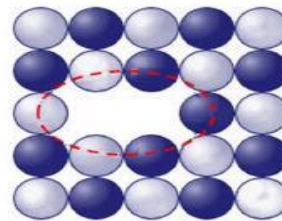
Impurity

### Point defects

In ceramic materials point defects occur in pair to maintain the electro neutrality. A cation-vacancy and a cation-interstitial pair is known as **Frenkel** defect. A cation vacancy-anion vacancy pair is known as a **Schottky** defect.



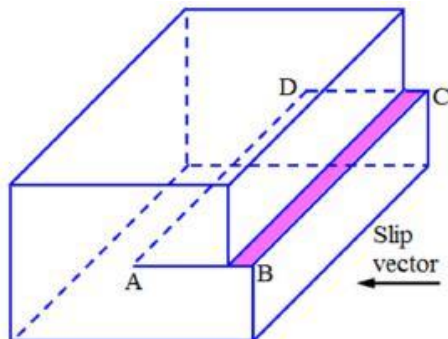
Frenkel defect



Schottky defect

### Line defects-Dislocations

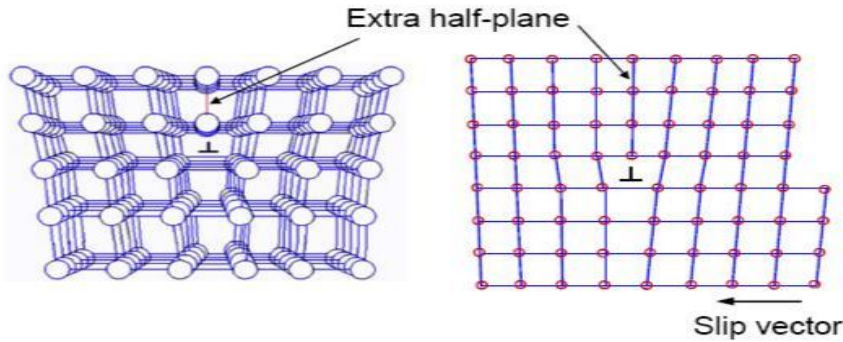
- Dislocation is the region of localized lattice distortion which separates the slipped and unslipped portion of the crystal.
- The upper region of the crystal over the slip plane has slipped relative to the bottom portion. The line (AD) between the slipped and unslipped portions is the dislocation.
- The magnitude and direction of slip produced by dislocation (pink shaded) is the Burger vector,  $b$ , of the dislocation.



### Edge Dislocations

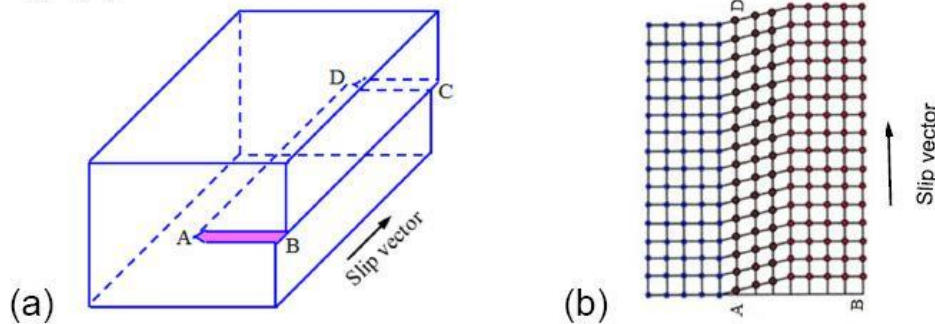
In one type of dislocations, the Burger vector is perpendicular to the dislocation line and the distortion produces an extra half-plane above the slip plane.





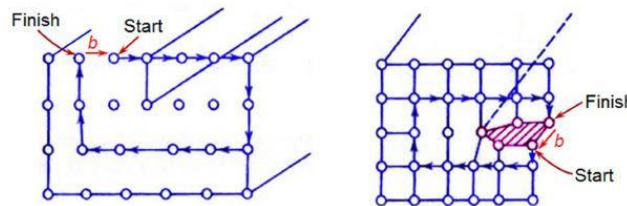
### Screw Dislocations

- The other type of dislocation is the screw dislocation where the Burger vector is parallel to the dislocation line (AD).
- The trace of the atomic planes around the screw dislocation makes a spiral or helical path (pink shade) like a screw and hence, the name.
- Atomic positions along a screw dislocation are represented in Fig. (b)



### Burger Circuit

The Burger vector can be found by the gap in the Burger circuit which is obtained by moving equal distances in each direction around the dislocation.



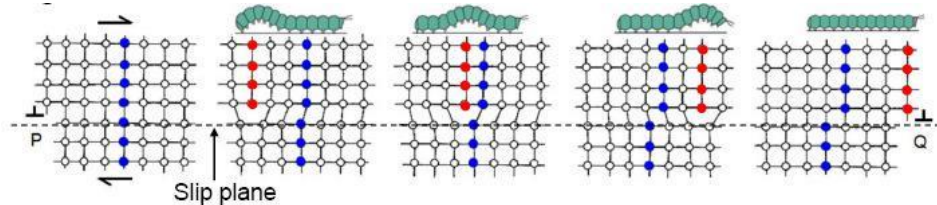
### Dislocation movement and deformation

- The theoretical shear stress to produce plastic deformation in metals,  $\tau = G/2$
- $G$ , the shear modulus for metals is in the range of  $= 20 - 150$  GPa yielding  $\tau = 3 - 30$  GPa
- However, actual measured values of  $\tau = 0.5 - 10$  MPa.
- This discrepancy can be explained by the presence of dislocations in the lattice.

### Dislocation movement

- Dislocations move in steps. The edge dislocation at P moves to Q in steps as depicted by the red (half-plane) and blue atoms. This movement is analogous to movement of a caterpillar.

- When the half-plane reaches a free surface it produces a slip step.
- Edge dislocations can move only on the slip plane while screw dislocations do not have a fixed glide plane.
- Since plastic deformation takes place by movement of dislocations, any hindrance to their motion will increase the strength of metals.
- Dislocations assist in plastic deformation since it is easier to move the atoms at the dislocations core.
- The movement of dislocations produces a slip step of one Burger vector or one interatomic distance.



### Observing dislocations

Dislocations appear as lines when observed under transmission electron microscope (TEM)



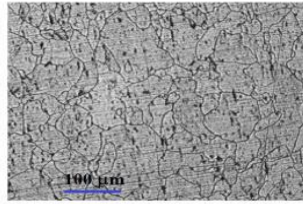
### Surface defects

- Most crystalline solids are an aggregate of several crystals. Such materials are called polycrystalline.
- Each crystal is known as a grain. The boundary between the grains is the grain boundary (the irregular lines in Fig.a)
- A grain boundary is a region of atomic disorder in the lattice only a few atomic diameter wide.
- The orientation of the crystals changes across the grain boundary as shown schematically in Fig. b.
- Grain boundaries act as obstacles to dislocation motion. Hence, presence of more grain boundaries (finer grain size) will increase the strength.

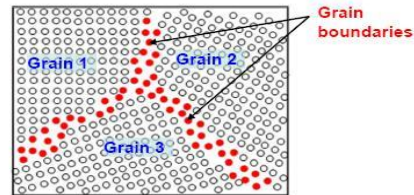
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## Grain boundaries



(a) Optical micrograph of a polycrystalline material



(b) Schematic of orientation change across the grain boundary

## Bulk or volume defects

- Porosity
- Inclusions
- Cracks

These defects form during manufacturing processes for various reasons and are harmful to the material.

### Bulk defects

- Casting blow holes, porosity – Gas entrapment during melting and pouring. Improper welding parameters/practice
- Shrinkage cavity due to improper risering
- Non-metallic inclusions – Slag, oxide particles or sand entrapment
- Cracks – Uneven heating/cooling, thermal mismatch, constrained expansion/contraction all leading to stress development

### Weld defect / Casting defect



Weld defect



Casting defect

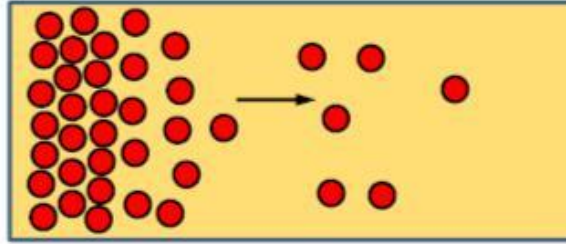


Shrinkage cavity

## Diffusion

### Diffusion Phenomena

- Diffusion is a process of mass transport by atomic movement under the influence of thermal energy and a concentration gradient.
- Atoms move from higher to lower concentration region.
- If this movement is from one element to another e.g. Cu to Ni, then it is termed *inter-diffusion*. If the movement is within similar atoms as in pure metals, it is termed *self-diffusion*.

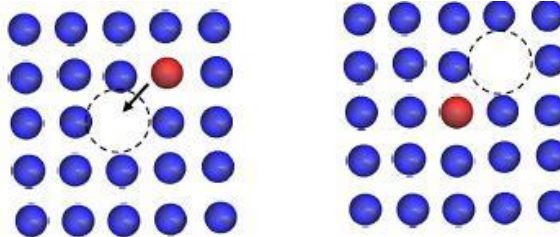


### Diffusion Mechanism

Diffusion of atoms involves movement in steps from one lattice site to the another. An empty adjacent site and breaking of bonds with the neighbor atoms are the two necessary conditions for this.

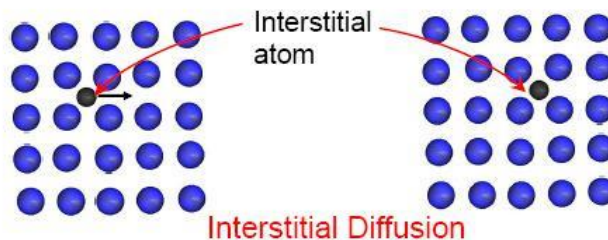
### Vacancy Diffusion

This mechanism involves movement of atoms from a regular lattice site to an adjacent vacancy. Since vacancy and atoms exchange position, the vacancy flux is in the opposite direction.



### Diffusion Mechanism-Interstitial Diffusion

- This mechanism involves migration of atoms from one interstitial site to a neighboring empty interstitial site.
- This mechanism is more prevalent for impurity atoms such as hydrogen, carbon, nitrogen, oxygen which are small enough to fit in to an interstitial position.
- For substitutional diffusion atoms exchange their places directly or along a ring (ring diffusion mechanism).



**Steady-state diffusion** is the situation when the diffusion flux is independent of time (e.g. diffusion of a gas through solid medium where concentration/pressure of the gas is kept constant at both the end).

**Fick's first law** Describes steady-state diffusion and is given by

$$J = -D \frac{dC}{dx}$$

Where,  $J$  is the diffusion flux or the mass transported per unit time per unit area and  $dC/dx$  is the concentration gradient.  $D$  is known as the diffusion coefficient.

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## **Fick's Second Law** Non- Steady state diffusion

In most practical situations, diffusion is non-steady state i.e. diffusion flux and concentration gradient varies with time. This is described by Fick's second law

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$

### **Factors affecting Diffusion**

#### **Diffusing species**

The magnitude of the diffusion coefficient,  $D$ , is an indication of the rate at which atoms diffuse. As the value of  $D$  is fixed for a given element in a given material, the extent of diffusion is first decided by the diffusing species itself.

#### **Temperature**

Temperature is a major factor which affects diffusion.

Temperature dependence of the diffusion coefficient is expressed as

$$D = D_0 \exp\left(-\frac{Q}{RT}\right)$$

Where,  $D_0$  is the pre-exponential factor and the  $Q$  is the activation energy for diffusion

### **Summary**

Atomic arrangements in crystalline solids can be described by a network of lines called a space lattice. In metals most common crystal structure unit cells are BCC, FCC, and HCP. Crystal imperfections are present in all real crystalline materials. Dislocations occur in metal crystals and are created during solidification process. Grain boundaries are surface imperfections in metals created by crystals of different orientation meeting each other during solidification. Atomic diffusion occurs in metallic solids mainly by vacancy or substitutional mechanism and interstitial mechanism. Fick's first law and second law states about the dependency of rate of diffusion on temperature, concentration.

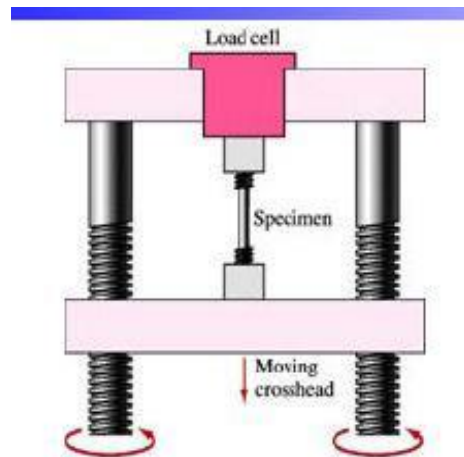
### **Self assessment questions**

1. Explain APF, coordination number, space lattice, unit cell, vacancy, interstitialcy, schottky defect, Frankel defect, lattice parameters.
2. Calculate the packing efficiency of a BCC structure.
3. Define diffusion. What are the factors affecting diffusion.
4. How do you distinguish between steady state and non-steady state diffusion?
5. Discuss the principle types of point defects found in crystals. Explain their significance.
6. Calculate atomic radius and packing factor for BCC structure.
7. State and explain the first Fick's law of diffusion.
8. Sketch the unit cell of HCP crystal structure. Calculate no of atoms per unit cell. Derive an expression for the density of atomic packing. Given  $C = 1.633a$ .
9. Calculate the packing efficiency of a FCC structure.
10. Discuss the role of dislocation in metals. Differentiate between screw and edge dislocations with sketches.
11. Explain point line and surface imperfections
12. Copper has a atomic radius of  $1.28 \times 10^{-8}$  cm, an FCC crystal structure and an atomic weight of 63.5. Calculate its density.
13. The unit cell of chromium is cubic and contains 2 atoms. Determine the dimensions of the chromium unit cell. [Given: atomic weight of Cr = 52 and density of Cr =  $7.19 \text{mgm}^{-3}$ ].

14. Copper has an FCC structure and an atomic and a n atomic radius of 0.1278mm. Calculate its density. Atomic weight of Cu = 63.54. avagadro number is =  $0.602 \times 10^{24}$
15. Calculate the diffusion rate of carbon in iron at  $700^{\circ}\text{C}$ . assuming the constants  $A = 4.9 \times 10^{-5} \text{ m}^2/\text{s}$  and  $E = 153.2\text{KJ/mol}$ .
16. Nickel has FCC structure with a lattice parameter of 0.352nm. What is the value of atomic radius in nanometers?
17. Iron has an atomic radius of 0.124nm, BCC structure and an atomic weight of 55.85g/mol. Calculate its density.



## Mechanical Behavior



### Introduction

Every engineering material is known by its set of properties. Testing of material is one of the important and essential steps for judging suitability for engineering applications. A variety of tests are conducted in the laboratory to evaluate and compare the mechanical properties of different materials. Following are some of the destructive tests which are carried out to evaluate mechanical properties.

- Hardness test
- Tensile test
- Compression test
- Flexural test
- Impact test

### Mechanical Properties of Metals

Mechanical Properties refers to the behavior of material when external forces are applied,

Stress and strain  $\longrightarrow$  fracture

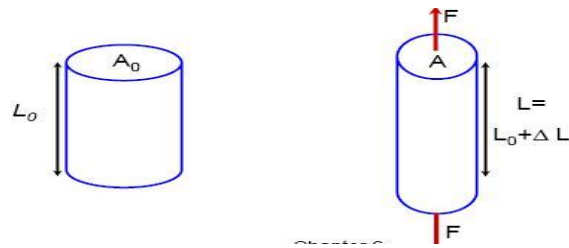
For **engineering point of view**: allows predicting the ability of a component or a structure to withstand the forces applied to it

For **science** point of view: what makes materials strong  $\rightarrow$  helps us to design a better new one

### Elastic and Plastic Deformation

- Metal piece is subjected to a uniaxial force leading to deformation
- When force is removed: - metal returns to its original dimensions  $\longrightarrow$  **elastic** deformation (atoms return to their original position)

Metal deformed to an extent that it cannot fully recover its original dimensions leads to **plastic** deformation (shape of the material changes, atoms are *permanently displaced* from their positions)



## Concept of Stress and Strain

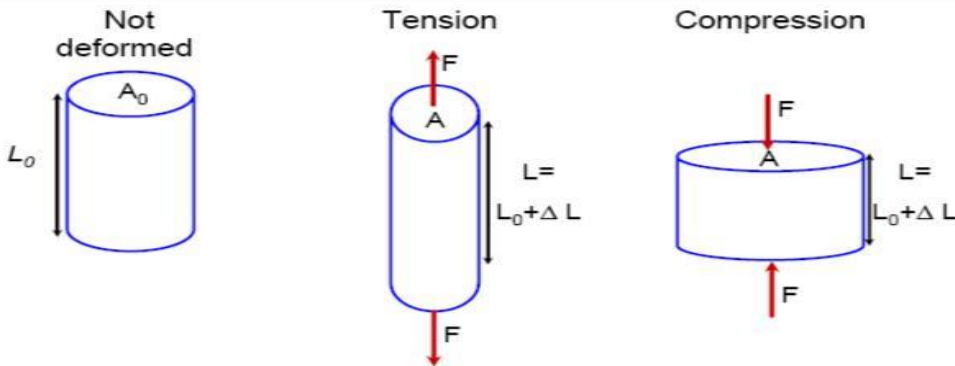
Load can be applied to the material by applying axial forces:

### Stress ( $\sigma$ )

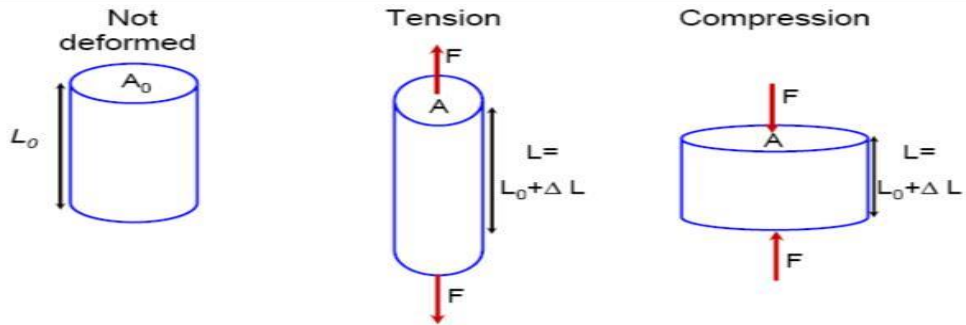
- defining  $F$  is not enough ( $F$  and  $A$  can vary)
- Stress  $\sigma$  stays constant

$$\sigma = \frac{F}{A}$$

Force / area = N / m<sup>2</sup> = Pa usually in MPa or GPa



$\Delta L$  can be measured as a function of the applied force; area  $A_0$  changes in response

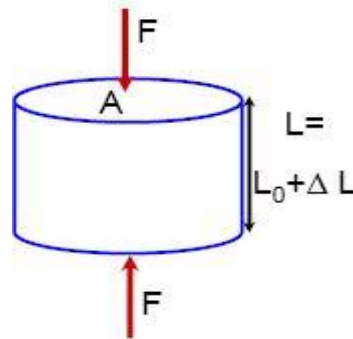


$\Delta L$  can be measured as a function of the applied force; area  $A_0$  changes in response

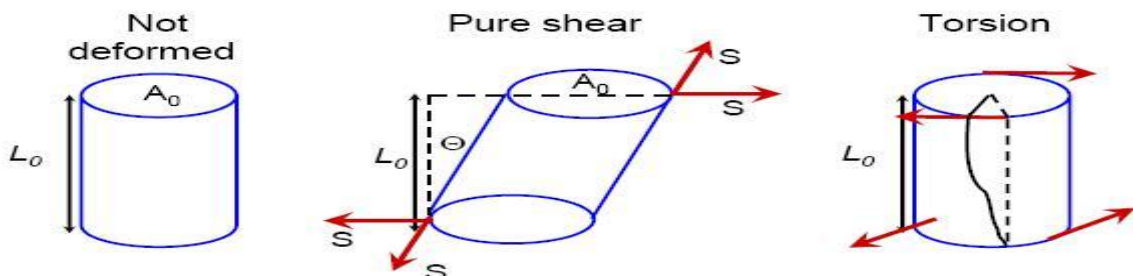
**Strain ( $\epsilon$ )** – result of stress

For tension and compression: change in length of a sample divided by the **original** length of sample  $L/L_0$

Block of metal



**Shear and Torsion (similar to shear)**



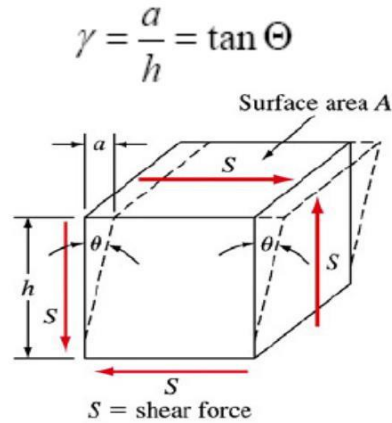
- Note: the forces are applied in this way, so that there is no net torque
  - If the forces are applied **along** the faces of the material, they are called **shear forces**
- Shear Stress and Shear Strain**

If the shear force  $S$  acts over an area  $A$ , the shear stress

$$\tau(\text{shear\_stress}) = \frac{S(\text{shear\_force})}{A(\text{area})}$$

$A$  area,  $S$  shear force

The shear strain  $\gamma$  is defined in terms of the amount of the shear displacement  $a$  divided by distance over which the shear acts:



### Elastic Properties of Materials

Most materials will get narrow when stretched and thicken when compressed

- This behaviour is qualified by Poisson's ratio, which is defined as the ratio of **lateral** and **axial** strain

$$\text{Poisson's Ratio : } \nu = -\frac{\epsilon_x}{\epsilon_z} = -\frac{\epsilon_y}{\epsilon_z}$$

- the minus sign is there because usually if  $\epsilon_z > 0$ , and  $\epsilon_x + \epsilon_y < 0 \Rightarrow \nu > 0$
- It can be proven that we must have  $\nu \leq \frac{1}{2}$ ;  $\nu = \frac{1}{2}$  is the case when there is no volume change

$$(l_x + \Delta l_x)(l_y + \Delta l_y)(l_z + \Delta l_z) = l_x \times l_y \times l_z$$

### Modulus of elasticity or Young's Modulus

- Stress and strain are properties that don't depend on the dimensions of the material (for small  $\epsilon$ ), just type of the material

$$E = \frac{\sigma(\text{stress})}{\epsilon(\text{strain})}$$

- $E$  – Young's Modulus, Pa Comes from the linear range in the stress-strain diagram

Behavior is related to **atomic bonding between the atoms**

Hydrogels and live cells <0.00001

Rubber 0.01

Polypropylene 1.5-2

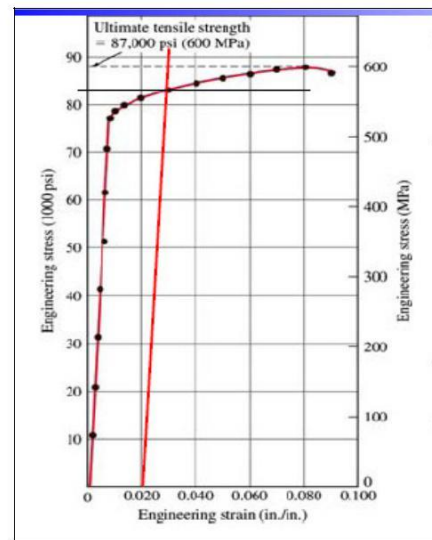
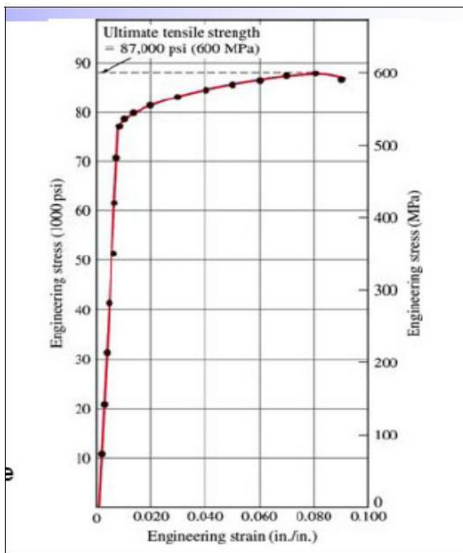
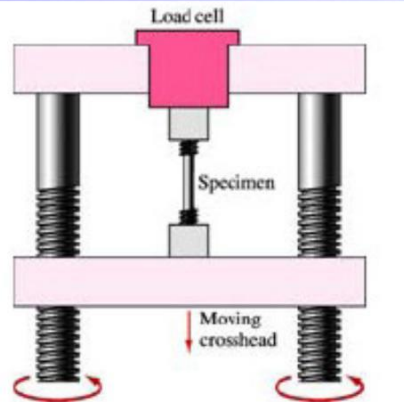
Metals 20-100

Material Young's Modulus [GPa]

Material	Young's Modulus [GPa]
Metals	20-100
Polypropylene	1.5-2
Rubber	0.01
Hydrogels and live cells	<0.00001

**Tensile Test** by conducting tensile test, the following can be evaluated.

1. Modulus of elasticity
2. Yield strength at 0.2% offset
3. Ultimate tensile strength
4. Percent elongation at fracture
5. Percent reduction in area at fracture



**Yield strength (at 0.2% offset)**

**Ultimate Tensile Strength (UTS):** the maximum strength reached in the stress strain curve

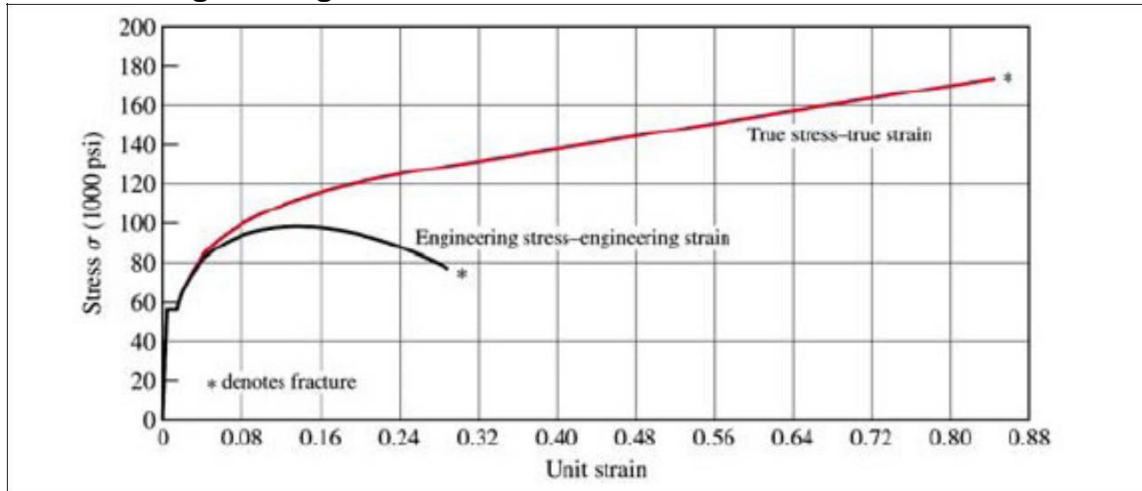
- Percent elongation at fracture (measure of **ductility** of the metal)
- Percent reduction in area at fracture

$$\sigma = \frac{F}{A(\text{original})} = E \times \frac{\Delta L}{L}$$



$$\% \text{ reduction in area} = \frac{A_{initial} - A_{final}}{A_{initial}} \times 100\%$$

### True and Engineering Stress



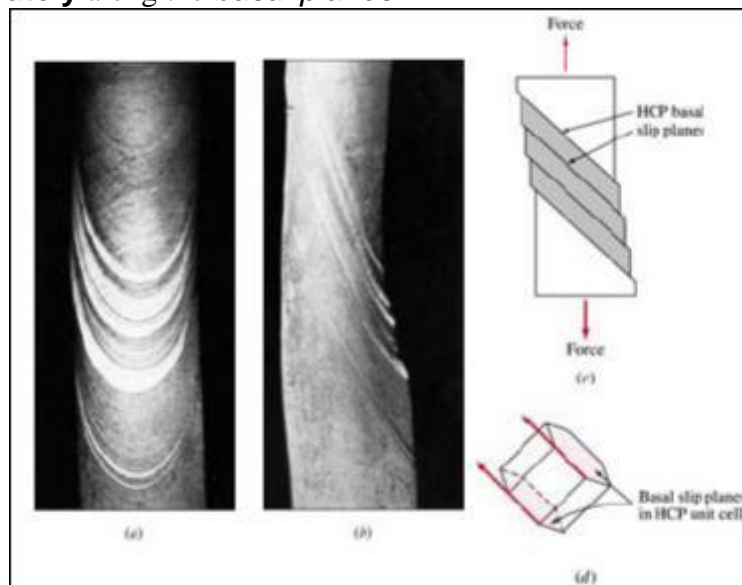
$$\sigma_{engineering} = \frac{F}{A_{initial}} = E \times \frac{\Delta L}{L}$$

$$\sigma_{true} = \frac{F}{A_{instant}}$$

### Plastic deformations of single crystal metals

A rod of a single crystal **Zn (hcp)** stressed beyond its elastic limit:

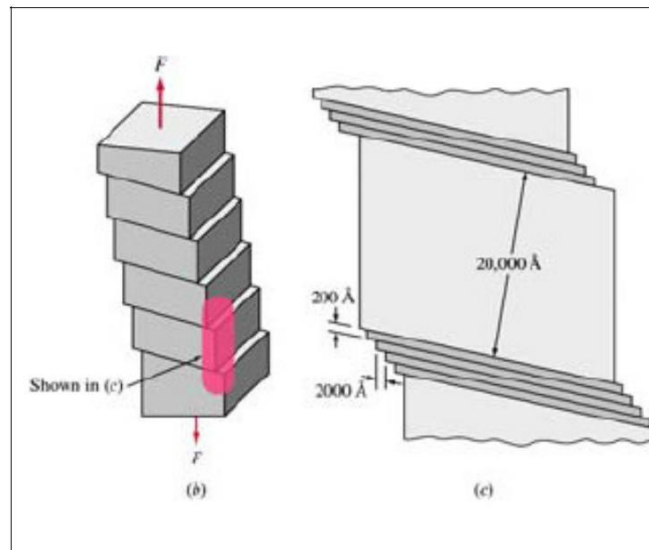
- Slip bands: slip of metal atoms on specific crystallographic planes (*slip planes*)
- Slip is **predominately** along the *basal planes*



A rod of a single crystal **Cu (fcc)** during plastic deformation:

- slip lines: 50-500 atoms apart
- slipbands: separated by  $\sim >10,000$  atomic planes





Other mechanical characteristics

**Ductility:** amount of plastic deformation that occurs before fracture. if ductility is high, the material can be deformed by applying stresses.

Ex.: gold

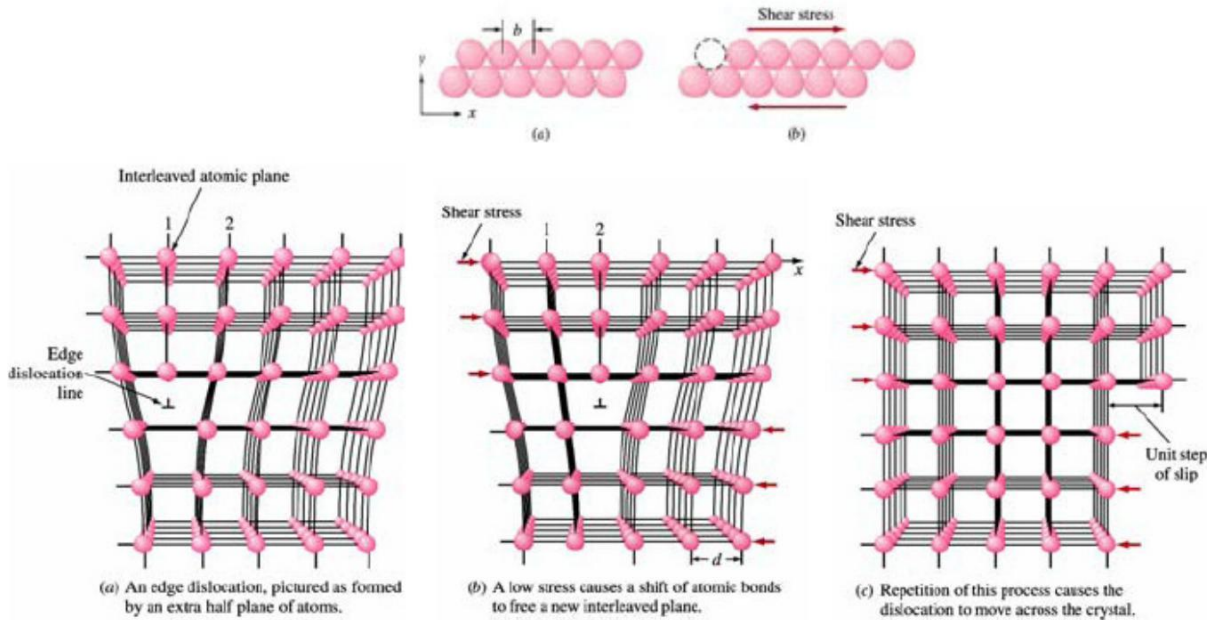
- if it is low, material breaks first, without significant deformation (material is brittle). depend on T: at low T many metals become brittle and can break as a glass

• **Resilience:** ability to have high yield strength and low E. Ex.: good springs

• **Toughness:** ability to absorb energy up to a fracture

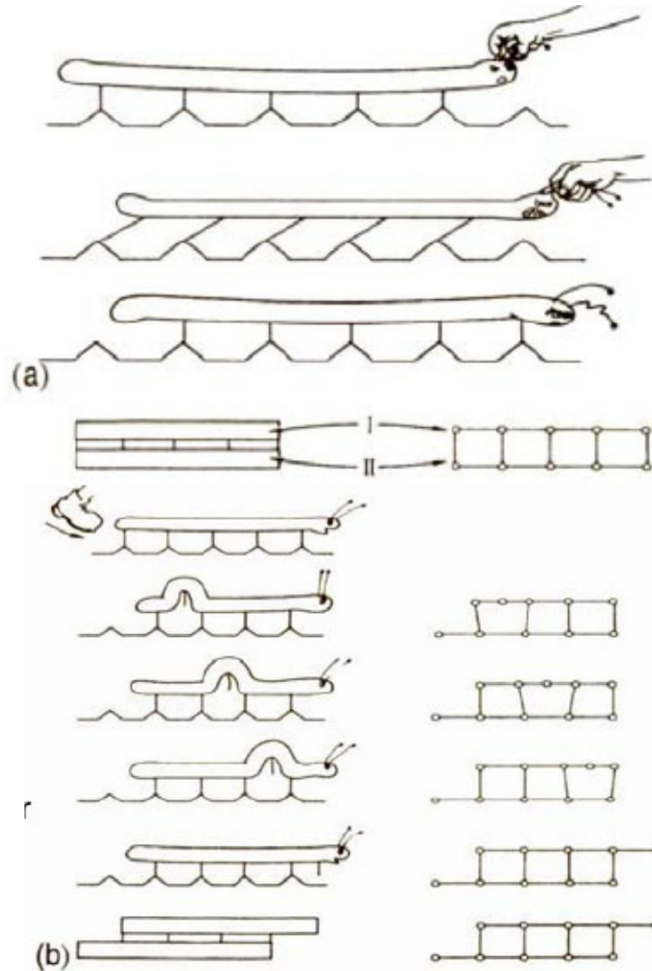
**Mechanism of Slip deformation**

The group of atoms do NOT slide over each other during plastic shear deformation. The process requires too much energy



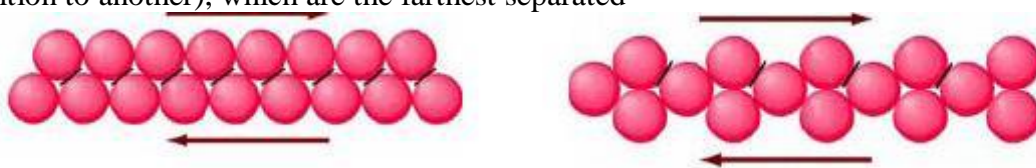
The process takes less energy!!!

**Motion of Dislocations** In the metal slip mechanism, dislocations move through the metal crystals like wave fronts, allowing metallic atoms to slide over each other under **low shear stress** deformation without fracture.



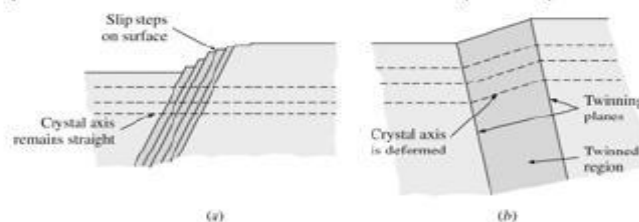
**Slip Systems**

Typically slip planes are the most densely packed planes (less energy is required to move from one position to another), which are the farthest separated



**Mechanical Twinning**

Another important plastic deformation mechanism (low T)



Schematic diagram of surfaces of a deformed metal after (a) slip and (b) twinning

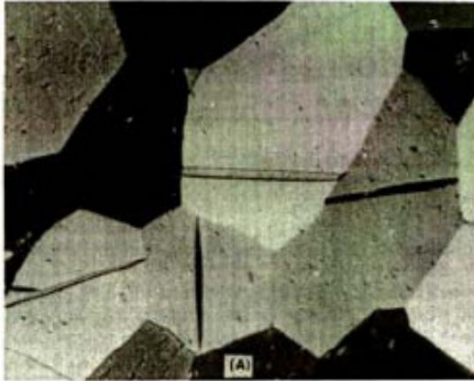
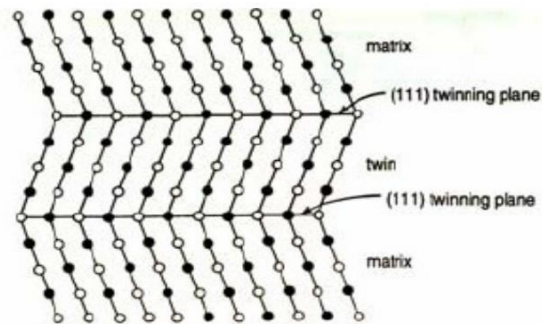


Fig. 6.22. Deformation twins in zirconium.

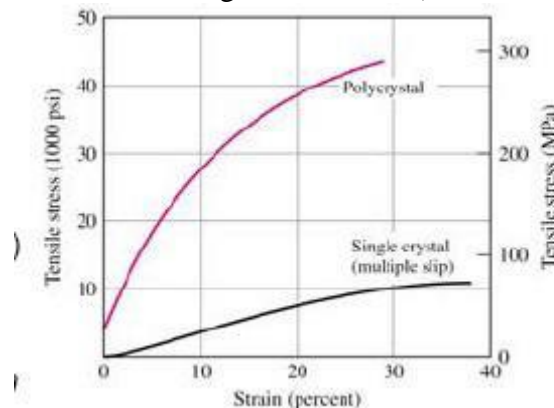


z. 6.23. Atomic configuration in matrix and twin of a fcc lattice.

## Plastic Deformations in Polycrystalline Metals

Majority of engineering alloys and metals are **polycrystalline**

- Grain boundaries – act as diffusion barriers for dislocation movements
- In practice: fine grain materials are stronger and harder (but less resistant to creep and corrosion)



## Summary

When a uniaxial stress is applied to a long metal bar, the metal deforms elastically at first and then plastically, causing permanent deformation. For many engineering designs the engineer is interested in the 0.2 percent offset yield strength, ultimate tensile strength, and elongation of a metal or alloy. These quantities are obtained from the engineering stress-strain diagram originating from a tensile test. The hardness of the material is also of engineering importance.

Plastic deformation in metals takes place by the slip process, involving dislocations. Grain boundaries at lower temperatures usually strengthen metals by providing barriers to dislocation movement.

## Self assessment questions

1. Explain in detail the mechanical properties in elastic and plastic region.
2. Discuss how the slip mechanism differs in case of a poly crystal to the single crystal
3. Distinguish between slip and twinning
4. With the help of a schematic diagram explain stress-strain for mild steel under tension; explain clearly the behaviour of material till fracture.
5. Explain non linear elastic properties when a material is subjected to static tension.
6. What is work hardening? Explain the reasons for the same
7. Draw stress strain diagram for a ductile material and explain the salient points. Also explain elastic modulus, ductility and toughness.

8. Differentiate between 1) toughness and resilience 2) Ductility and brittleness
9. Draw the stress strain diagram for 1, mild steel 2. Copper 3.cast iron 4. Rubber.
10. A cylindrical specimen of medium carbon steel, having an original diameter of 20mm when subjected to a tension test has fracture strength of 450Mpa. If its final diameter at fracture is 12mm, calculate the engineering stress, engineering strain and true stress.
11. A steel bar 100mm long and of square section 20mmX20mm is pulled in tension with a load of 89000N and experiences a elongation of 0.1mm. Assuming the elongation to be entirely elastic, calculate the elastic modulus of the steel.
12. A copper wire has a nominal breaking strength of 300Mpa. Its ductility is 77% reduction of area. Calculate the true stress for failure.

## FRACTURE



### OBJECTIVES:

- To learn and understand the concepts of
- Fracture and types such as ductile and brittle fracture
- Creep, propagation of creep, creep properties
- Fatigue and its type, evaluation of fatigue parameters, factors affecting fatigue strength of a material and fatigue testing.

### OUT COMES

The student should be able to understand failure of materials by different types of loads in real world.

## Introduction

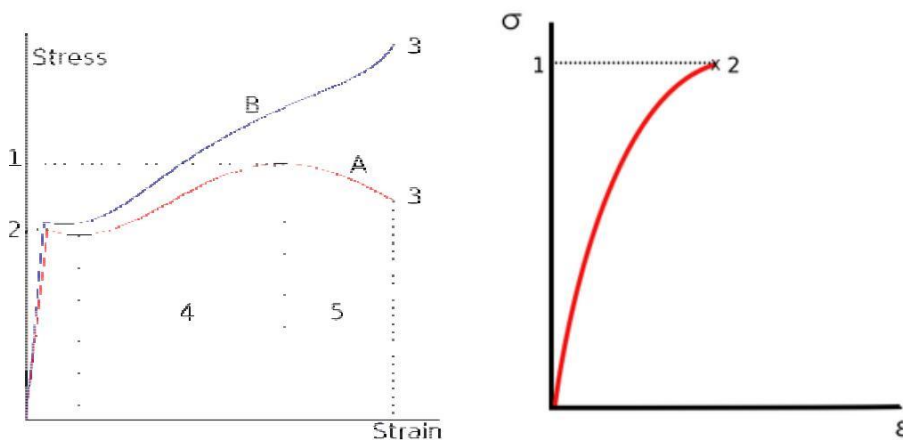
One of the important and practical aspects of material selection in the design, development and production of new components is the possibility of failure of the component under normal operation. Failure may be defined as the inability of a material to perform the intended function, meet performance criteria although it may be still operational or perform safely and reliably even after deterioration. Every engineer should be completely aware of the concept of fracture and failure of materials. Fracture is a separation of a solid body in to two or more parts under the action of load.

### Types of Fracture

**Ductile materials**, which includes structural steel, as well as many alloys of other metals, are characterized by their ability to yield at normal temperatures. Low carbon generally exhibits a very linear stress–strain relationship up to a well defined yield point (*Fig.2*). The linear portion of the curve is the elastic region and the slope is the modulus of elasticity or Young's Modulus. After the yield point, the curve typically decreases slightly because of dislocations escaping from Cottrell atmospheres. As deformation continues, the stress increases on account of strain hardening until it reaches the ultimate strength. Until this point, the cross-sectional area decreases uniformly and randomly because of Poisson contractions. The actual rupture point is in the same vertical line as the visual rupture point.

However, beyond this point a *neck* forms where the local cross-sectional area decreases more quickly than the rest of the sample resulting in an increase in the true stress. As shown in Fig.2. On an engineering stress–strain curve this is seen as a decrease in the *apparent*

*stress*. However if the curve is plotted in terms of *true stress* and *true strain* the stress will continue to rise until failure. Eventually the neck becomes unstable and the specimen ruptures (fractures).



### Stress strain curves for ductile and brittle materials

Less ductile materials such as medium to high carbon steels do not have a well-defined yield point. There are generally two types of yield points, upper and lower yield point. For these materials the yield strength is typically determined by the "offset yield method", by which a line is drawn parallel to the linear elastic portion of the curve and intersecting the abscissa at some



arbitrary value (generally from 0.1% to 0.2%). The intersection of this line and the stress–strain curve is reported as the yield point. The elastic region is the portion of the curve where the material will return to its original shape if the load is removed. The plastic region is the portion where some permanent deformation will occur, even if the load is removed. Failure point is when the object ruptures.

**Brittle materials**, which include cast iron, glass, and stone, are characterized by the fact that rupture occurs without any noticeable prior change in the rate of elongation.

Brittle materials such as concrete or carbon fiber do not have a yield point, and do not strain-harden. Therefore the ultimate strength and breaking strength are the same. A typical stress-strain curve is shown in *Fig.3*. Typical brittle materials like glass do not show any plastic deformation but fail while the deformation is elastic. One of the characteristics of a brittle failure is that the two broken parts can be reassembled to produce the same shape as the original component as there will not be a neck formation like in the case of ductile materials. A typical stress strain curve for a brittle material will be linear. Testing of several identical specimen, cast iron, or soil, tensile strength is negligible compared to the compressive strength and it is assumed zero for many engineering applications. Glass fibers have a tensile strength stronger than steel, but bulk glass usually does not. This is because of the stress intensity factor associated with defects in the material. As the size of the sample gets larger, the size of defects also grows. In general, the tensile strength of a rope is always less than the sum of the tensile strengths of its individual fibers.

A **fracture** is the separation of an object or material into two, or more, pieces under the action of stress. The fracture of a solid almost always occurs due to the development of certain displacement discontinuity surfaces within the solid. If a displacement develops in this case perpendicular to the surface of displacement, it is called a normal tensile crack or simply a crack; if a displacement develops tangentially to the surface of displacement, it is called a shear crack, slip band, or dislocation.

**Fracture strength**, also known as **breaking strength**, is the stress at which a specimen fails via fracture. This is usually determined for a given specimen by a tensile test, which charts the stress-strain curve (see image). The final recorded point is the fracture strength.

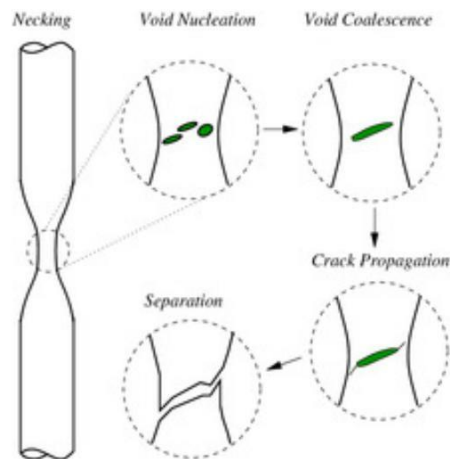
Ductile materials have fracture strength lower than the ultimate tensile strength (UTS), whereas in brittle materials the fracture strength is equivalent to the UTS. If a ductile material reaches its ultimate tensile strength in a load-controlled situation, it will continue to deform, with no additional load application, until it ruptures. However, if the loading is displacement-controlled,<sup>[Note 2]</sup> the deformation of the material may relieve the load, preventing rupture.

Brittle fracture, no apparent plastic deformation takes place before fracture. In brittle crystalline materials, fracture can occur by *cleavage* as the result of tensile stress acting normal to crystallographic planes with low bonding (cleavage planes). In amorphous solids, by contrast, the lack of a crystalline structure results in a conchoidal fracture, with cracks proceeding normal to the applied tension.



1 Brittle fracture in [glass](#) 2. Fracture of an aluminum crank arm. Bright: brittle fracture. Dark: fatigue fracture

Ductile fracture



1 Ductile failure of a specimen strained axially. 2 Schematic representation of the steps in ductile fracture (in pure tension).

In ductile fracture, extensive plastic deformation (necking) takes place before fracture. The terms rupture or ductile rupture describes the ultimate failure of tough ductile materials loaded in tension. Rather than cracking, the material "pulls apart," generally leaving a rough surface. In this case there is slow propagation and absorption of large amount energy before fracture. Many ductile metals, especially materials with high purity, can sustain very large deformation of 50–100% or more strain before fracture under favorable loading condition and environmental condition. The strain at which the fracture happens is controlled by the purity of the materials. At room temperature, pure iron can undergo deformation up to 100% strain before breaking, while cast iron or high-carbon steels can barely sustain 3% of strain. Because ductile rupture involves a high degree of plastic deformation, the fracture behavior of a propagating crack as modeled above changes fundamentally. Some of the energy from stress concentrations at the crack tips is dissipated by plastic deformation before the crack actually propagates. The basic steps are: void formation, void coalescence (also known as crack formation), crack propagation, and failure, often resulting in a cup-and-cone shaped failure surface.

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## Crack separation modes

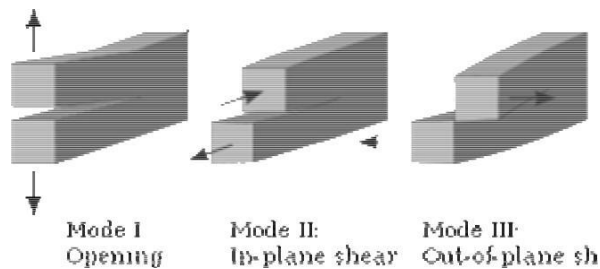
There are three ways of applying a force to enable a crack to propagate:

**Mode I crack** – Opening mode (a tensile stress normal to the plane of the crack)

**Mode II cracks** – Sliding mode (a shear stress acting parallel to the plane of the crack and perpendicular to the crack front)

**Mode III crack** – Tearing mode (a shear stress acting parallel to the plane of the crack and parallel to the crack front)

Crack initiation and propagation accompany fracture. The manner through which the crack propagates through the material gives great insight into the mode of fracture. In ductile materials (ductile fracture), the crack moves slowly and is accompanied by a large amount of plastic deformation. The crack will usually not extend unless an increased stress is applied. On the other hand, in dealing with brittle fracture, cracks spread very rapidly with little or no plastic deformation. The cracks that propagate in a brittle material will continue to grow and increase in magnitude once they are initiated. Another important mannerism of crack propagation is the way in which the advancing crack travels through the material. A crack that passes through the grains within the material is undergoing transgranular fracture. However, a crack that propagates along the grain boundaries is termed an intergranular fracture.



## Creep

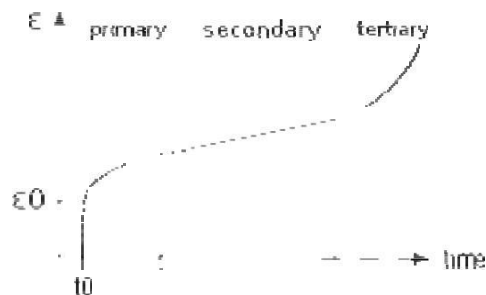
In materials science, **creep** (sometimes called **cold flow**) is the tendency of a solid material to move slowly or deform permanently under the influence of mechanical stresses. It can occur as a result of long-term exposure to high levels of stress that are still below the yield strength of the material. Creep is more severe in materials that are subjected to heat for long periods, and generally increases as they near their melting point.

The rate of deformation is a function of the material properties, exposure time, exposure temperature and the applied structural load. Depending on the magnitude of the applied stress and its duration, the deformation may become so large that a component can no longer perform its function — for example creep of a turbine blade will cause the blade to contact the casing, resulting in the failure of the blade. Creep is usually of concern to engineers and metallurgists when evaluating components that operate under high stresses or high temperatures. Creep is a deformation mechanism that may or may not constitute a failure mode. For example, moderate creep in concrete is sometimes welcomed because it relieves tensile stresses that might otherwise lead to cracking.

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Unlike brittle fracture, creep deformation does not occur suddenly upon the application of stress. Instead, strain accumulates as a result of long-term stress. Therefore, creep is a "time-dependent" deformation.

The temperature range in which creep deformation may occur differs in various materials. For example, tungsten requires a temperature in the thousands of degrees before creep deformation can occur, while ice will creep at temperatures near 0 °C (32 °F).<sup>[1]</sup> As a general guideline, the effects of creep deformation generally become noticeable at approximately 30% of the melting point (as measured on a thermodynamic temperature scale such as kelvin or rankine) for metals, and at 40–50% of melting point for ceramics. Virtually any material will creep upon approaching its melting temperature. Since the creep minimum temperature is related to the melting point, creep can be seen at relatively low temperatures for some materials. Plastics and low-melting-temperature metals, including many solders, can begin to creep at room temperature, as can be seen markedly in old lead hot-water pipes. Glacier flow is an example of creep processes in ice.



In the initial stage, or primary creep, the strain rate is relatively high, but slows with increasing time. This is due to work hardening. The strain rate eventually reaches a minimum and becomes near constant. This is due to the balance between work hardening and annealing (thermal softening). This stage is known as secondary or steady-state creep. This stage is the most understood. The characterized "creep strain rate" typically refers to the rate in this secondary stage. Stress dependence of this rate depends on the creep mechanism. In tertiary creep, the strain rate exponentially increases with stress because of necking phenomena.

### Mechanisms of creep

The mechanism of creep depends on temperature and stress. Various mechanisms are:

- Bulk diffusion (Nabarro-Herring creep)
- Climb — here the strain is actually accomplished by climb
- Climb-assisted glide — here the climb is an *enabling* mechanism, allowing dislocations to get around obstacles
- Grain boundary diffusion (Coble creep)
- Thermally activated glide — e.g., via cross-slip

### Fatigue

**Fatigue** is the weakening of a material caused by repeatedly applied loads. It is the progressive and localized structural damage that occurs when a material is subjected to cyclic loading. The nominal maximum stress values that cause such damage may be much less than the strength of the material typically quoted as the ultimate tensile stress limit, or the yield stress limit.

Fatigue occurs when a material is subjected to repeat loading and unloading. If the loads are above a certain threshold, microscopic cracks will begin to form at the stress concentrators such as the surface, persistent slip bands (PSBs), and grain interfaces. Eventually a crack will reach a critical size, the crack will propagate suddenly, and the structure will fracture. The shape of the structure will significantly affect the fatigue life; square holes or sharp corners will lead to elevated local stresses where fatigue cracks can initiate. Round holes and smooth transitions or fillets will therefore increase the fatigue strength of the structure.

### Characteristics of fatigue

- In metal alloys, when there are no macroscopic or microscopic discontinuities, the process starts with dislocation movements, which eventually form persistent slip bands that become the nucleus of short cracks.
- Macroscopic and microscopic discontinuities as well as component design features which cause stress concentrations (holes, keyways, sharp changes of direction etc.) are common locations at which the fatigue process begins.
- Fatigue is a process that has a degree of randomness (stochastic), often showing considerable scatter even in well controlled environments.
- Fatigue is usually associated with tensile stresses but fatigue cracks have been reported due to compressive loads.<sup>[7]</sup>
- The greater the applied stress range, the shorter the life.
- Fatigue life scatter tends to increase for longer fatigue lives.
- Damage is cumulative. Materials do not recover when rested.
- Fatigue life is influenced by a variety of factors, such as temperature, surface finish, metallurgical microstructure, presence of oxidizing or inert chemicals, residual stresses, scuffing contact (fretting), etc.
- Some materials (e.g., some steel and titanium alloys) exhibit a theoretical fatigue limit below which continued loading does not lead to fatigue failure.
- In recent years, researchers have found that failures can occur below the theoretical fatigue limit at very high fatigue lives ( $10^9$  to  $10^{10}$  cycles). An ultrasonic resonance technique is used in these experiments with frequencies around 10–20 kHz.
- High cycle fatigue strength (about  $10^4$  to  $10^8$  cycles) can be described by stress-based parameters. A load-controlled servo-hydraulic test rig is commonly used in these tests, with frequencies of around 20–50 Hz. Other sorts of machines—like resonant magnetic machines—can also be used, to achieve frequencies up to 250 Hz.
- Low cycle fatigue (loading that typically causes failure in less than  $10^4$  cycles) is associated with localized plastic behavior in metals; thus, a strain-based parameter should be used for fatigue life prediction in metals. Testing is conducted with constant strain amplitudes typically at 0.01–5 Hz.

### Factors that affect fatigue-life

**Cyclic stress state:** Depending on the complexity of the geometry and the loading, one or more properties of the stress state need to be considered, such as stress amplitude, mean stress, biaxiality, in-phase or out-of-phase shear stress, and load sequence,

**Geometry:** Notches and variation in cross section throughout a part lead to stress concentrations where fatigue cracks initiate.

**Surface quality:** Surface roughness can cause microscopic stress concentrations that lower the fatigue strength. Compressive residual stresses can be introduced in the surface by e.g. shot peening to increase fatigue life. Such techniques for producing surface stress are often referred to as *peening*, whatever the mechanism used to produce the stress. Low plasticity burnishing, laser peening, and ultrasonic impact treatment can also produce this surface compressive stress and can increase the fatigue life of the component. This improvement is normally observed only for high-cycle fatigue.

**Material Type:** Fatigue life, as well as the behavior during cyclic loading, varies widely for different materials, e.g. composites and polymers differ markedly from metals.

**Residual stresses:** Welding, cutting, casting, grinding, and other manufacturing processes involving heat or deformation can produce high levels of tensile residual stress, which decreases the fatigue strength.

**Size and distribution of internal defects:** Casting defects such as gas porosity voids, non-metallic inclusions and shrinkage voids can significantly reduce fatigue strength.

**Air or Vacuum:** Certain materials like Metals are more prone to fatigue in air than in a vacuum. Depending upon the level of humidity and temperature, the lifetime for metals such as aluminum or iron might be as much as 5 to 10 times greater in a vacuum. This is mostly due to the effect of the oxygen and water vapour in the air which will aggressively attack the material and so encourage the propagation of cracks. Other environments such as oil or seawater may reduce the fatigue life at an even greater rate.

**Direction of loading:** For non-isotropic materials, fatigue strength depends on the direction of the principal stress.

**Grain size:** For most metals, smaller grains yield longer fatigue lives, however, the presence of surface defects or scratches will have a greater influence than in a coarse grained alloy.

**Environment:** Environmental conditions can cause erosion, corrosion, or gas-phase embrittlement, which all affect fatigue life. Corrosion fatigue is a problem encountered in many aggressive environments.

**Temperature:** Extreme high or low temperatures can decrease fatigue strength.

**Crack Closure:** Crack closure is a phenomenon in fatigue loading, during which the crack will tend to remain in a closed position even though some external tensile force is acting on the material. During this process the crack will open only at a nominal stress above a particular crack opening stress. This is due to several factors such as plastic deformation or phase transformation during crack propagation, corrosion of crack surfaces, presence of fluids in the crack, or

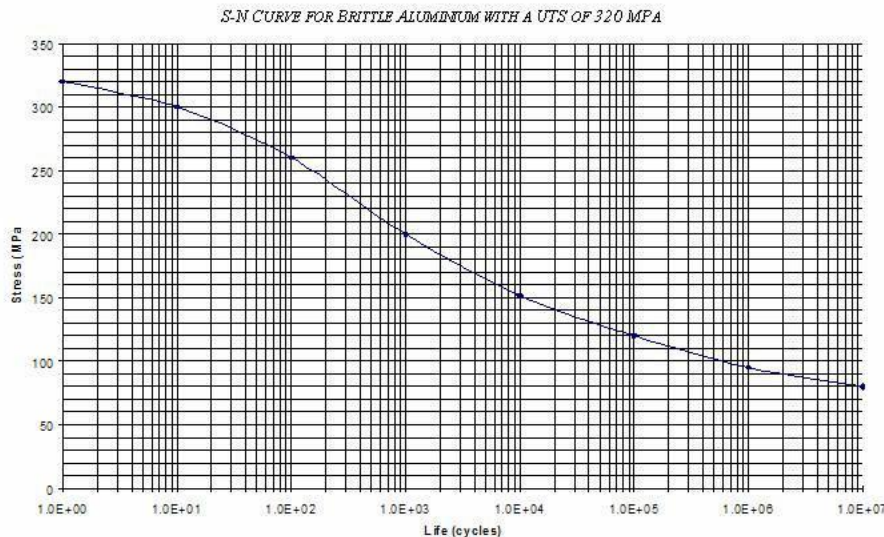


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roughness at cracked surfaces etc. this will provide a longer fatigue life for the material than expected, by slowing the crack growth rate.

### S-N curve

In high-cycle fatigue situations, materials performance is commonly characterized by an *S-N curve*, also known as a *Wöhler curve*. This is a graph of the magnitude of a cyclic stress (*S*) against the logarithmic scale of cycles to failure (*N*).



S-N curves are derived from tests on samples of the material to be characterized (often called *coupons*) where a regular sinusoidal stress is applied by a testing machine which also counts the number of cycles to failure. This process is sometimes known as *coupon testing*. Each coupon test generates a point on the plot though in some cases there is *arunout* where the time to failure exceeds that available for the test (see censoring). Analysis of fatigue data requires techniques from statistics, especially survival analysis and linear regression.

The progression of the *S-N curve* can be influenced by many factors such as corrosion, temperature, residual stresses, and the presence of notches. The Goodman-Line is a method to estimate the influence of the mean stress on the fatigue strength.

### Summary

Metals under load fail by fracture. Fracture is the separation of an object or material into two, or more, pieces under the action of stress. A fracture may be ductile or brittle. A ductile fracture is preferred over brittle fracture. **Creep** (sometimes called **cold flow**) is the tendency of a solid material to move slowly or deform permanently under the influence of mechanical stresses. It can occur as a result of long-term exposure to high levels of stress that are still below the yield strength of the material. **Fatigue** is the weakening of a material caused by repeatedly applied loads. It is the progressive and localized structural damage that occurs when a material is subjected to cyclic loading.

### Self assessment questions

1. How fractures are classified? State and explain different types of fracture giving appearance of the fracture in each case.

2. Explain with neat figure ductile fracture using both stress-strain and stages of fracture
3. Explain with sketch brittle fracture in materials.
4. Why brittle fracture is dangerous?
5. Explain with sketch, the ductile to brittle transition in the materials.
6. Derive an expression for the critical resolved shear stress for slip
7. Explain Griffith's theory of brittle fracture.
8. Sketch a typical creep curve and explain different stages of creep.
9. Discuss any two mechanisms for creep.
10. Define creep strength, creep life and creep limit.
11. How fatigue strength of materials is determined?
12. Discuss on fatigue properties.
13. With the help of a sketch, discuss the different types of stress cycles which bring about fatigue failure.
14. What is meant by stress relaxation? Explain with figure.
15. Explain factors affecting fatigue life.