

Module 2

Imperfections in Crystals

1. Thermal Expansion

- Tendency of a matter to change in volume in response to change in temperature
- When a substance is heated, its constituent particles begin moving and become active, thus maintaining a greater average separation
- Degree of expansion divided by change in temperature is material's **Coefficient of Thermal Expansion** (varies with temp)

Thermal Expansion Coefficient

$$\alpha = \frac{1}{V} \left(\frac{\partial V}{\partial T} \right)$$

- **Common engineering solids usually have thermal expansion coefficients that do not vary significantly over the range of temp where they are designed to be used**
- **Materials with anisotropic structures, such as crystals and composites, will generally have different expansion coefficients in different orientations**

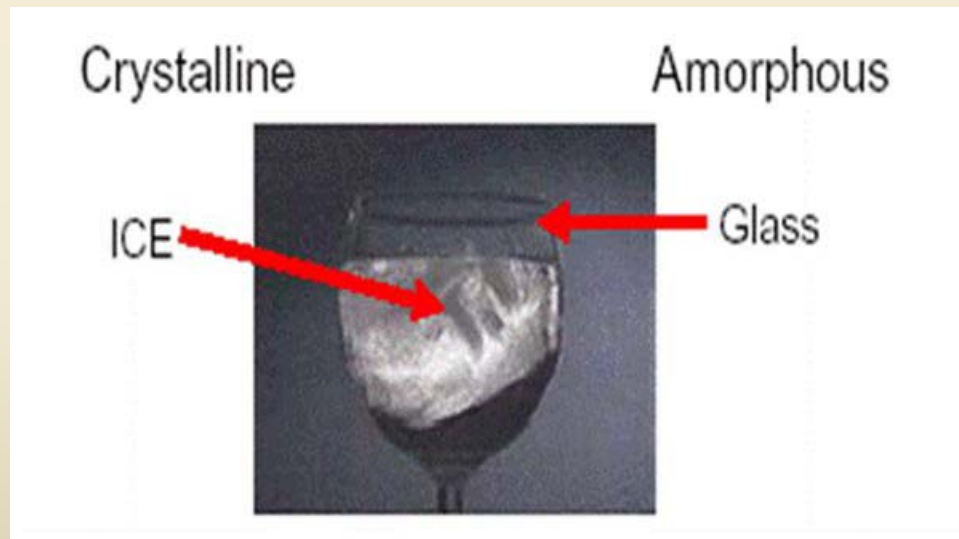
2. Introduction to Crystal Geometry

- Materials may be classified as **Crystalline** or **Non-Crystalline** structures
- Crystalline solid can be either **Single Crystal Solid** (crystal lattice of entire sample is continuous and unbroken to edges of sample with no grain boundary) or **Poly Crystal Solid** (aggregate of many crystals separated by well-defined boundaries)
- Cluster of crystals with identical structure (same crystallographic planes & directions) are known as **Grains** separated by **Grain Boundaries**
- X-ray diffraction analysis shows that atoms in metal crystal are arranged in a regular, repeated 3-D Pattern known as **Crystalline Structure**

➤ **Example:**

Ceramic: Inorganic non-metallic crystalline (regular internal Structure) materials

Glass: Inorganic non-metallic non-crystalline / amorphous (completely disordered form) material



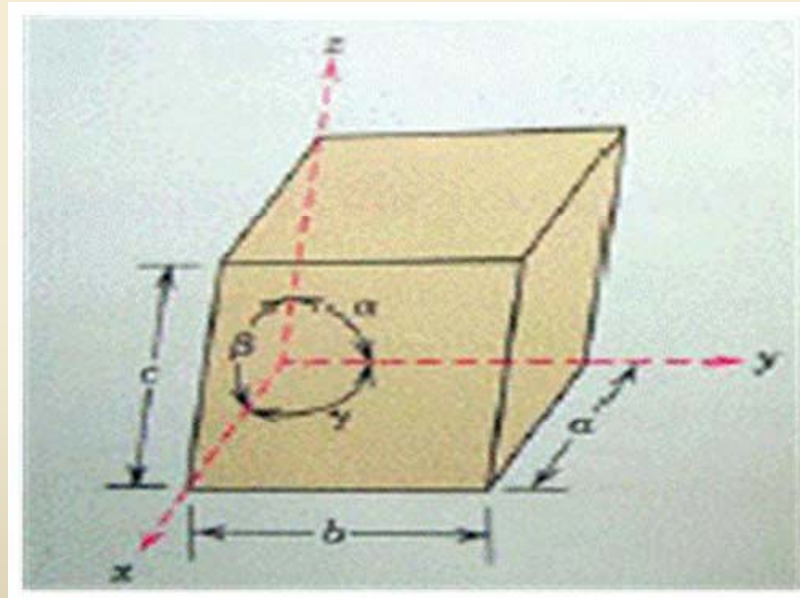
- Arrangement of atoms can be most simply portrayed by *Crystal Lattice*, in which atoms are visualized as, *Hard Balls* located at particular locations
- *Space Lattice / Lattice*: Periodic arrangement of points in space with respect to three dimensional network of lines
- Each atom in lattice when replaced by a point is called *Lattice Point*, which are the intersections of above network of lines
- Arrangement of such points in 3-D space is called *Lattice Array* and 3-D space is called *Lattice Space*

➤ Tiny block formed by arrangement of small group of atoms is called ***Unit Cell***. It is chosen to represent the symmetry of crystal structure, and may be defined as:

- Finite representation of infinite lattice
- Small repeat entity
- Basic structural unit
- Building block of crystal structure
- Can generate entire crystal by translation

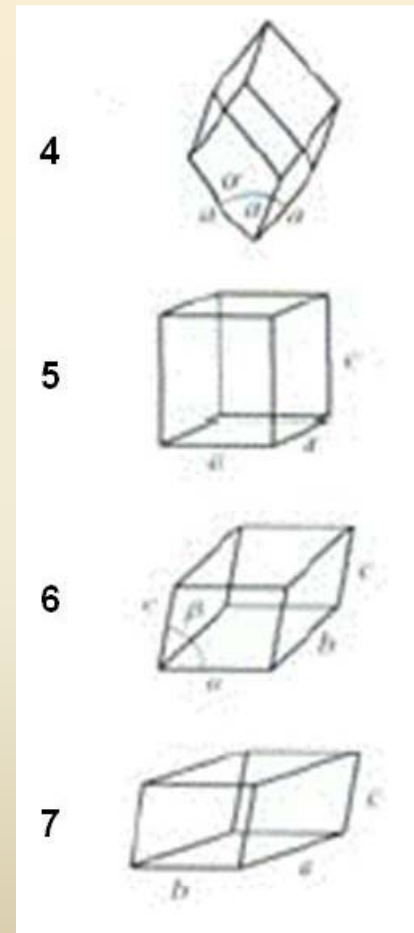
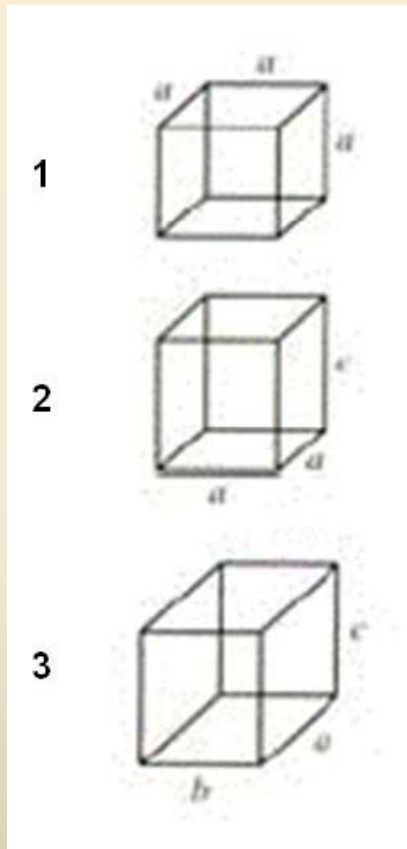
Lattice Parameters

- Six lattice parameters a , b , c , α , β , γ
- Typically in the order of few Angstroms (few tenths of nanometer)
- **Example:** Cubic structure has following lattice parameters:
 $a = b = c$ and $\alpha = \beta = \gamma = 90^\circ$



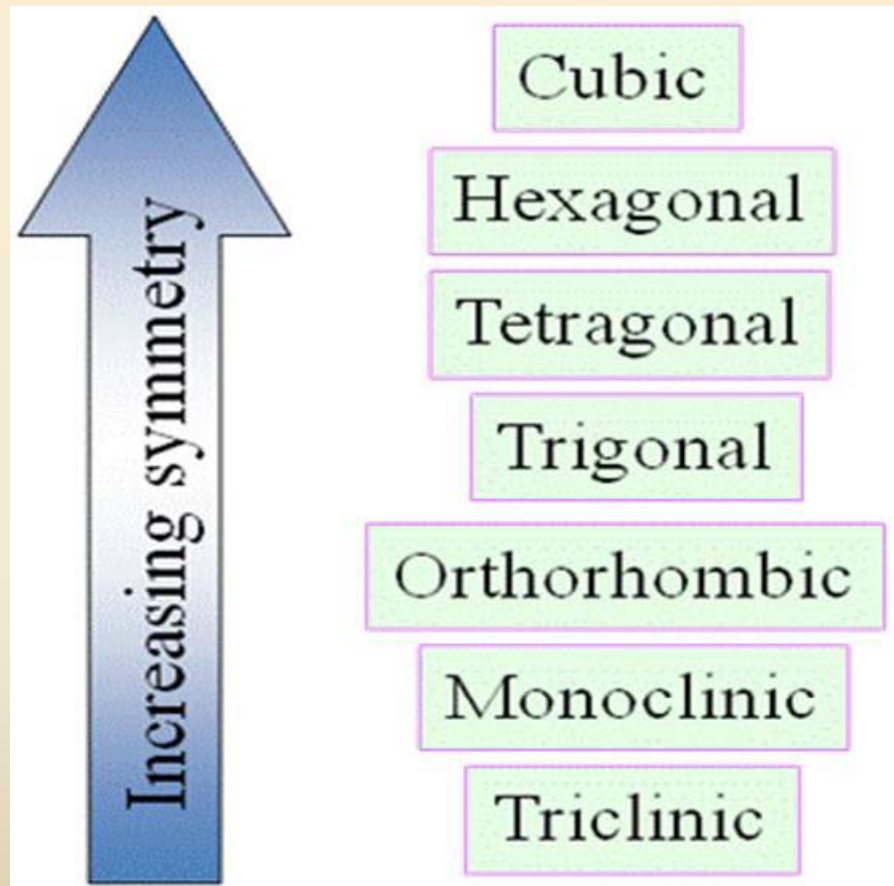
Types of Crystal

Cubic, Monoclinic, Triclinic, Tetragonal, Orthorhombic, Rhombohedral and Hexagonal



No.	Crystal Type	Lattice Parameters	Examples
1.	Cubic	$a = b = c, \alpha = \beta = \gamma = 90^\circ$	Fluorite, Garnet, Pyrite
2.	Tetragonal	$a = b \neq c, \alpha = \gamma = 90^\circ = \beta$	Zircon
3.	Orthorhombic	$a \neq b \neq c, \alpha = \gamma = \beta = 90^\circ$	Topaz
4.	Rhombohedral	$a = b = c, \alpha = \beta = \gamma \neq 90^\circ$	Tourmaline
5.	Hexagonal	$a = b \neq c, \alpha = \beta = 90^\circ, \gamma = 120^\circ$	Corundum
6.	Monoclinic	$a \neq b \neq c, \alpha = \gamma = 90^\circ \neq \beta$	Kunzite
7.	Triclinic	$a \neq b \neq c, \alpha \neq \gamma \neq \beta \neq 90^\circ$	Amazonite

Order of Symmetry



Examples of Crystal Types



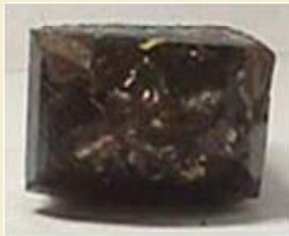
Fluorite Octahedron



Garnet Dodecahedron



Pyrite Cube



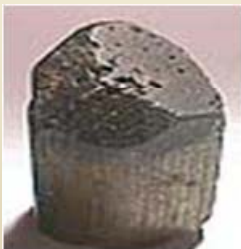
Zircon



Topaz



Corundum



Tourmaline



Kunzite



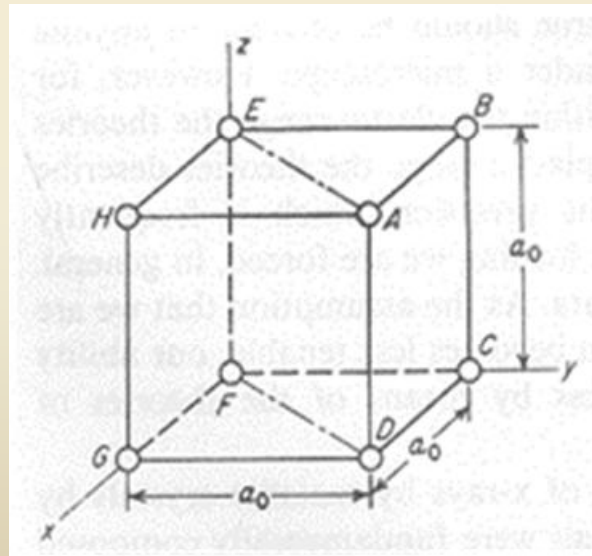
Amazonite

Principal Metal Crystal Structures

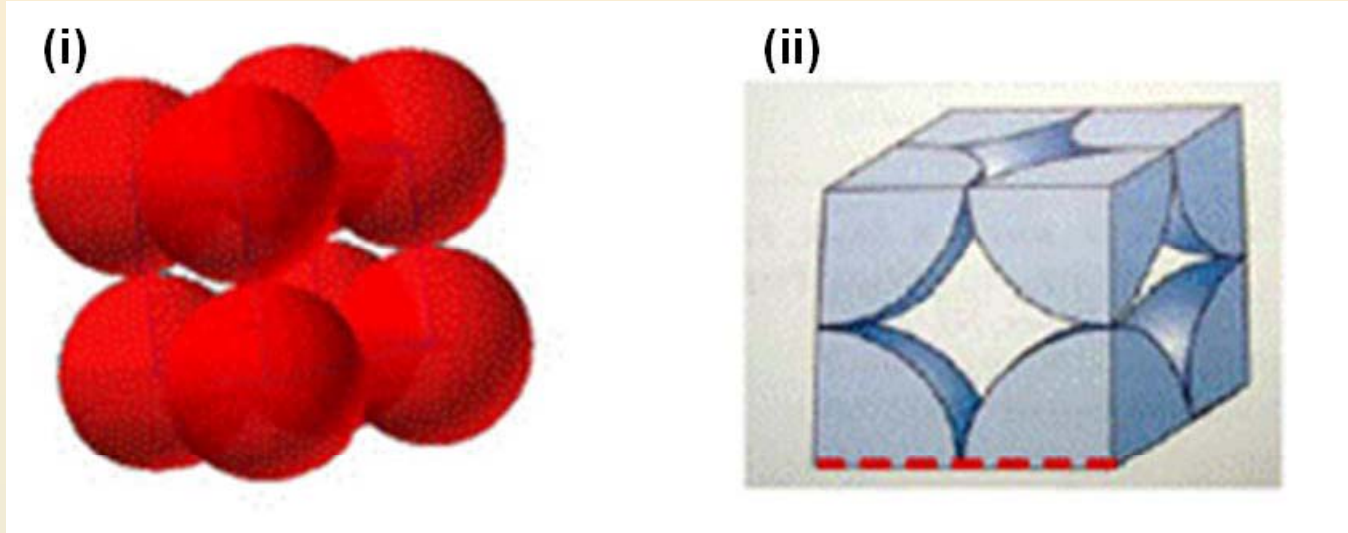
- ***Simple Cubic Lattice Structure***
- ***Body Centered Cubic (BCC) Structure***
- ***Face Centered Cubic (FCC) Structure***

Simple Cubic Lattice

- Most elementary crystal structure with three mutually perpendicular axes arbitrarily placed through one of the corners of a cell
- Each corners occupied with one atom



SC Structure

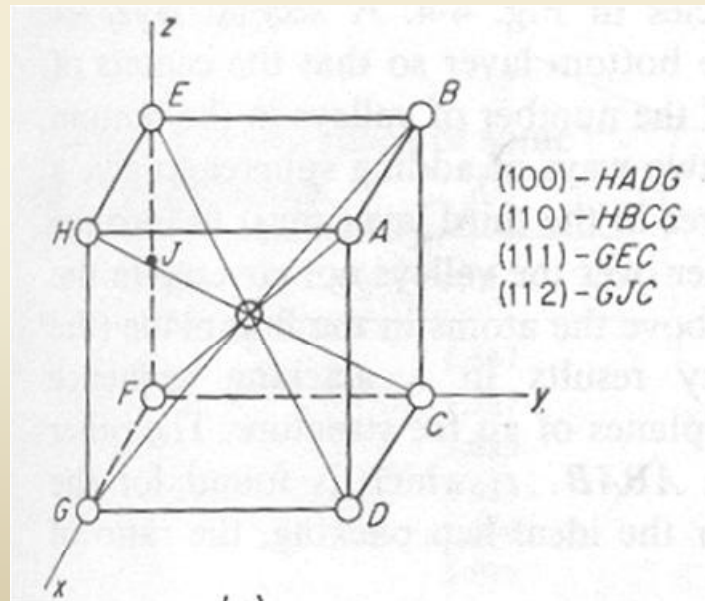


(i). Aggregate of atoms

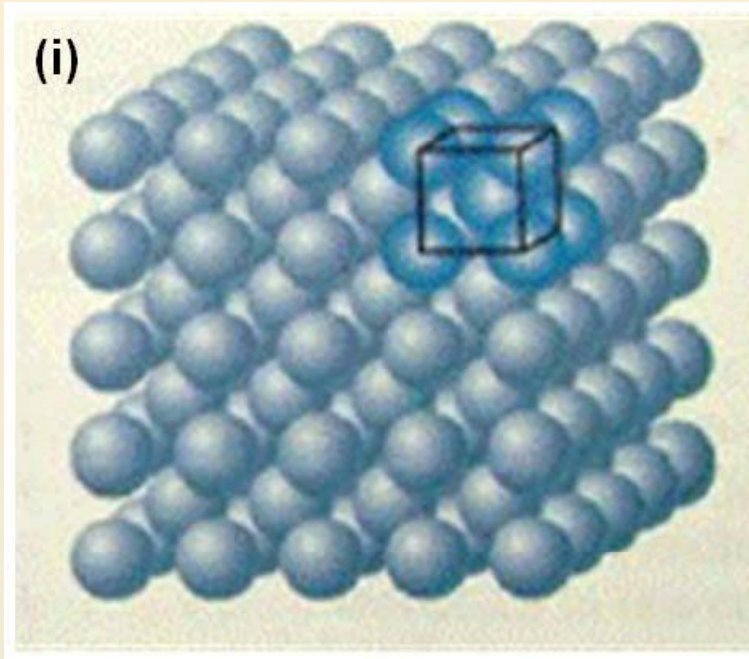
(ii). Hard Sphere Unit Cell

Body Centered Cubic (BCC) Structure

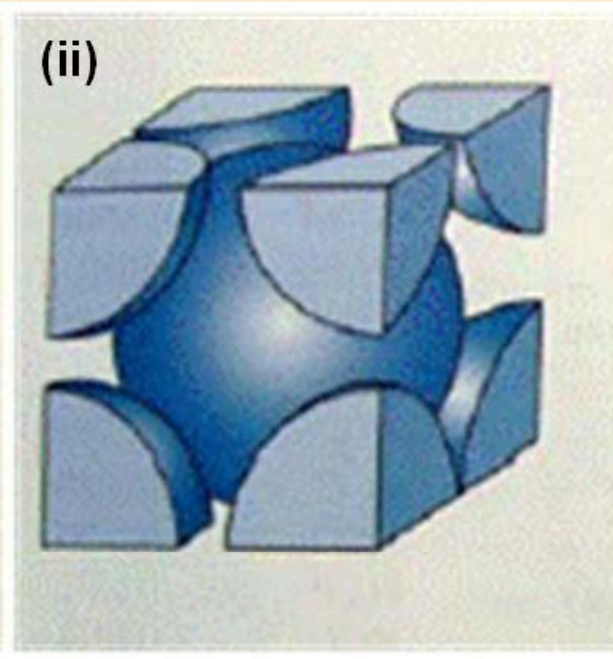
- BCC cell has an atom at each corner and another atom at body center of cube
- Each atom at corner is surrounded by eight adjacent atoms
- Example: alpha iron, chromium, molybdenum & tungsten



BCC Structure



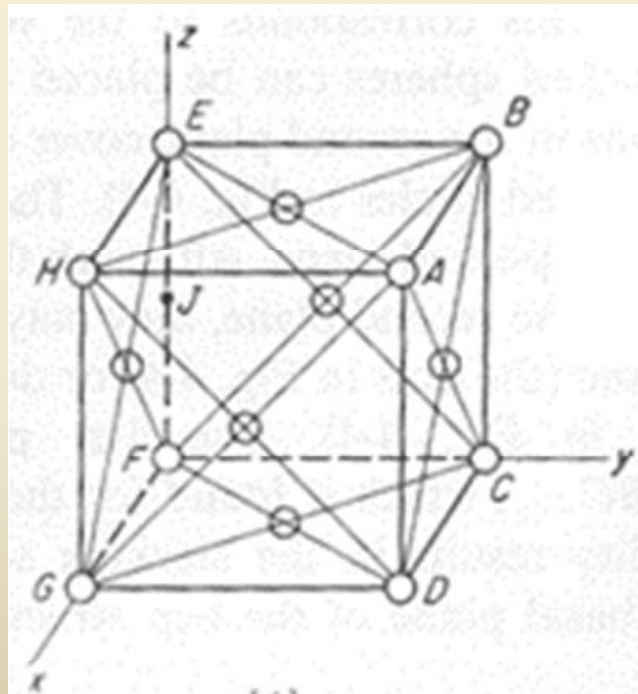
(i). Aggregate of atoms



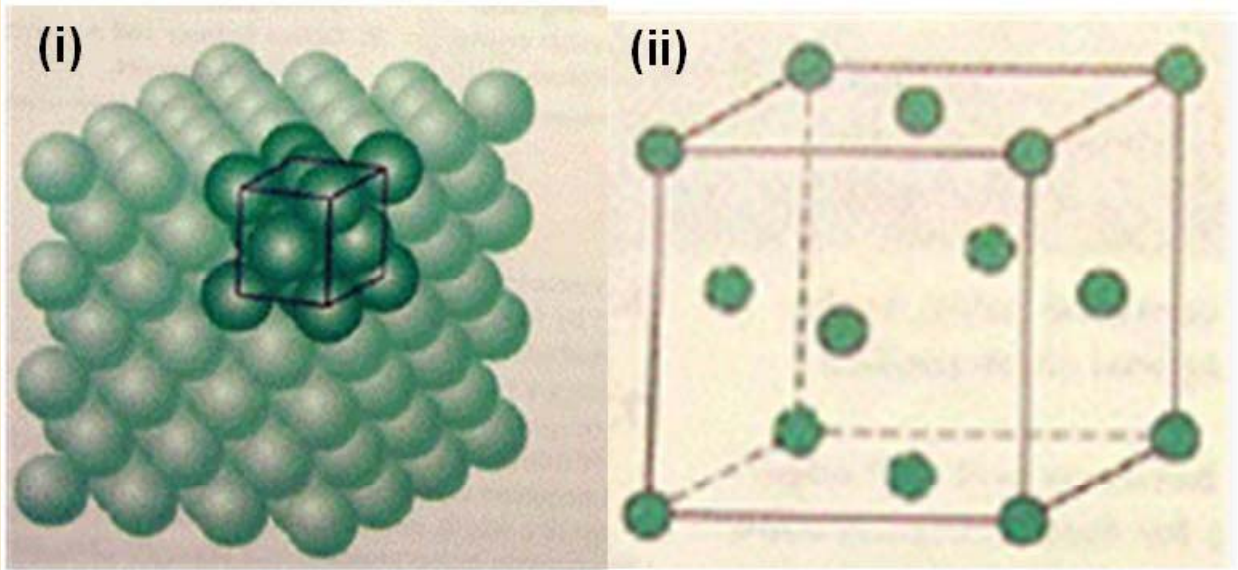
(ii). Hard Sphere Unit Cell

Face Centered Cubic (FCC) Structure

- Atoms at each corner of cube, and in addition there is an atom at the center of each cube's face
- Example: aluminium, copper, gold, lead, silver and nickel



FCC Structure

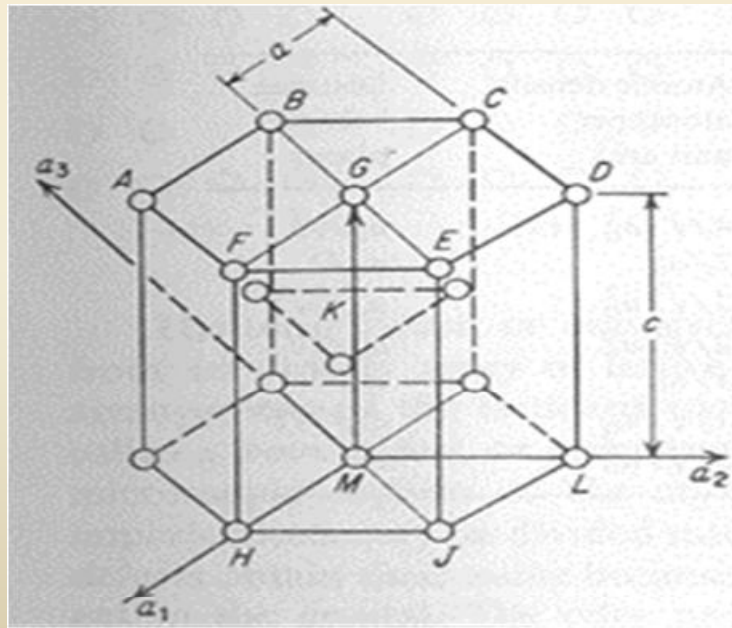


(i). Aggregate of atoms

(ii). Hard Sphere Unit Cell

Hexagonal Close-packed (HCP) Structure

- Unit cell has an atom at each of twelve corners of hexagonal prism, with one atom at centre of each of two hexagonal faces and three atoms in body of cell
- Example: zinc, lithium, magnesium, beryllium

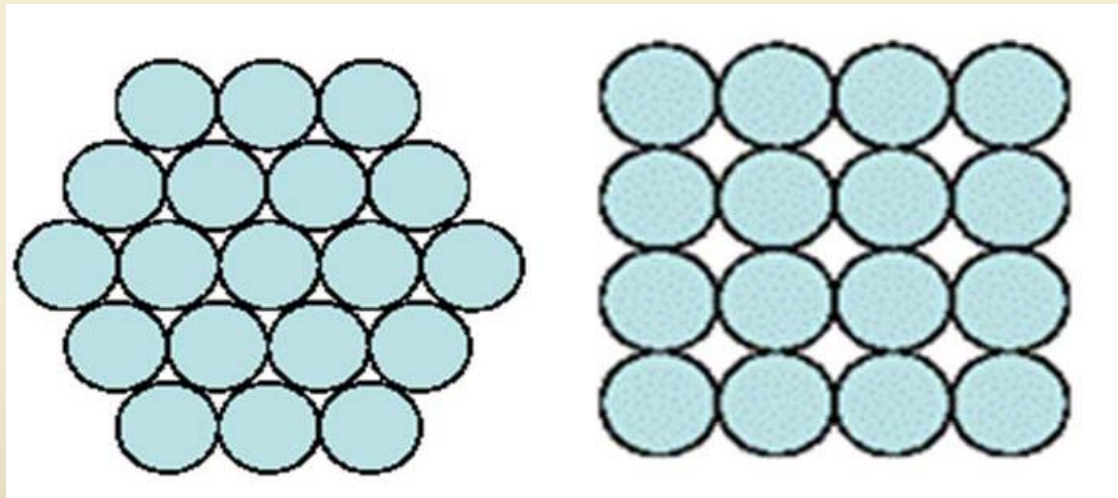


Comparison

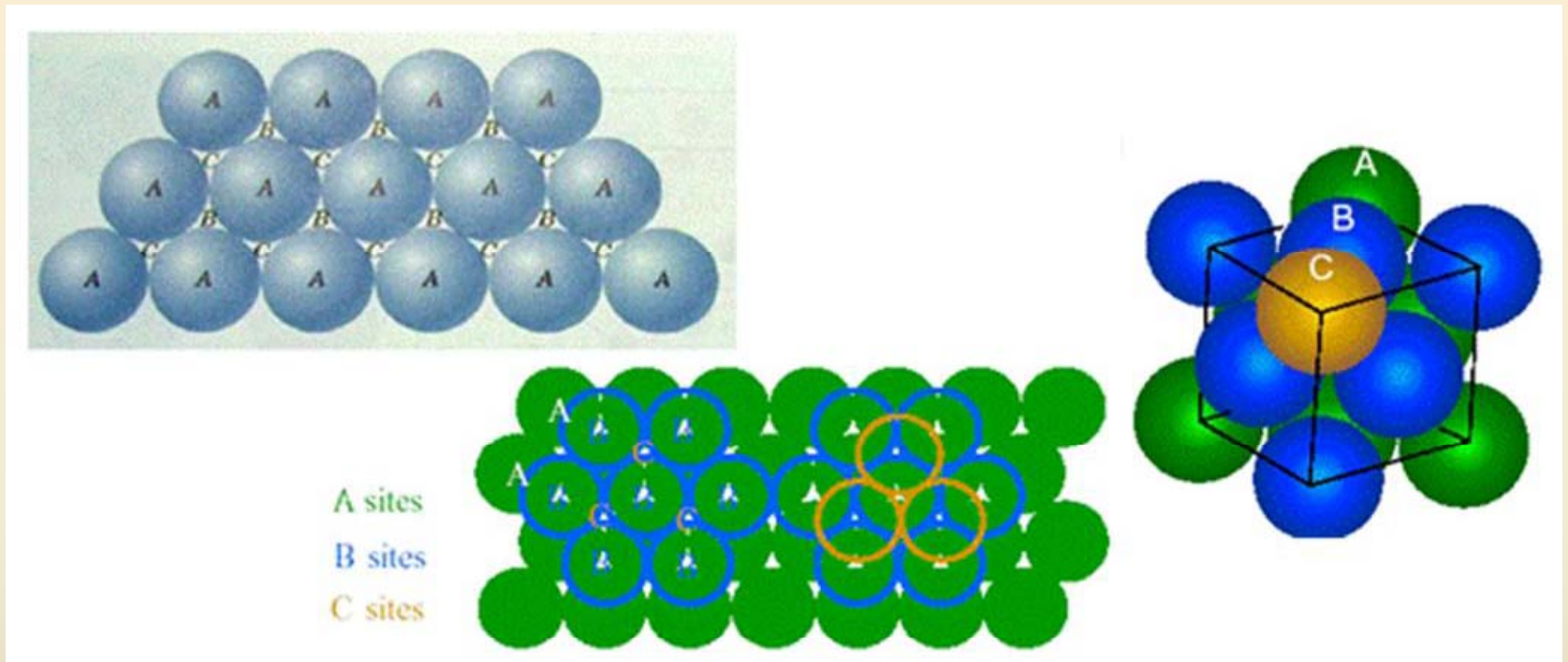
Sl. No.	APF (Atomic Packing Factor) (Ratio of vol . of atoms in unit cell to unit cell vol.)	Co-ordination Number (No. of nearest neighbor atoms)
SC	0.52	6
BCC	0.68	8
FCC	0.72	12

Close-Packed Structures

- How can metal atoms be stacked to fill empty spaces in the lattice?
- Can these 2-D layers be stacked to make 3-D structures

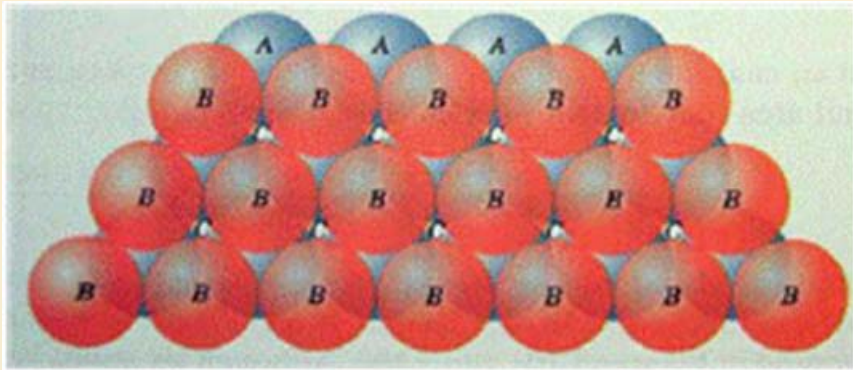


Example: Close-Packed FCC Structure

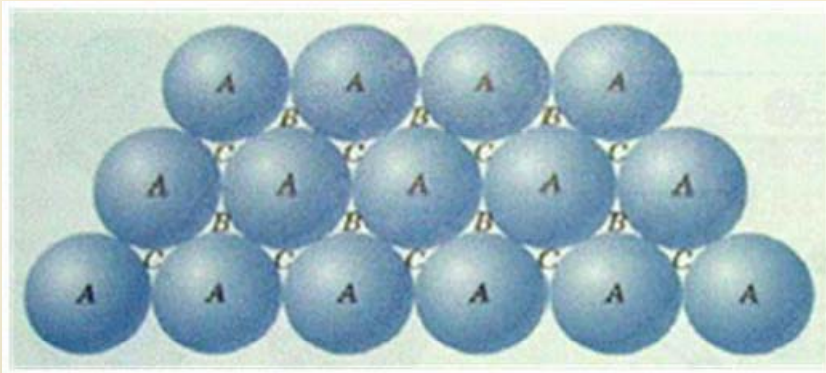


ABC Stacking Sequence

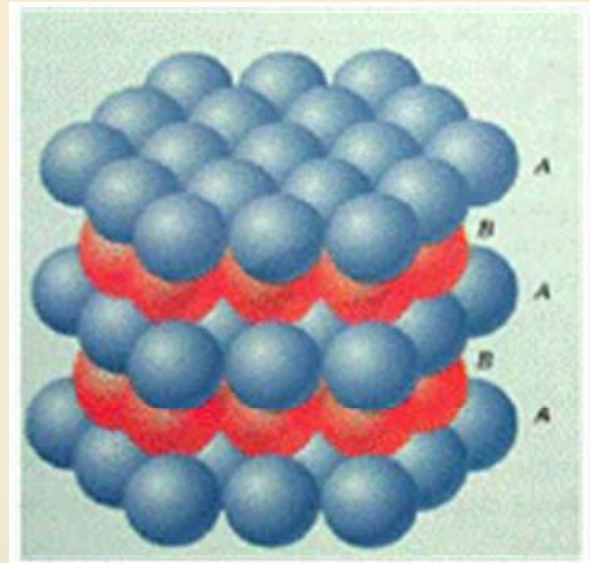
Example: Close-Packed HCP Structure



AB Stacking Sequence

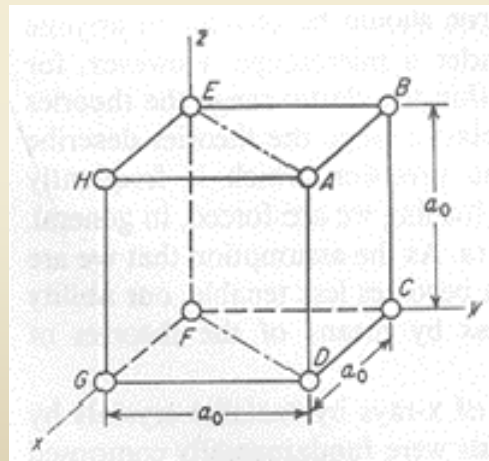


ABC Stacking Sequence



Crystallographic Planes & Directions

- **Crystallographic Planes & Directions** are specified with respect to the reference axes in terms of '**Miller Indices**', which is the system of notation of planes within a crystal of space lattice
- **Example:** SC structure is chosen for understanding

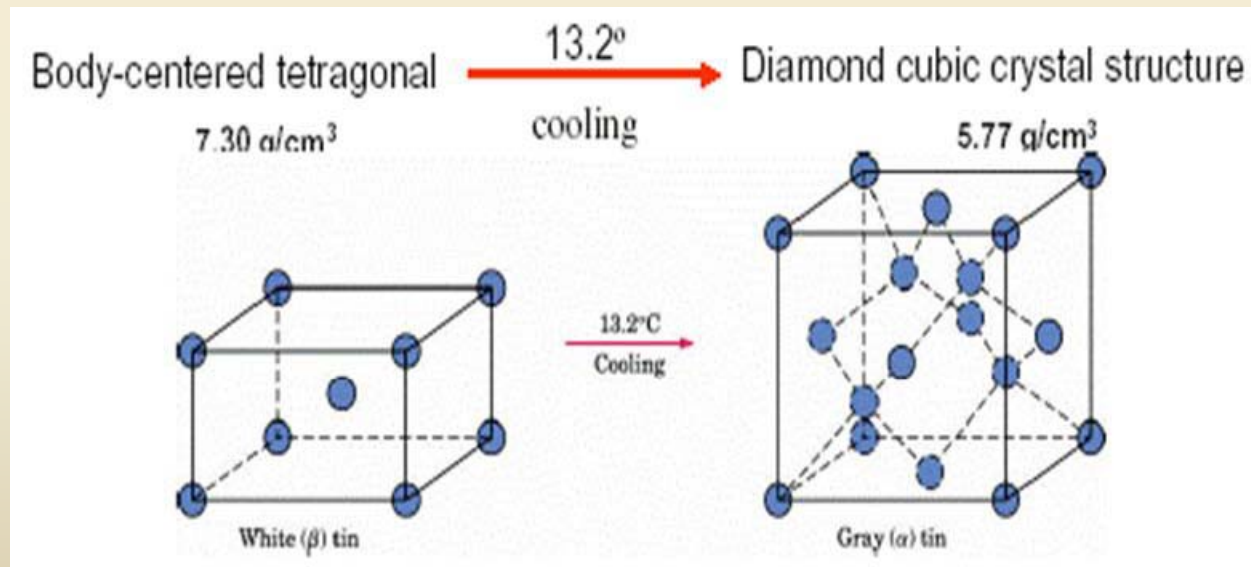


- **Crystallographic Plane** is specified in terms of length of its intercepts on three mutually perpendicular axes. To simplify it, reciprocals of these intercepts reduced to lowest common denominator (LCM) are used as miller indices,
- e.g. plane ABCD in figure is parallel to x and z axes and intersects y-axis at one interatomic distance ' a_0 ', therefore miller indices of the plane are $1/\infty, 1/\infty, 1/\infty$ or $(hkl) = (010)$
- Plane EBCF is designated as $(\bar{1} 00)$ plane, where bar indicates that plane intersects the axis in negative direction

- **Crystallographic Directions** are indicated by integers in brackets like $[uvw]$, where reciprocals are never used, e.g. direction 'FD' is obtained by moving out from origin, a distance ' a_0 ' along positive x-axis and moving same distance along positive y-axis also, therefore, the crystallographic direction will be given as $[110]$
- **Example:** Ionic crystals like NaCl, LiF (not for metals)
- **Note:** For simple cubic lattice only, direction is always perpendicular the plane having same indices

Allotropy / Polymorphism

- Two or more distinct crystal structures for the same material at different temperature & pressure
- Examples: iron (α -iron & γ -iron), carbon (graphite & diamond), tin (α -tin & β -tin)



3. Imperfection / Defects In Crystals

In actual crystals, imperfection or defects are always present, which are important to understand, as they influence the properties of material

Classifications of Defects

(i). Point Defects (Zero Dimensional Defects)

- (a). Vacancy**
- (b). Schottky Imperfections**
- (c). Interstitialcy**
- (d). Frenkel Defect**
- (e). Compositional Defect**
- Substitutional Defect**
- Interstitial Impurity**
- (f). Electronic Defect**

(ii). Line Defects / Dislocations (One Dimensional Defects)

(a). Edge Dislocations

(b). Screw Dislocations

(iii). Surface / Plane Defects (Two Dimensional Defects)

(a). External Defects

(b). Internal Defects

- **Grain Boundary Defect**
- **Tilt Boundary Defect**
- **Twin Boundary Defect**
- **Stacking Fault**

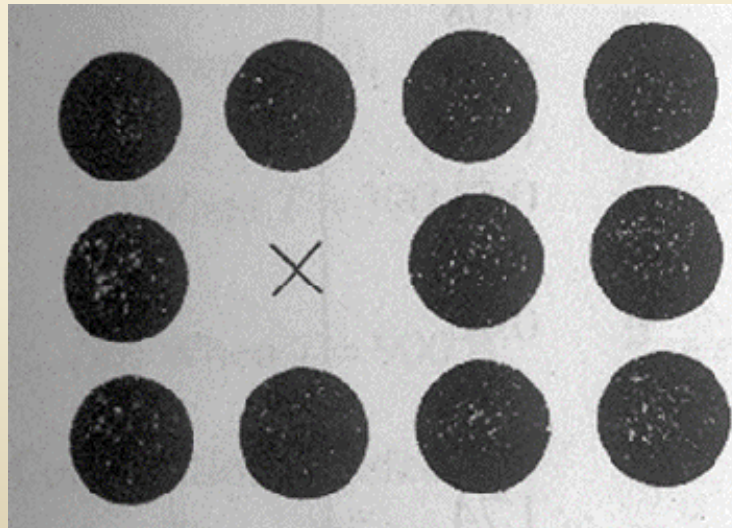
(iv). Volume Defects (Three Dimensional Defects)

(I). Point Defects (Zero Dimensional Defects)

- Imperfect point like regions in crystal (size is one or two atomic diameter)
- Completely local in effect, i.e. vacant lattice site
- Always present in crystals
- Created by thermal fluctuations, quenching (high rate of cooling), severe deformation of crystal lattice (hammering or rolling) or external bombardment by atoms / high energy particles

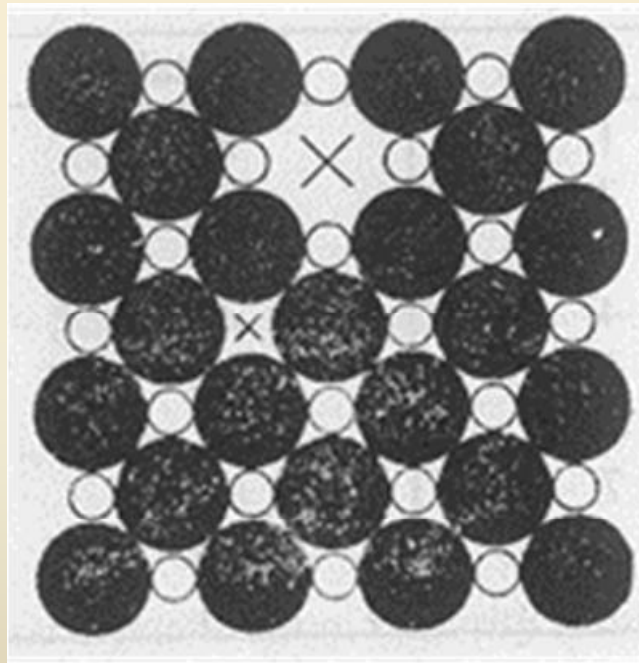
(a). Vacancy

Simplest type of point defect involving a missing atom within crystal lattice of metal, which results due to imperfect packing during original crystallization process or by thermal vibrations of atoms at very high temperature



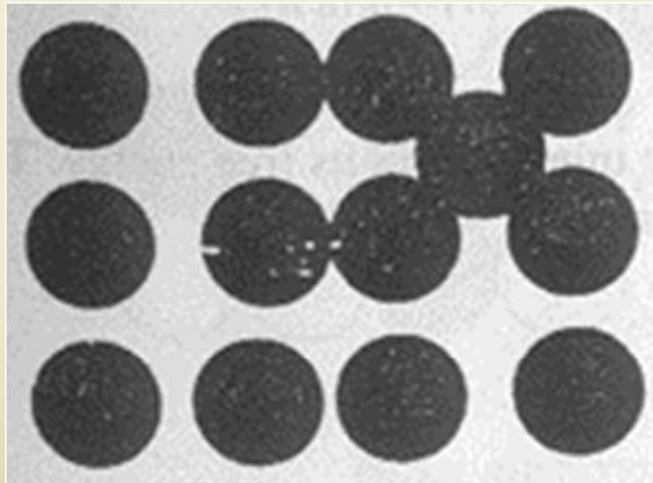
(b). Schottky Imperfections

Involve vacancies in pair of ions having opposite charges and are found in compounds, which maintain charge balance, e.g. alkali halides



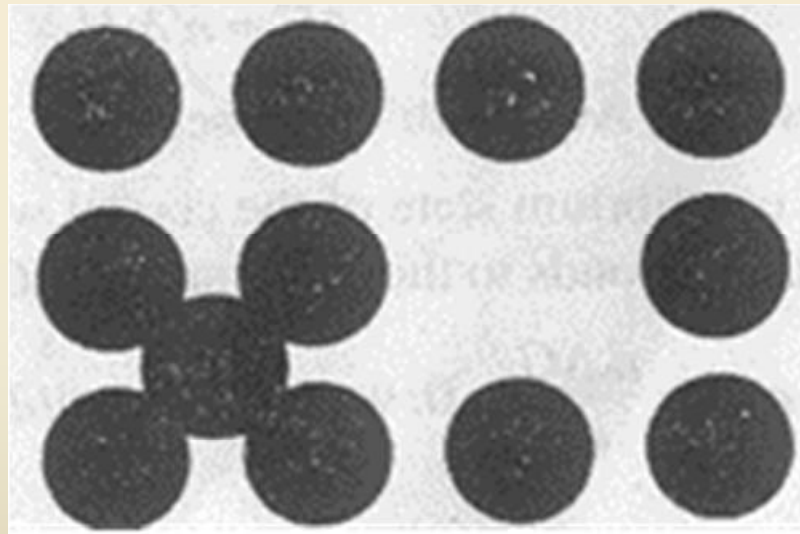
(c). Interstitialcy

Addition of an extra atom in the crystal lattice, when atomic packing density / factor is low and the foreign atom may be an impurity or alloying atom (generally very less in number as additional energy is required to force atom / ion to occupy new position)



(d). Frenkel Defect

Ion dislodged from its crystal lattice into an interstitial site (generally very less in number as additional energy is required to force the atom / ion to occupy the new position)



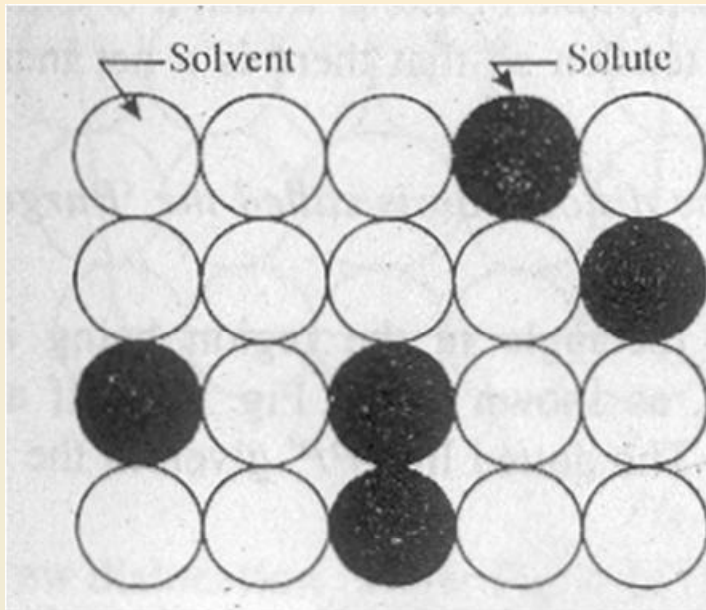
(e). Compositional Defect

Arises due to presence of impurity atom in crystal lattice of metal during original crystallization process (responsible for functioning of semi-conductor devices)

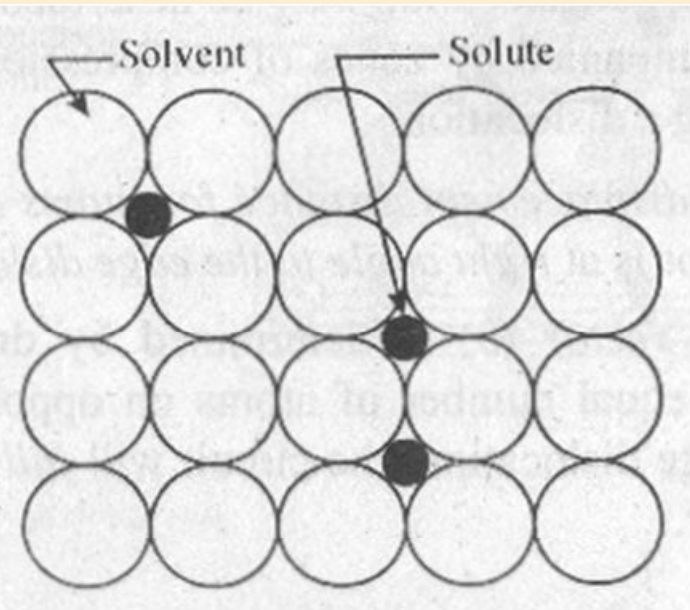
- Substitutional Defect: Original parent atom from its lattice is replaced
- Interstitial Impurity: Small impurity occupies interstitial spaces in lattice

(f). Electronic Defect

Errors in charge distribution in solids, e.g. diodes and transistors devices, where charges diffuse in opposite regions leading to change of their concentration in that region



Substitutional Defect



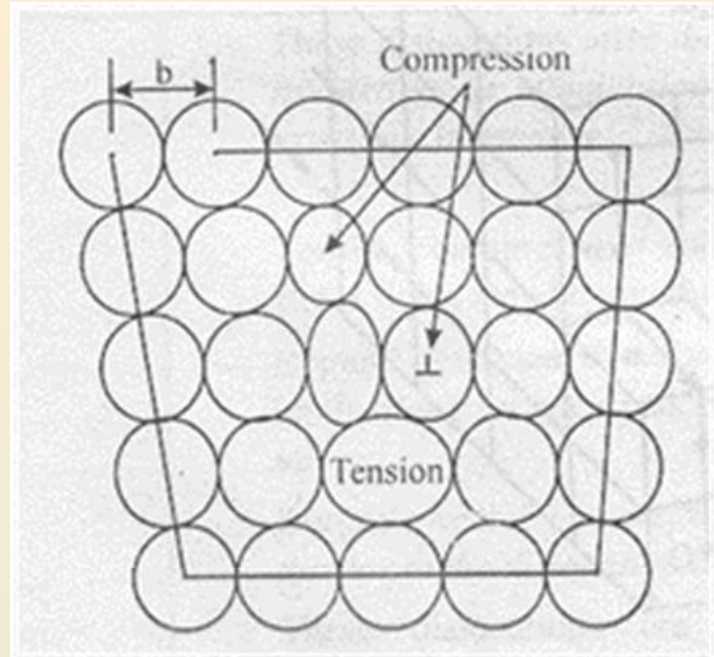
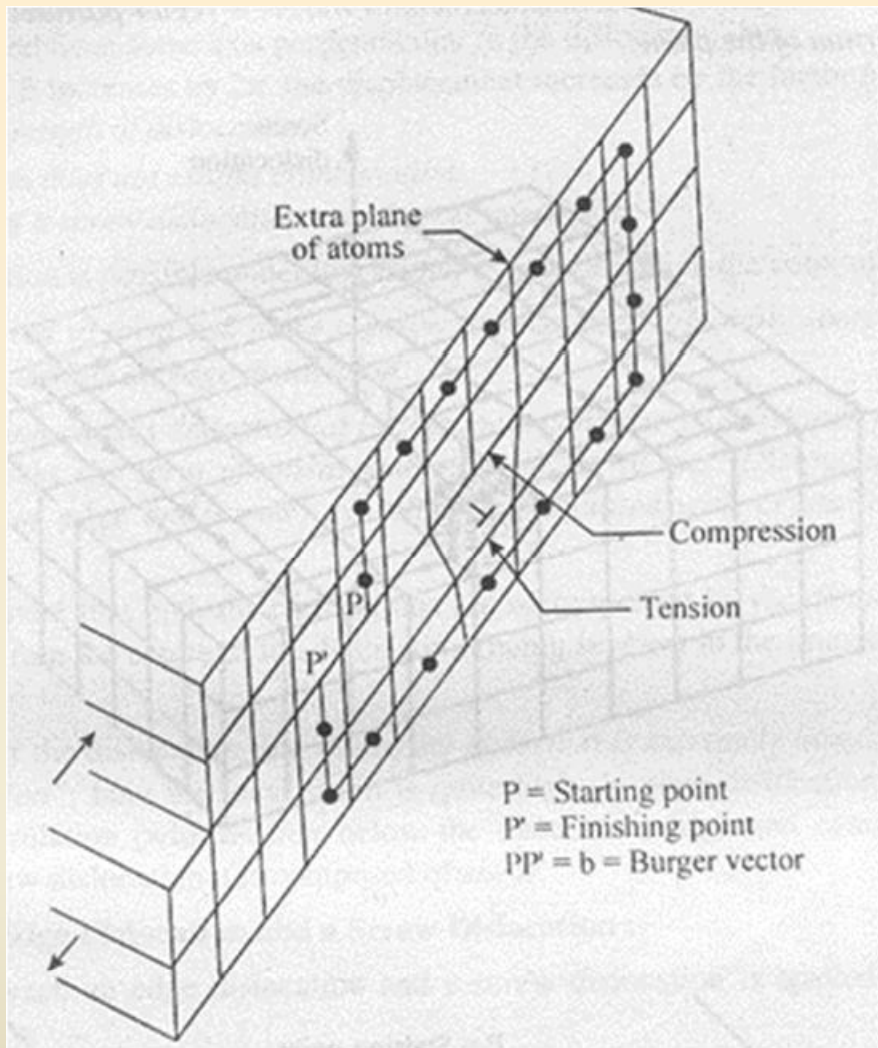
Interstitial Defect

(ii). Line Defects (One Dimensional Defects)

- Linear disturbance of atomic arrangement, which can move very easily on slip plane through crystal
- Occurs during recrystallization process or during slip
- Created along a line, which is also boundary between slipped and unslipped regions of crystals
- Defect is known as 'dislocation' and boundary is known as '*Dislocation Line*'
- Region near dislocation, where distortion is extremely large is called '*Core of Dislocation*' (very high local strain)

(a). Edge Dislocation

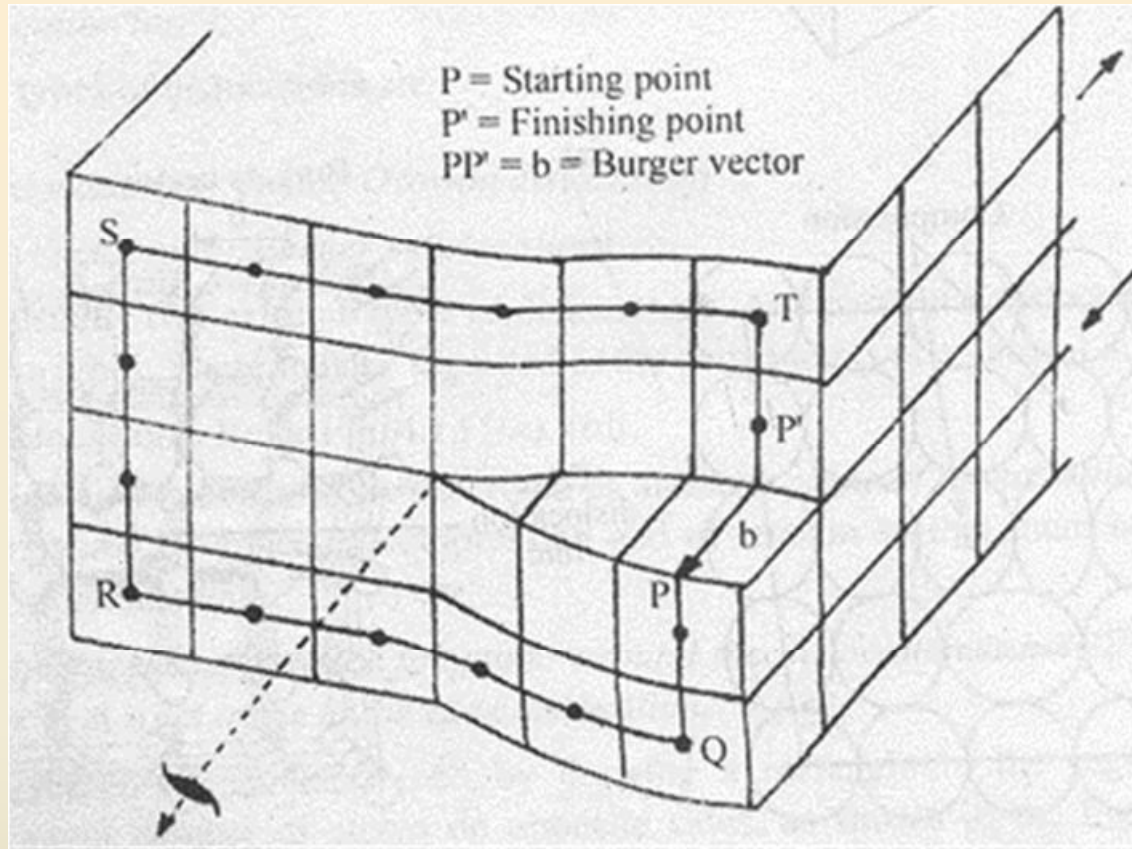
- Any extra plane of atoms within a crystal structure is edge dislocation
- Accompanied by zones of compression and tension and there is a net increase in energy along dislocation
- Displacement distance for atoms around dislocation is called '**Burger Vector**', which is at right angle to edge dislocation
- Berger vector is determined by drawing a rectangle in region by connecting an equal number of atoms on opposite sides (circuit fails to complete), i.e. PP' as shown in figure



Edge Dislocation

(b). Screw Dislocation

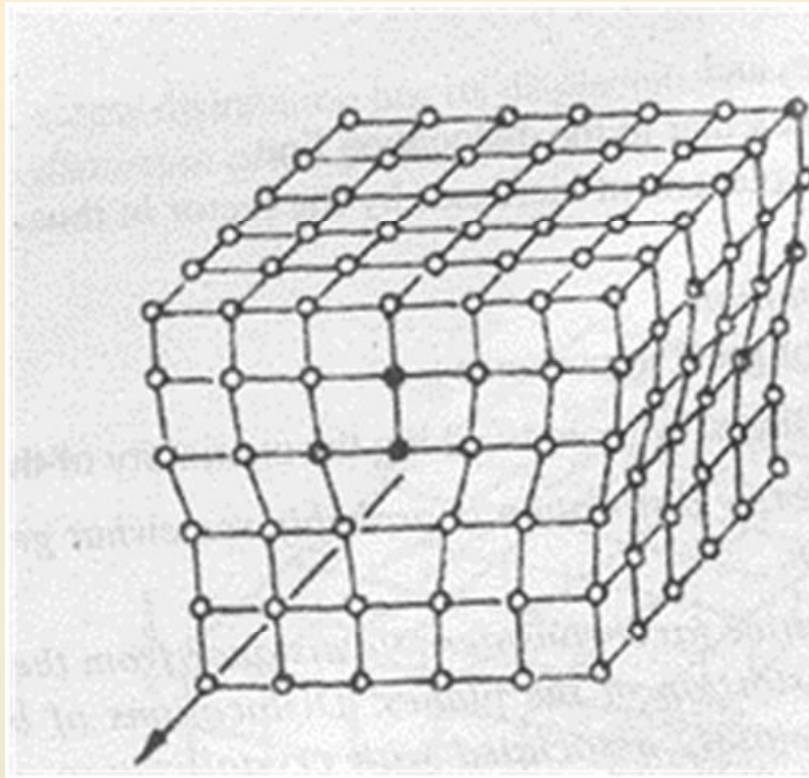
- Originate from partial slipping of a section of crystal plane
- Shear stresses are associated with adjacent atoms and extra energy is involved along the dislocation
- Successive atom planes are transformed into the *Surface of Helix of Screw* (plane is distorted), which accounts for its name as screw dislocation
- Displacement vector is parallel to the line defect



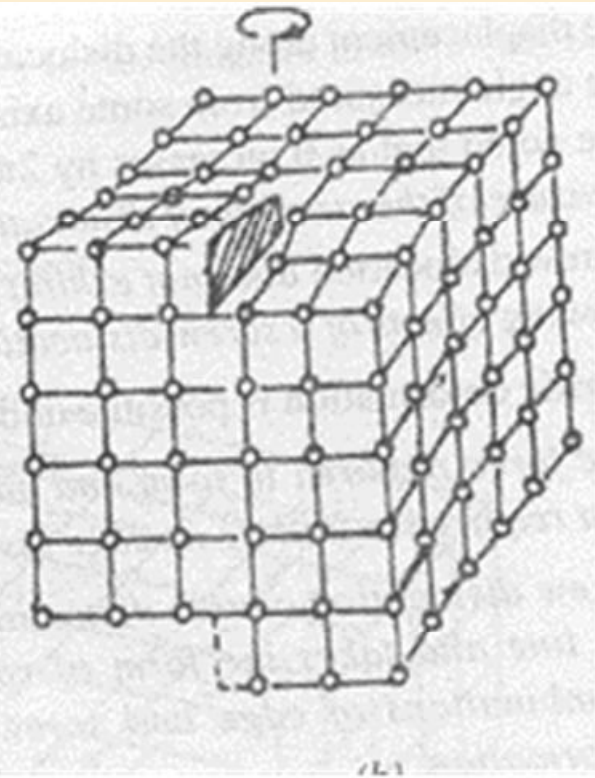
SCREW DISLOCATION

Comparison

Edge Dislocation	Screw Dislocation
Arise due to introduction or elimination of an extra row of atoms	Arise due to partial slipping of section of crystal plane, where planes of atoms are transformed into surface of helix of screw
Tensile, compressive or shear stress field may be present	Only shear stress field is present
Lattice disturbance extends along an edge inside crystal	Lattice disturbance extends into two separate planes at right angles to each other
Burger's vector is always perpendicular to dislocation line	Burger's vector is parallel to dislocation line
Dislocations can climb and glide	Dislocation can only glide
Force required is less as compared to that for screw dislocation	Force required is more as compared to that of edge dislocation

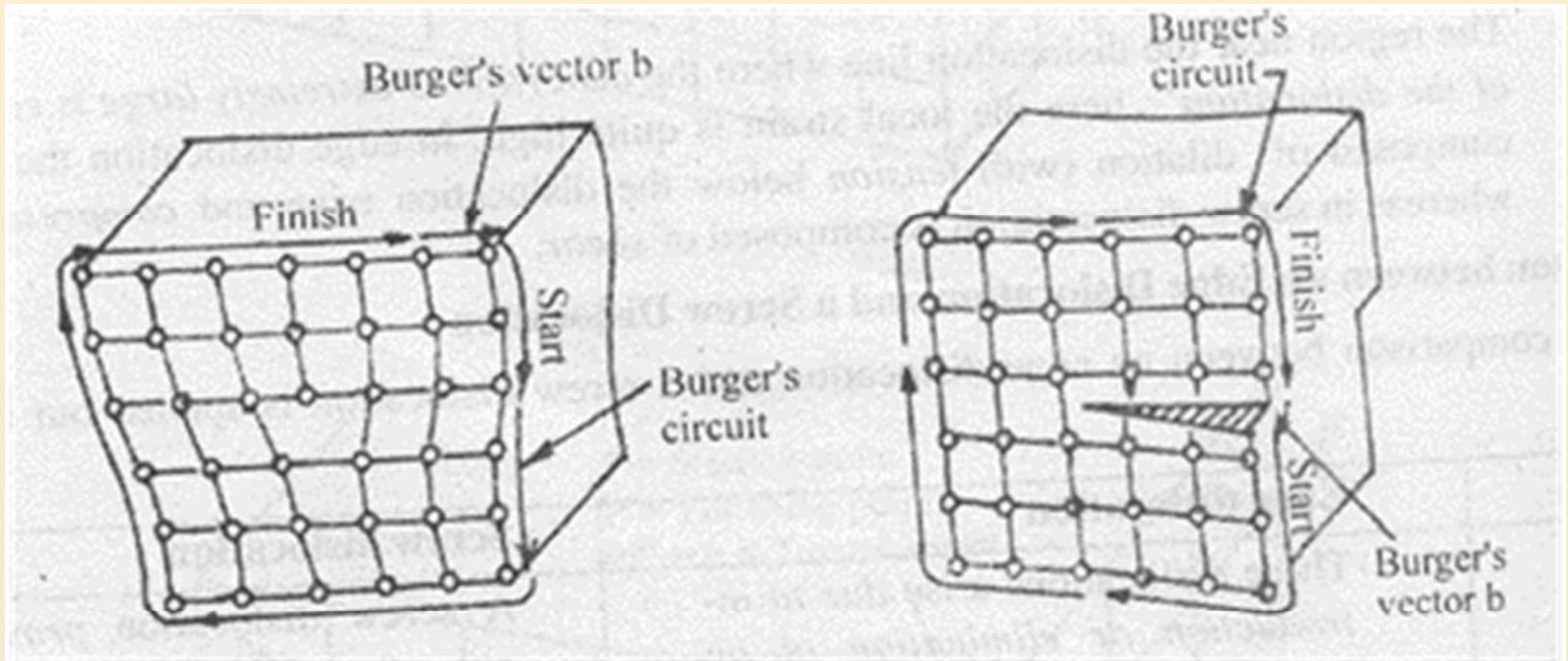


Edge Dislocation



Screw Dislocation

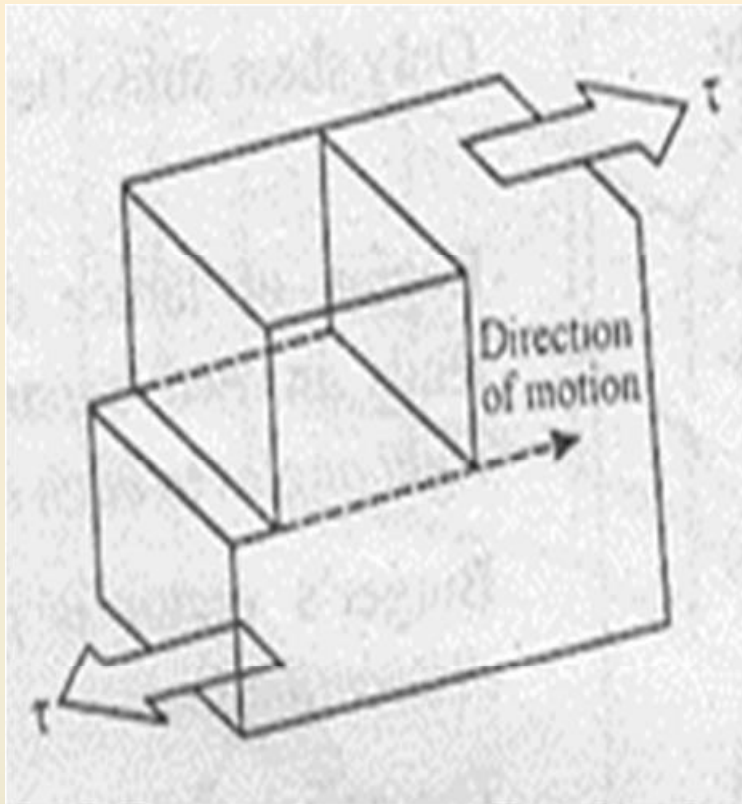
Geometry of Dislocation



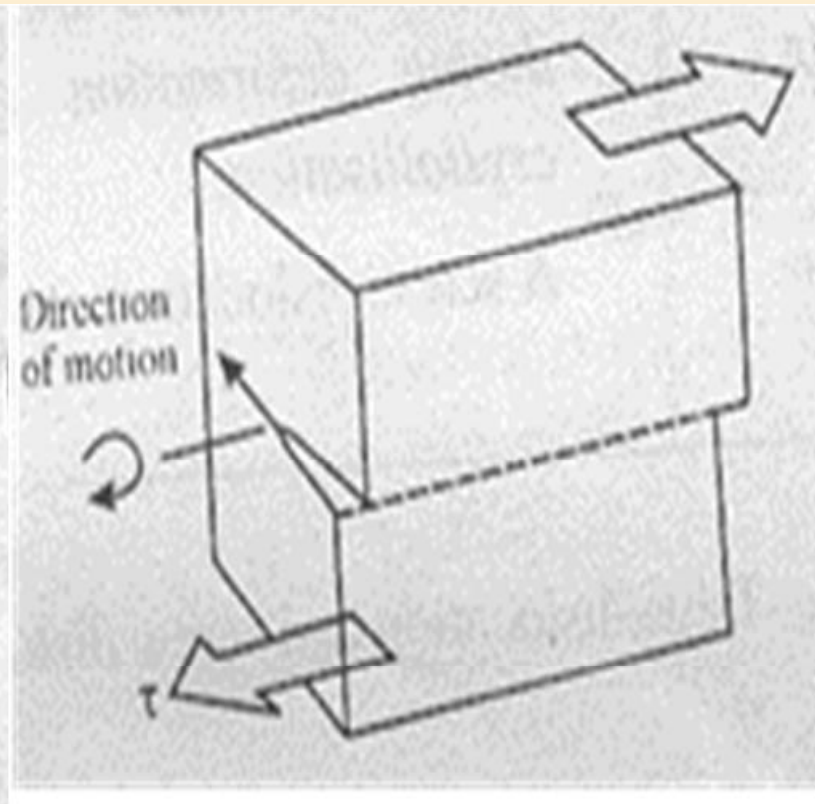
Edge Dislocation

Screw Dislocation

Burger's Vector



Edge Dislocation



Screw Dislocation

Formation of Step on Crystal Surface

(iii). Surface / Plane Defects (Two Dimensional Defects)

- **Two-dimensional regions in crystal and arise from change in stacking of atomic planes on or across boundary**

(a). External Defects

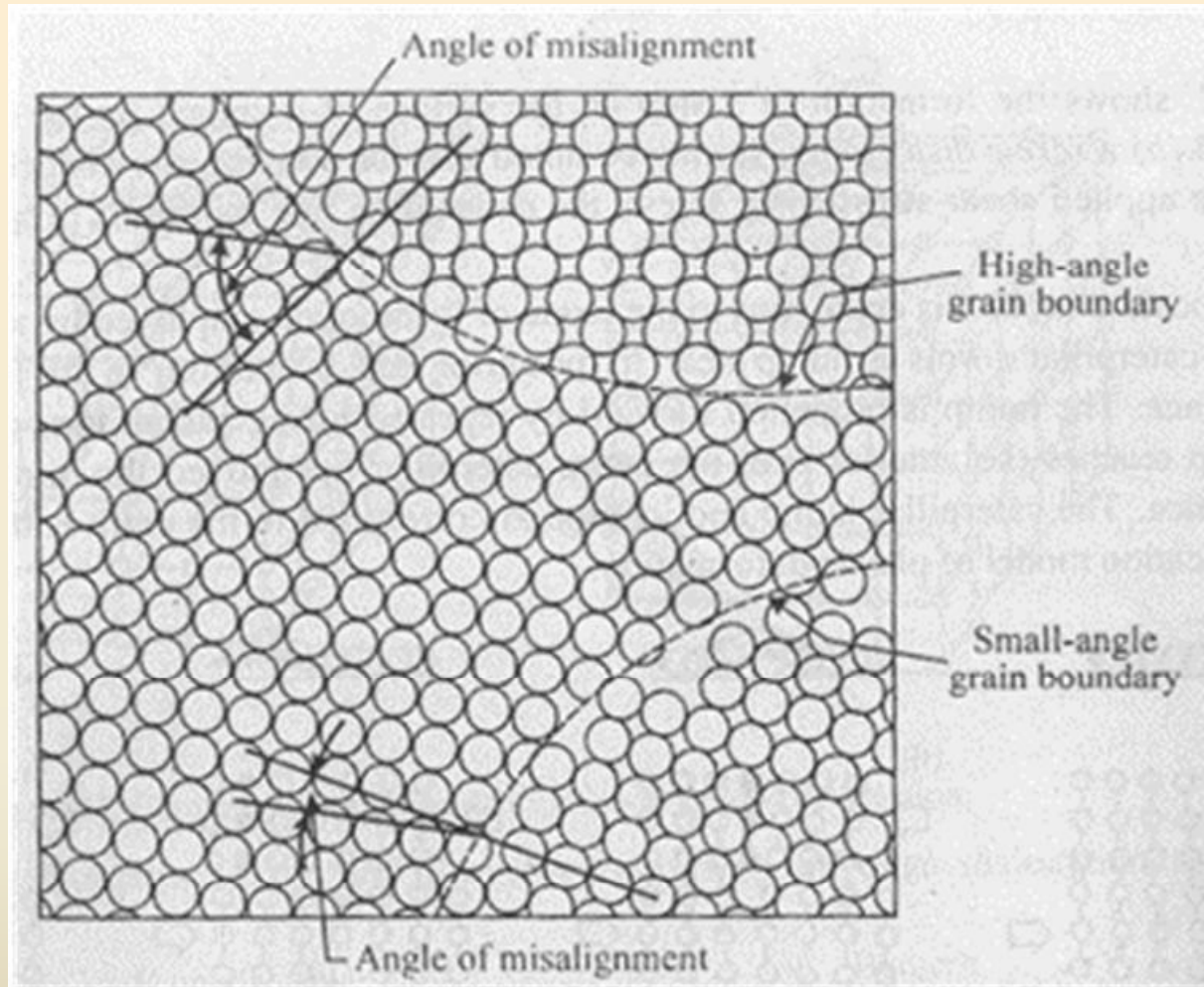
- **Defects or imperfections represented by a boundary**
- **External surface of material itself is an imperfection because atomic bonds do not extend beyond it**
- **Surface atoms do not have neighboring atoms on one side (as compared to atoms inside the material) and thus, have high energy (in the order of 1 J/m^2)**

(b). Internal Defects

▪ Grain Boundary Defect

- Imperfections, which separate crystals or grains of different orientation in polycrystalline aggregation during nucleation or crystallization
- Individual crystals with different orientation are called as '*Grains*', and boundary separating grains are called as '*Interface / Interface Boundary*'
- **Example:** copper metal

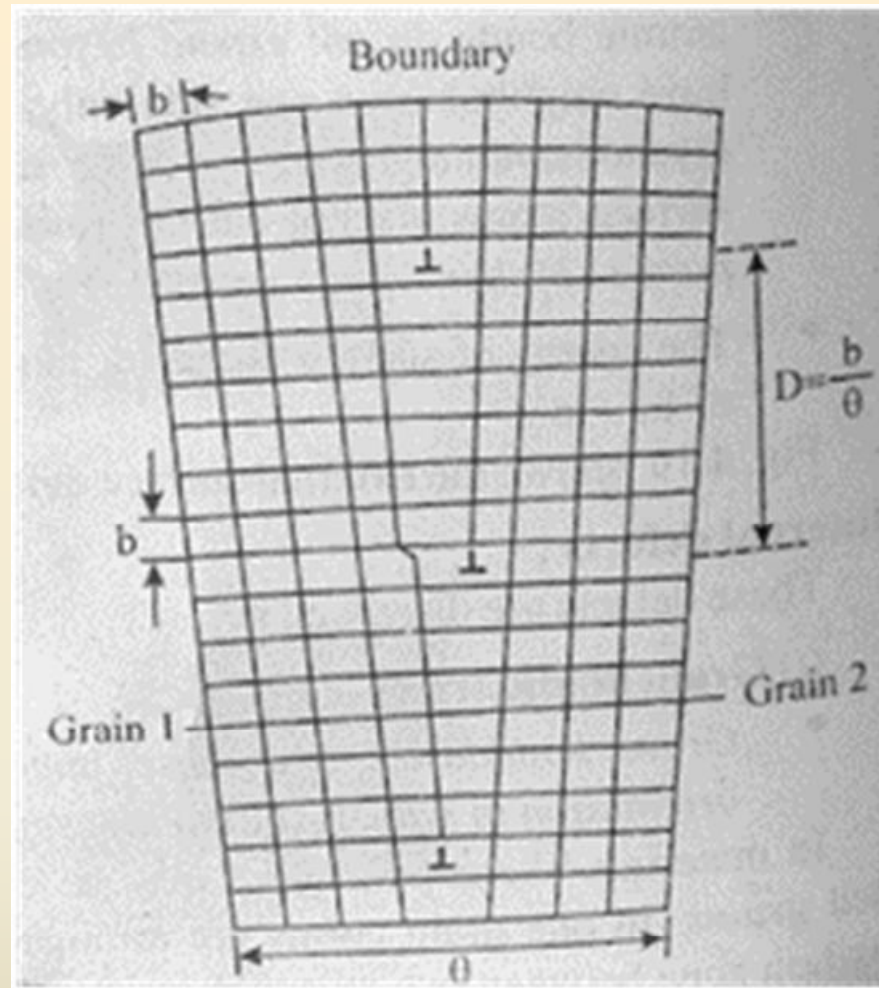
- **Atoms within a grain are arranged with one orientation and pattern, which does not aligns with orientation of atoms in neighboring grains**
- **Misalignment between adjacent grains may be of various degrees (small or high angle grain boundaries)**
- **Always a transition zones between two neighboring grains**
- **Leads to less efficient packing of atoms at boundary and thus, atoms at boundary have higher energy as compared to those at inside of grain boundaries**



Grain Boundary Defect

- **Tilt Boundary Defect**

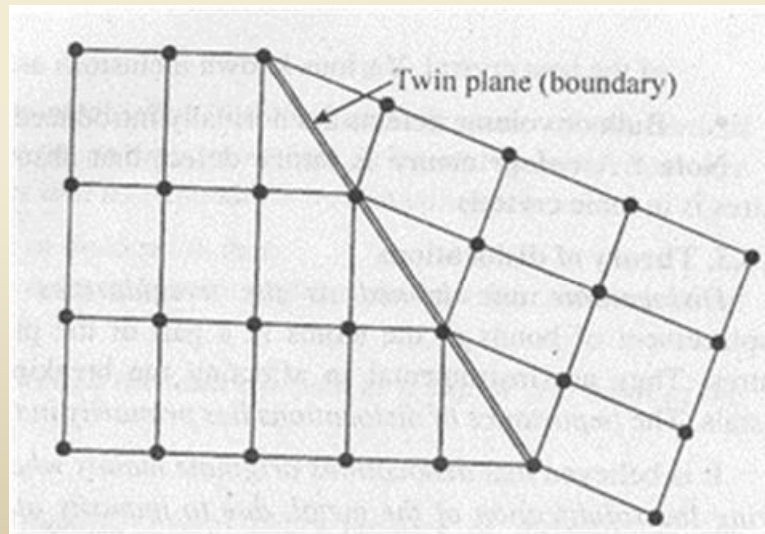
- Series of aligned dislocations, which tend to anchor (fasten) dislocation movements normally contributing to plastic deformation
- Associated with little energy
- Orientation difference between two neighboring grains is less than 10° , thus, it may be called as small / low angle grain boundary



Tilt Boundary Defect

▪ **Twin Boundary Defect**

- Special type of grain boundary across which, there is specific mirror lattice of symmetry, i.e. atoms on one side of boundary are located in mirror-image positions of atoms on other side
- Region of material between these boundaries is called as '**Twin**', which results due to basic twinning



- **Stacking Fault**

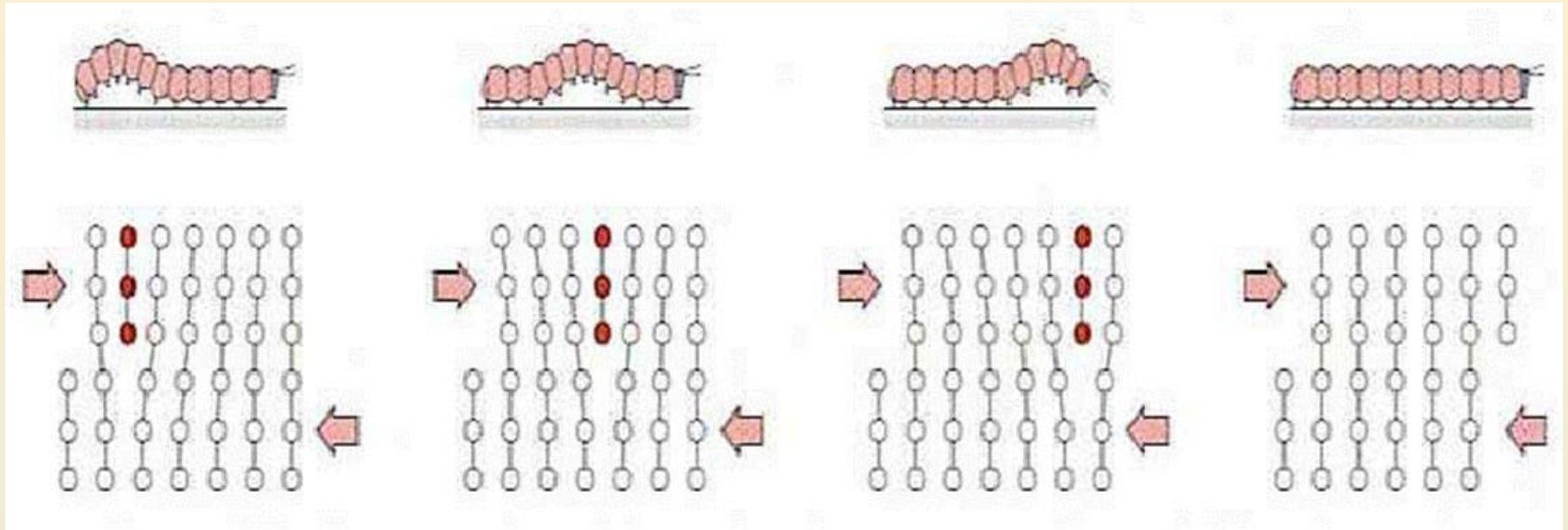
- Arise due to stacking of one atomic plane out of sequence on another, while lattice on either side of fault is perfect, i.e. one or more than one atomic plane may be missing from usual conventional style of stacking

- (iv). Volume Defects (Three Dimensional Defects)**

- Bulk defects, which includes pores, cracks, foreign inclusions or other phases

Slip by Dislocation Motion

- Slip is plastic deformation process produced by dislocation motion (Note: *Dislocations Can Move*)
- Dislocation motion is analogous to the mode of locomotion employed by caterpillar
- Caterpillar forms a hump near its posterior (later) end by pulling in its pair of legs unit leg distance and then this hump is propelled forward by repeating lifting and shifting of leg pairs
- When a hump moves forward, entire caterpillar moves forward by leg separation distance corresponding to extra half plane of atoms in its dislocation model of plastic deformation



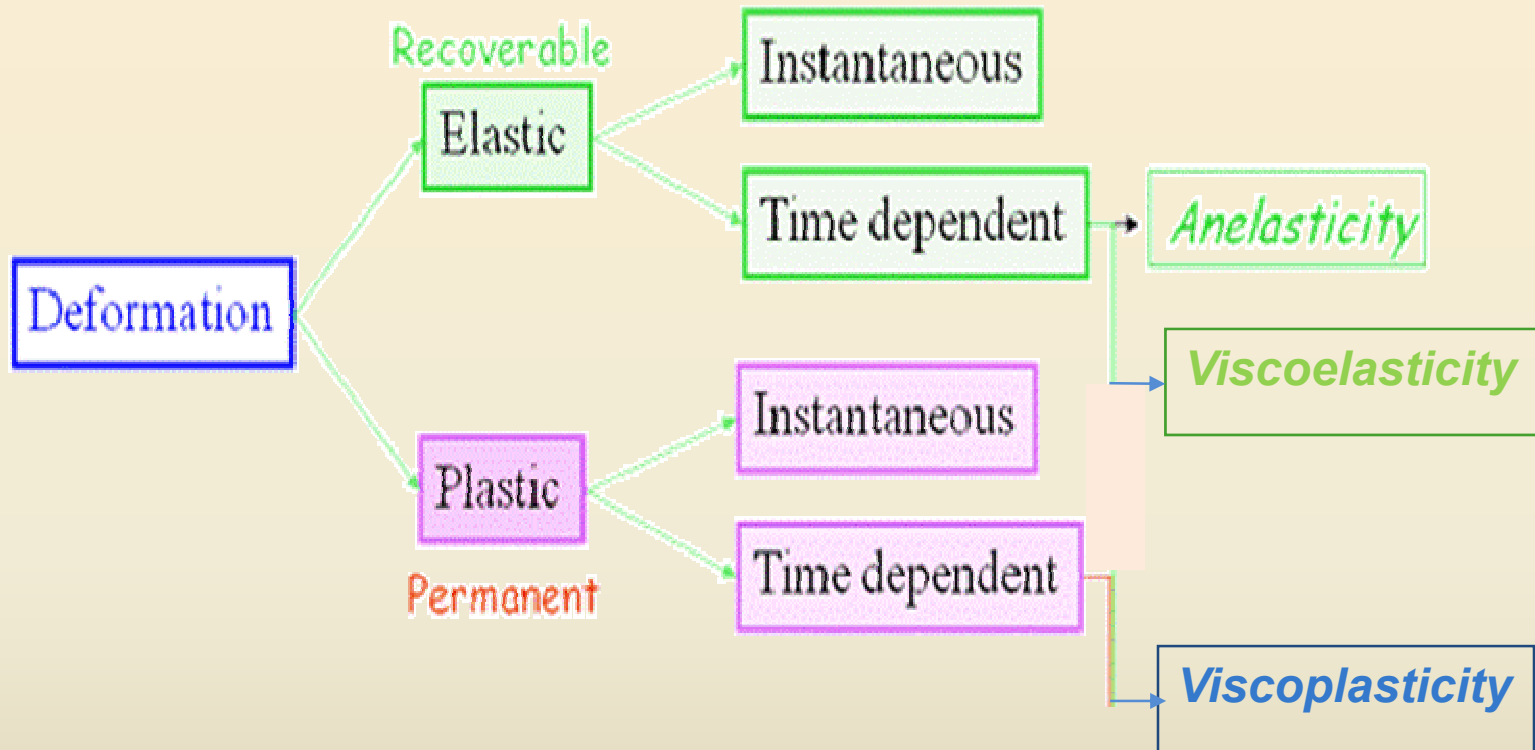
Analogy between Caterpillar & Dislocation Motion

4. Concept of Elastic & Plastic Deformation

Introduction:

- **Change in dimensions of material under action of applied forces**
- **Caused by mechanical action or by various physical and physio-chemical processes**
- **Deformed components are superior to cast components in performance**
- **Types: Elastic & Plastic deformations**

Classification of Deformation



Elastic Deformation

- Disappears, when load is removed & takes place before plastic deformation
- Strain is proportional to stress (*Hooke's Law*)
- Ratio of stress to strain is *Young's Modulus of Elasticity (E)*, which is a material characteristic (magnitude depends upon force of attraction between atoms of metal)
- Shear stress produces shear strains and ratio of shear stress to shear strain is *Shear Modulus of Rigidity (G)*
- Ratio of volumetric stress to volumetric strain is *Bulk Modulus of Elasticity (K)*

Young's Modulus of Elasticity

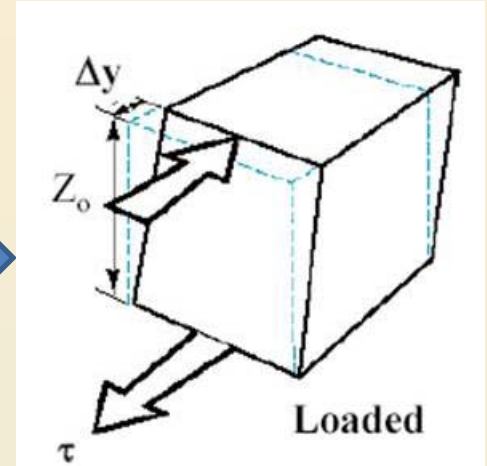
$$\nu = -\frac{\varepsilon_t}{\varepsilon_l}$$

Shear Modulus of Elasticity

$$G = \frac{E}{2(1+\nu)}$$

Bulk Modulus of Elasticity

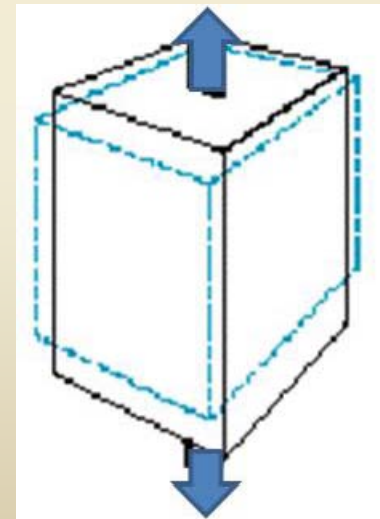
$$K = \frac{E}{3(1-2\nu)}$$



- **Perfect elastic material is one which regains back its original shape and size completely, after deforming force is removed**
- **During elastic deformation, material stores energy (strain or elastic energy), which is recovered, when load is removed**
- **Elastic strain energy is area under stress-strain curve (up to elastic limit)**

- **Materials subjected to tension shrink laterally & those subjected to compression, bulge**
- **Ratio of lateral and axial strains is called the Poisson's ratio (ν), which is a dimensionless quantity (sign shows that lateral strain is in opposite sense to longitudinal strain)**
- **Theoretical value is 0.25 & maximum value is 0.50 (typical value lies in between 0.24 to 0.30)**

$$\nu = -\frac{\epsilon_x}{\epsilon_z} = -\frac{\epsilon_y}{\epsilon_z}$$

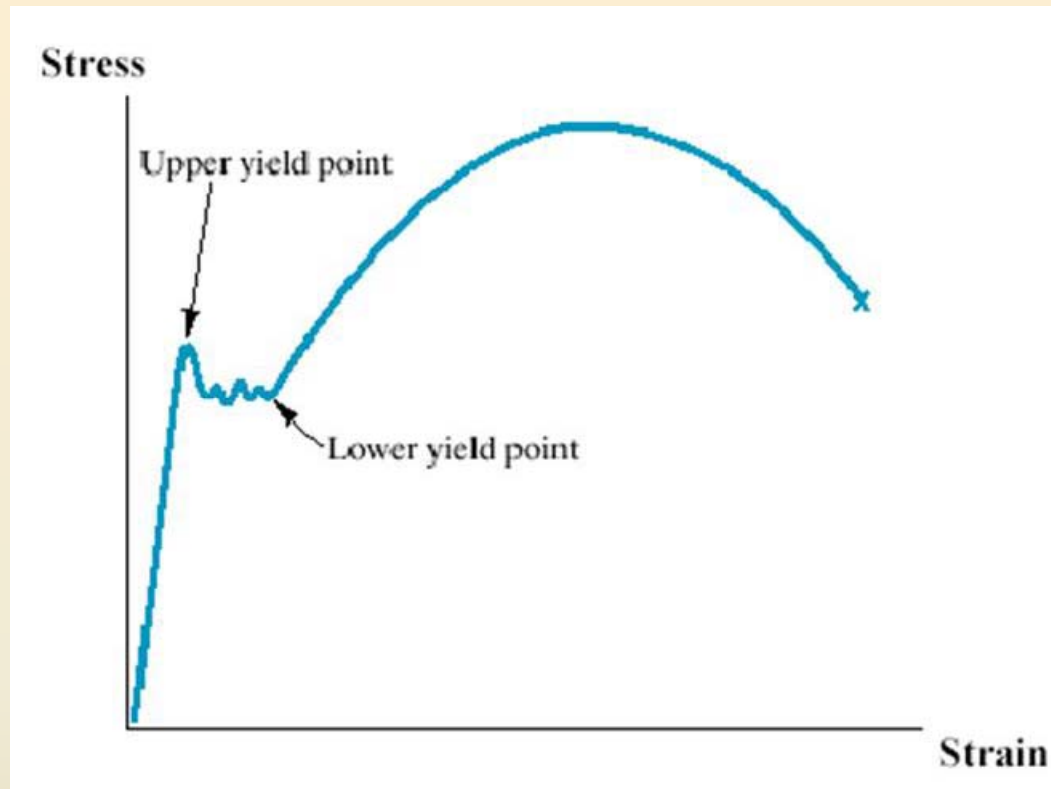


Plastic Deformation

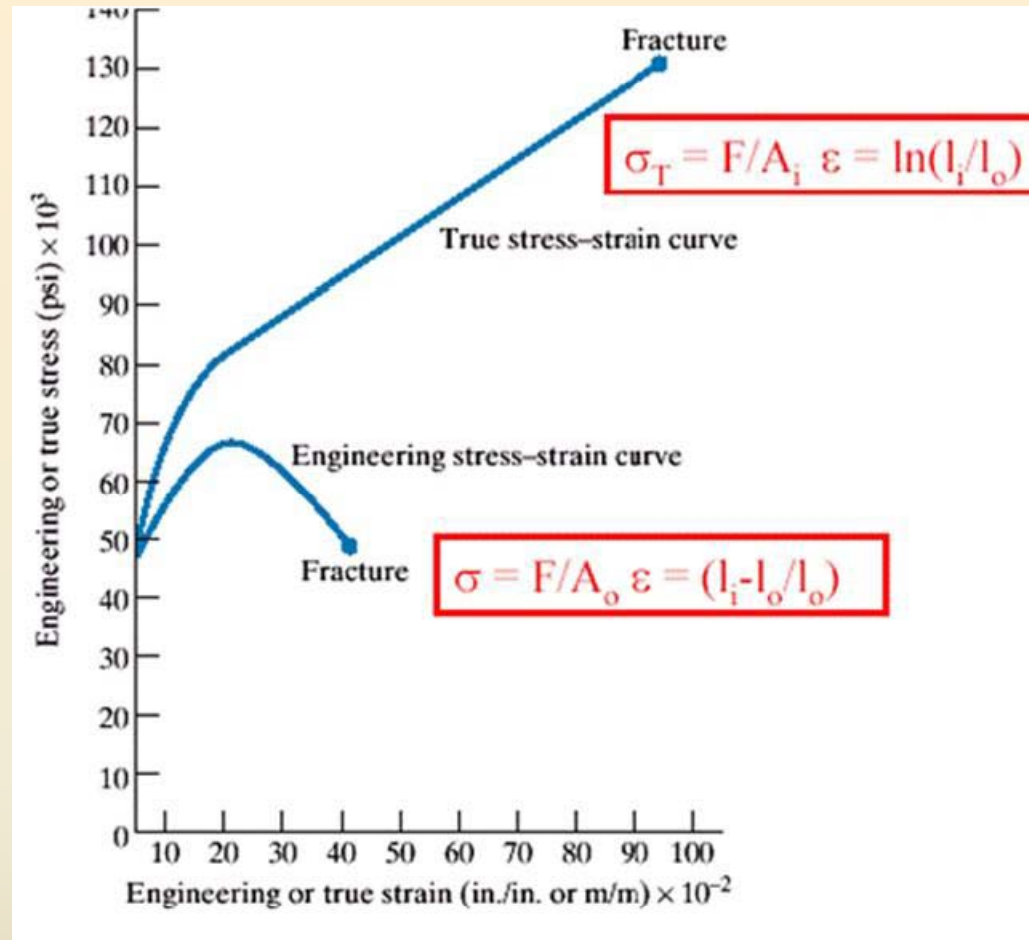
- **Permanent deformation, which persists even when deforming load is removed (function of stress, temperature & rate of straining)**
- **Caused by loads exceeding elastic limit & occurs after elastic deformation**
- **Non-linear relation between stress and strain (nature varies with material & deformation condition)**
- **Exhibit yield point phenomenon (yield stress)**
- **Continued plastic deformation leads to fracture (instantaneous fracture for brittle material & necking followed by fracture for ductile material)**

Yield Point Phenomenon

- Yielding starts at 1st higher point known as *Upper Yield Point* and 2nd lower point is known as *Lower Yield Point*
- Stress required to deform metal after yield point is always higher due to strain hardening, which causes curve to gradually rise upwards uptill ultimate tensile point (corresponding stress known as *Ultimate Tensile Strength*). After this specimen fails by fracture



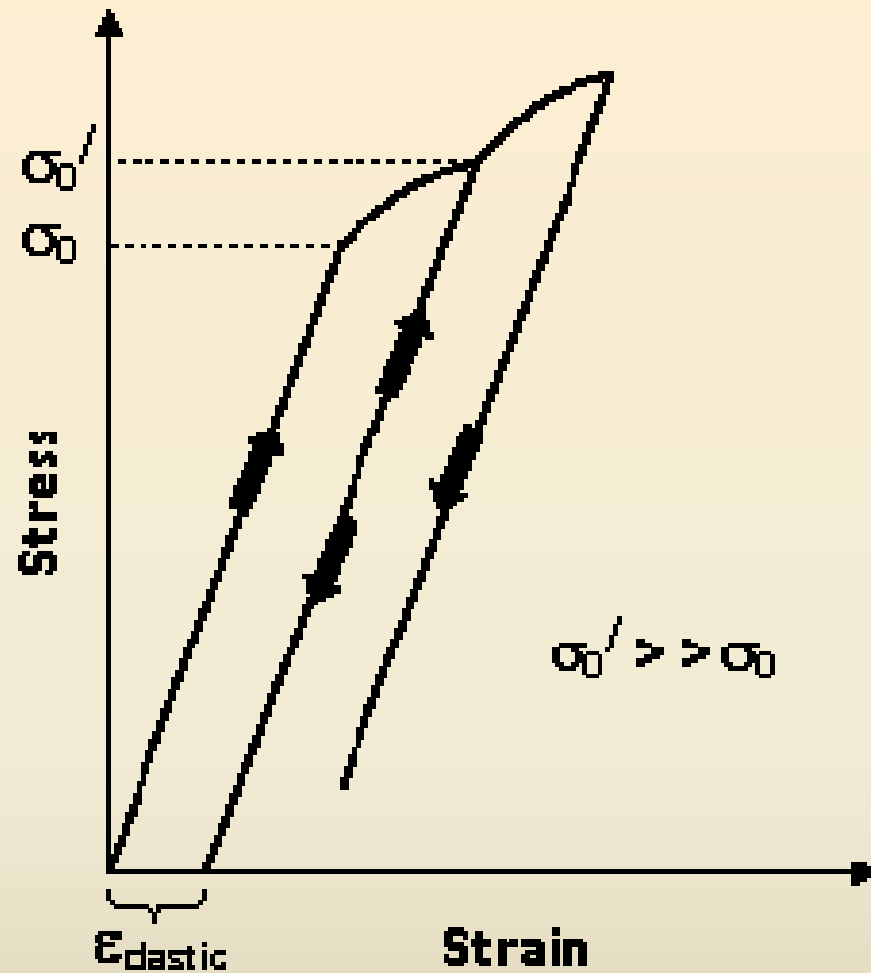
Stress-Strain curve for Mild Steel Specimen



True & Engineering Stress-Strain Curves

Strain Hardening

- Increase in yield stress of material when loaded subsequently in same direction again and again below recrystallization temperature
- When material is loaded in any direction (say tensile direction), it experiences linear elastic deformation till elastic limit. If load is removed, material comes back to its original shape and size and curve will retrace back loading path
- If material is further loaded (beyond yield stress ' σ_0 '), slight plastic deformation occurs leading to small permanent deformation. Now, if load is removed, material will retain this small plastic / permanent deformation and curve will not retrace original path, but will follow path parallel to original loading path

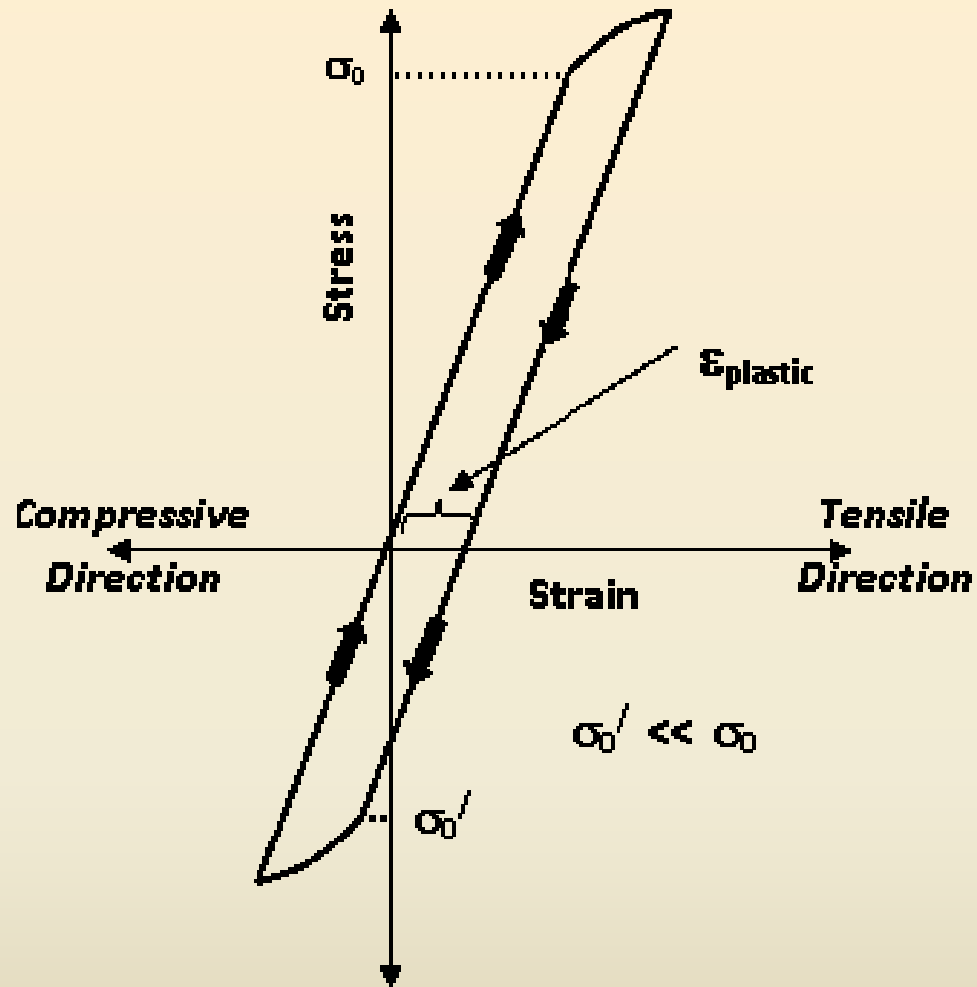


Strain Hardening

- If same material is loaded in same (tensile) direction again, it will start yielding at new yield stress ' σ_0' ', which will be higher than initial yield stress of material ' σ_0 '.
- This is because material becomes harder during plastic deformation by storing strain energy (some % of total deformation energy)
- Reduces ductility and plasticity of material
- At micro level, dislocation piles up during plastic deformation at slip planes, which interact with each other and create barriers to further motion / movement of dislocations through crystal lattice

Bauschinger Effect / Elastic Hysteresis

- **Decrease in yield stress of material when loaded initially in one direction (tensile) and then subsequently in opposite direction (compressive) below recrystallization temperature**
- **When a material is loaded in any direction (say tensile direction), it experiences linear elastic deformation till elastic limit. If it is further loaded (beyond yield stress ' σ_0 '), slight plastic deformation will occur leading to small permanent deformation**
- **Now, even if load is removed, material will retain this small plastic / permanent deformation and curve will not retrace original path, but will follow path parallel to original loading path**



Bauschinger Effect

- Further, loaded in opposite direction (compressive), it will start yielding at new yield stress ' σ_0' ', which will be very less than initial yield stress of material ' σ_0 '.
- This is because residual tensile stress stored in material during tensile loading need to be removed / compensated before elastic deformation in reversal (compressive) direction starts
- At micro level, dislocations piles up during tensile loading along at slip planes, which can be easily moved in opposite direction (compressive loading) by residual stresses

Anelasticity:

Time-dependent, recoverable low strain with linear behavior and relatively low damping

Viscoelasticity:

Time-dependent, recoverable higher strains with nonlinear behavior and higher damping

Viscoplasticity:

Time-dependent, non-recoverable strain with nonlinear behavior and higher damping

Superplasticity:

Materials demonstrate remarkably high strain to failure (strain rate around 0.001/s), generally at high temperatures ($T > 0.5 T_m$). It is used to form complex shapes, which are impossible to obtain using traditional methods like rolling, forging, extrusion or drawing processes, e.g. fuel tank of pulsar motorcycle

COLD WORKING

- **Mechanical processing of materials below its recrystallization temperature**
- **Produces improved surface finish and closer dimensional tolerance**
- **Grains are permanently distorted & residual stresses are set-up**
- **Heat treatment is must to restore original microstructure of metal**
- **Excessive cold working also leads to fracture before desired shape is imparted, hence it is carried at successive steps with intermediate heat treatment**
- **Example: drawing, squeezing, bending, shearing, hobbing, cold extrusion, shot peening etc**

HOT WORKING

- Mechanical processing of materials above its recrystallization temperature
- Work hardening effect is neutralized by effect of high temperature
- Facilitates metal forming at lower loads, power requirements
- High tooling life but costly operation
- Loss of metal due to scaling & no fine tolerances
- Defects like cavities, pores etc are removed
- More refined grain structure
- Example: hot rolling, hot forging, hot pipe bending, hot piercing, hot spinning, hot extrusion etc

DIFFERENCE

COLD WORKING	HOT WORKING
Carried below recrystallization temp.	Carried above recrystallization temp.
Hardening is not eliminated, rather accompanied by strain hardening	Strain hardening is completely eliminated
Elongation, area reduction, ductility and impact strength are reduced	Ductility, elongation, area reduction and impact strength are increased
Crystallization does not occur	Crystallization occurs again
Uniformity of material is lost and properties are greatly affected	Grain refinement occurs
Chances of crack propagation is more	Cracks and defects like blow holes, cavities are welded
Increases ultimate tensile strength, yield point, hardness, fatigue strength	Does not affect ultimate tensile strength, yield point, hardness, fatigue strength

Resistance to corrosion decreases due to presence of residual stresses	Resistance to corrosion is not affected
Internal and residual stresses are produced	Internal and residual stresses are not produced
Load and energy requirements are high	Load and energy requirements are low
Tooling life is decreased	High tooling life
Less costly	High cost operation
No oxidation of metal occurs	High scaling and oxidation occurs
No metal loss	High metal loss
Surface decarbonization of steel does not occur	Surface decarbonization of steel occurs
Good surface finish	Surface finish is not good
Easy to control dimensions within tolerance limits	Difficult to control dimensions within tolerance limits
Material handling is easy	Material handling is difficult