

# MATERIAL SCIENCE AND ENGINEERING



## UNIT 1

# INTRODUCTION OF MATERIALS

---

**Dr. SWATI GANGWAR**

**Mr. KAPIL KUMAR**

Department Of Mechanical Engineering, MMMUT Gorakhpur

## **BME-11 MATERIAL SCIENCE AND ENGINEERING**

<b>Course category</b>	: Basic Science & Maths (BSM)
<b>Pre-requisite Subject</b>	: NIL
<b>Contact hours/week</b>	: Lecture : 3, Tutorial : 1 , Practical: 2
<b>Number of Credits</b>	: 5
<b>Course Assessment methods</b>	: Continuous assessment through tutorials, attendance, home assignments, quizzes, practical work, record, viva voce and Three Minor tests and One Major Theory & Practical Examination
<b>Course Outcomes</b>	: The students are expected to be able to demonstrate the following knowledge, skills and attitudes after completing this course

1. Understand the importance of numerous materials with their basic concepts including crystallography and imperfections.
2. The understanding about the advanced materials testing by different testing methods such as strength, hardness, fatigue, NDT, etc.
3. The knowledge of different surface behavior studies of engineering materials including heat treatment processes, TTT diagram and other related processes.
4. The knowledge of different concepts regarding materials and electrical, magnetic, electronic, etc. properties.

## **UNIT-I**

9

### **Introduction**

Historical perspective, importance of materials, Crystallography and imperfections: Concept of unit cell, space lattice, Bravais lattices, common crystal structures, Atomic packing factor and density. Miller indices, X-ray crystallography techniques, imperfections, Defects & Dislocations in solids

## **UNIT-II**

9

### **Mechanical Properties and Testing**

Stress strain diagram, Ductile and brittle materials, stress Vs strength, toughness, hardness, fracture, fatigue and creep. Testing, such as Strength testing, Hardness testing, Impact tests, Fatigue testing Creep testing, Non-destructive testing (NDT). Performance of materials in service: Brief theoretical consideration of fracture, fatigue, and corrosion and its control.

### **Micro Structural Examination**

Microscope principle and methods, Preparation of samples and microstructure exam and grain size determination, comparative study of microstructure of various metals and alloys, such as Mild steel, CI, Brass.

### **Phase Diagram and Equilibrium Diagram**

Unary and Binary diagrams, Phase rules, Types of equilibrium diagrams: solid solution type, eutectic type and combination type, Iron-carbon equilibrium diagram.

## **UNIT-III**

9

### **Ferrous & Non-ferrous materials**

Iron and steel manufacture, furnaces, various types of carbon steels, alloy steels and cast irons, its properties and uses. 3 Heat Treatment: various types of heat treatment, such as Annealing, Normalizing, Quenching, Tempering and Case hardening. Time Temperature Transformation (TTT) diagrams.

### **Non-Ferrous metals and alloys**

Non-ferrous metals, such as Cu, Al, Zn, Cr, Ni etc. and its applications

## **UNIT-IV**

9

### **Magnetic properties**

Concept of magnetism- Dia, para, ferro magnetic materials, Hysteresis, Soft and hard magnetic materials, Magnetic Storages.

### **Electrical Properties**

Energy band, concept of conductor, insulator and semi conductor. Intrinsic and extrinsic semi-conductors, P-n junction and transistors, Basic devices and their applications. diffusion of Solid, Super conductivity and its applications, Messier effect. Type I & II superconductors. High Temp. superconductors

Brief description of other material such as optical and thermal materials, Composite Materials and its uses. Smart materials & Nano-materials and their potential applications

## **EXPERIMENTS**

**Minimum Eight experiments are to be conducted from the following:**

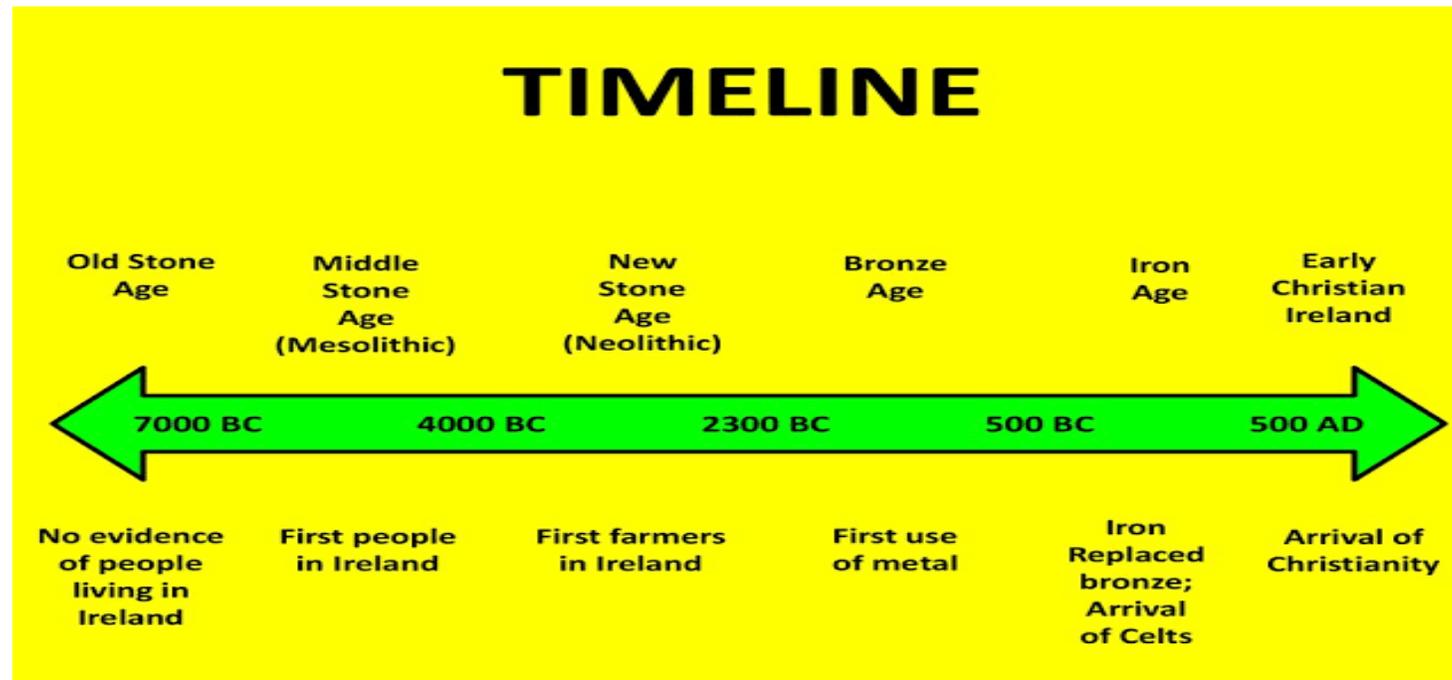
1. Tensile test on universal testing machine
2. Compressive on universal testing machine
3. Torsion test of a rod on torsion testing machine
4. Creep test on creep testing machine
5. Fatigue test on fatigue testing machine
6. Hardness testing of given specimen on Vicker/Brinell/Rockwell hardness testing machine
7. Determination of deflection of cantilever under point/uniformly distributed loading
8. Determination of deflection of beam under point/uniformly distributed loading
9. Study of corrosion and its effects.
10. Comparative study of microstructures of different specimens of different materials (mild steel, gray C.I., brass, copper etc.)
11. Study of heat treatment processes such as annealing, normalizing, quenching, case hardening and comparison of hardness before and after heat treatment.
12. Study of non destructive testing methods such as ultrasonic flaw detector, magnetic flaw detector and eddy current testing machine

## **Books & References**

1. Material Science and Engineering – Smith, Hashemi and Prakash (Tata McGraw Hill)
2. Material Science- Narula (Tata McGraw Hill)
3. Material Science for Engineering Students- Fischer (Academic Press)
4. Material Science & Engineering - Van Vlash (John Wiley & Sons)
5. Elements of Material Science & Engineering -W.D. Callister (Wiley India Pvt. Ltd.)
6. Technology of Engineering Materials- Philip and Bolton (Butterworth-Heinamann)
7. Material Science -V. Raghvan (Prentice Hall of India)
8. Elements of Material Science & Engineering- Van Vlack (Pearson)

## Historical Perspective

- Materials are so important in the **development of human civilization** that the historians have identified early periods of civilization by the name of most significantly used material. Materials constitute foundation of technology.
- The history of human civilization evolved from the **Stone Age to the Bronze Age, the Iron Age, the Steel Age, and to the Space Age** (contemporaneous with the Electronic Age). Each age is marked by the advent of certain materials.



- From the historical point of view, it can be said that **human civilization started with *Stone Age*** where people used only natural materials, like stone, clay, skin, and wood for the purposes like to make weapons, instruments, shelter, etc.
- However, the increasing need for better quality tools brought forth exploration that led to ***Bronze Age***, followed by ***Iron Age***.
- When people found copper and how to make it harder by alloying, **the *Bronze Age* started about 3000 BC.**



*Stone age tools and materials*



*Bronze Age tools and materials*

- **The use of iron and steel**, a stronger material that gave advantage in wars **started at about 1200 BC**. Iron was abundant and thus availability is not limited to the affluent.
- This commonness of the material affected every person in many aspects, gaining the name *democratic material*. One of the most significant features of the *democratic material* is that number of users just exploded.
- The next big step in human civilization was the **discovery of a cheap process to make steel around 1850 AD**, which enabled the railroads and the building of the modern infrastructure of the industrial world.

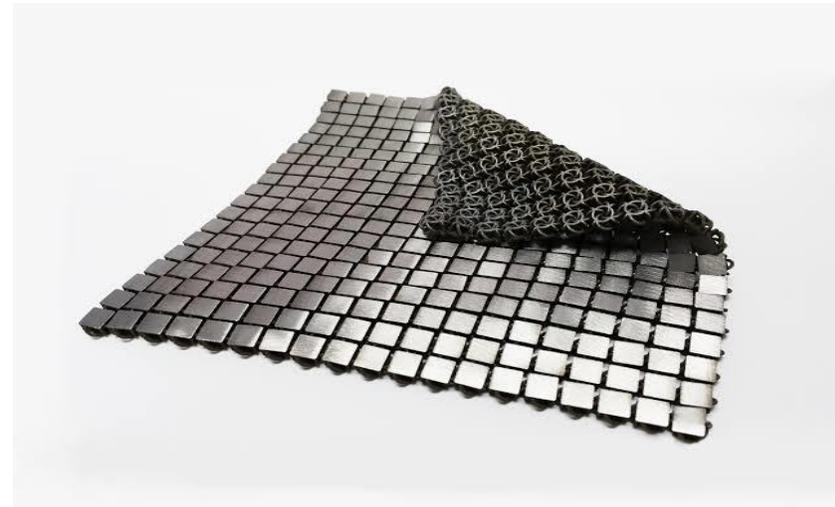


**Iron age tools**

- The **Iron Age** brought tools and utensils.
- The **Steel Age** brought railroads, instruments, and the Industrial Revolution.
- The **Space Age** brought the materials for stronger and light structures (e.g., composite materials).
- The **Electronic Age** brought semiconductors, and thus many varieties of electronic gadgets.
- We are presently in **Space Age** marked by many technological developments towards development materials resulting in **stronger and light materials** like composites, electronic materials like semiconductors, materials for space voyage like high temperature ceramics, biomaterials, etc.



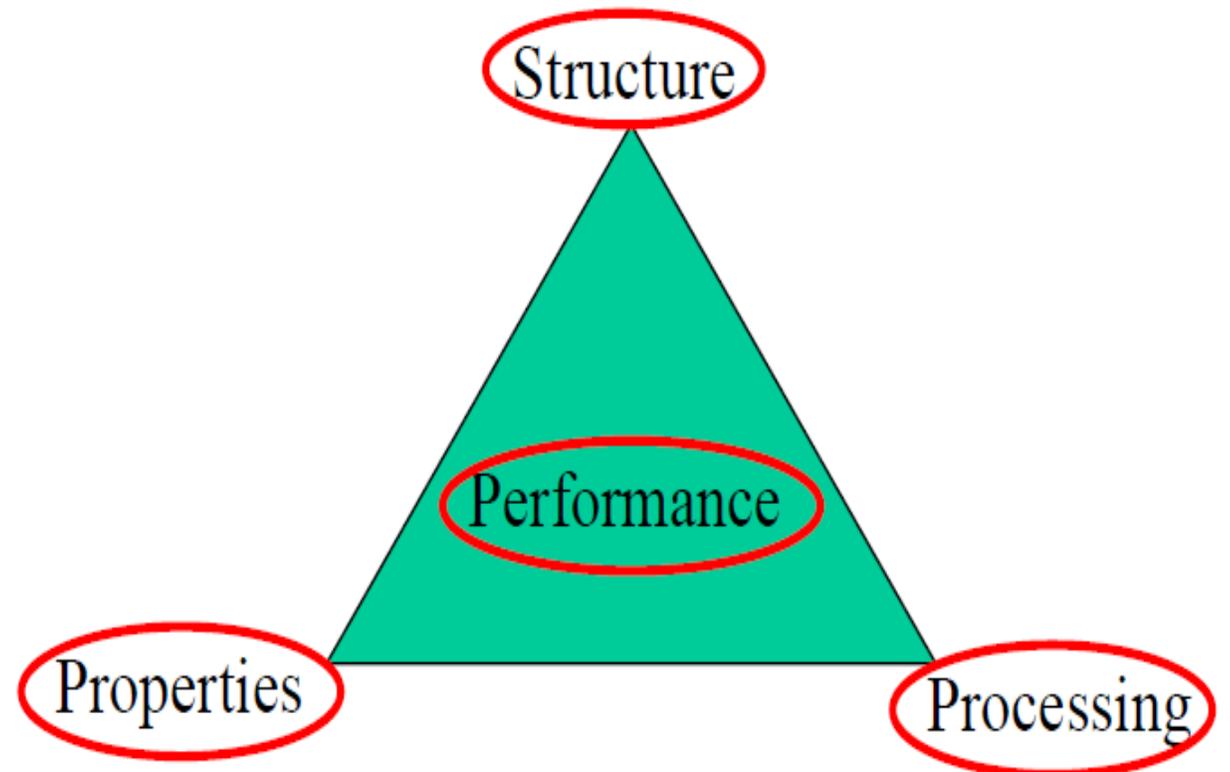
Lightest wheel chair material



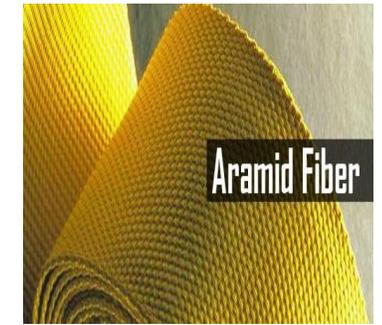
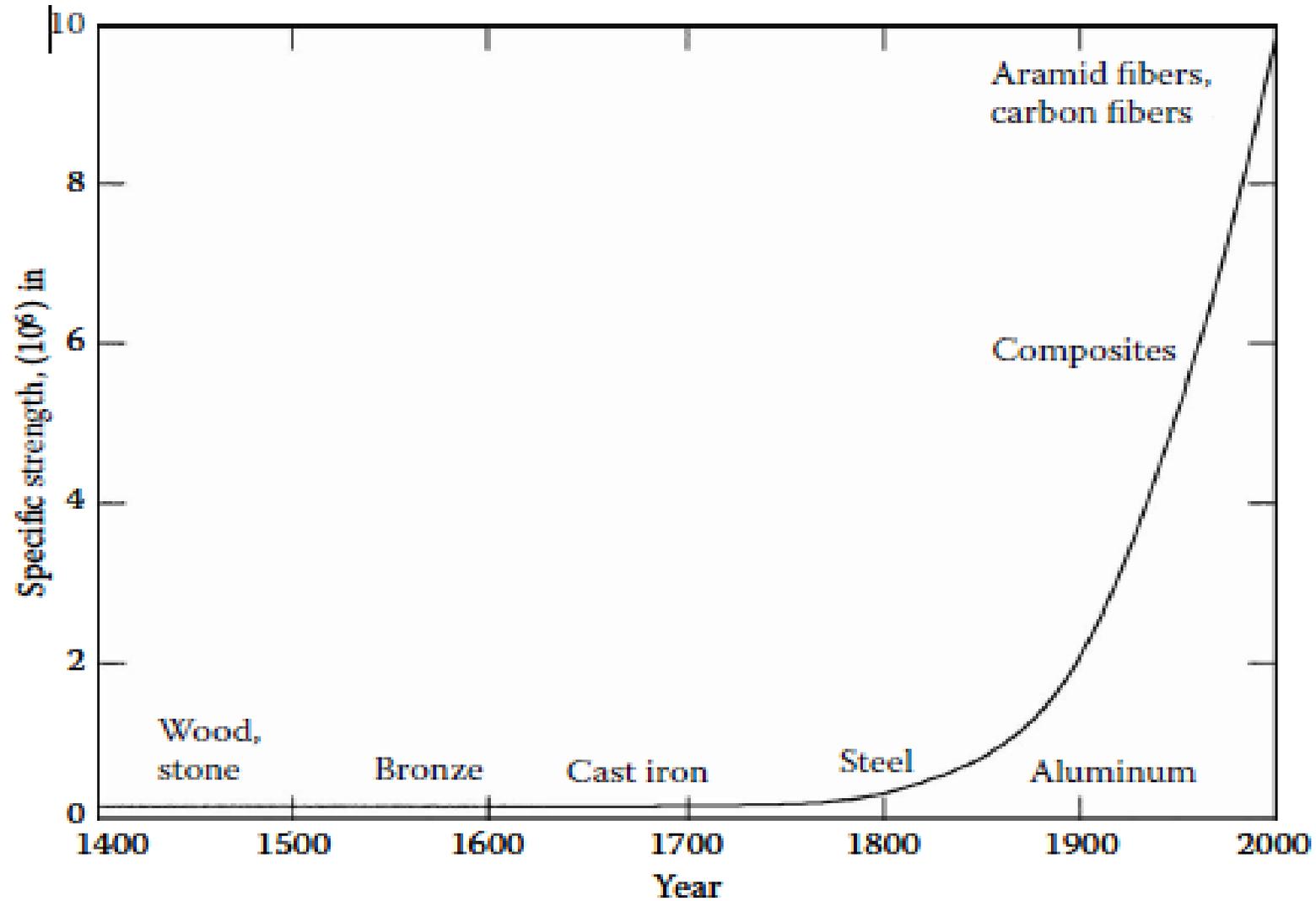
3D printed space fabric material

## *Materials Science*

- As engineering materials constitute foundation of technology, it's not only necessary but a must to understand how materials behave like they do and why they differ in properties.
- This is only possible with the atomistic understanding allowed by quantum mechanics that first explained atoms and then solids starting in the 1930s.
- The combination of physics, chemistry, and the focus on the relationship between the properties of a material and its microstructure is the domain of Materials Science.



**Interrelation between four components of Materials Science.**



Variation of specific strength as a function of time of use of materials

## *Why Study Materials Science and Engineering?*

- All engineers need to know about materials. Even the most "immaterial", like software or system engineering depend on the development of new materials, which in turn alter the economics, like software-hardware trade-offs.
- Increasing applications of system engineering are in materials manufacturing (industrial engineering) and complex environmental systems.
- Thus it is very important that every engineer must study and understand the concepts of Materials Science and Engineering. This enables the engineer
  - To select a material for a given use based on considerations of cost and performance.
  - To understand the limits of materials and the change of their properties with use.
  - To be able to create a new material that will have some desirable properties.
  - To be able to use the material for different application.

# *Classification of Materials*

materials can classify based on many criteria, for example crystal structure (arrangement of atoms and bonds between them), or properties, or use.

- Metals,
- Ceramics,
- Polymers,
- Composites,
- Semiconductors, and
- Biomaterials.

# ENGINEERING MATERIAL



**Ceramic (bottle)**



**Metal (can)**

**Polymer**



## Metals:

These materials are characterized by

- High thermal and electrical conductivity;
  - Strong yet deformable under applied mechanical loads;
  - Opaque to light (shiny if polished).
- These characteristics are due to valence electrons that are detached from atoms, and spread in an *electron sea* that *glues* the ions together, i.e. atoms are bound together by metallic bonds and weaker vanderwalls forces.
- Pure metals are not good enough for many applications, especially structural applications. Thus metals are used in alloy form i.e. a metal mixed with another metal to improve the desired qualities. E.g.: aluminum, steel, brass, gold.



# Metallic Material



## *Ceramics:*

- These are inorganic compounds, and usually made either of oxides, carbides, nitrides, or silicates of metals. Ceramics are typically partly crystalline and partly amorphous.
- Atoms (ions often) in ceramic materials behave mostly like either positive or negative ions, and are bound by very strong Coulomb forces between them.

These materials are characterized by

- Very high strength under compression,
- Low ductility;
- Usually insulators to heat and electricity.

Examples: Glass, porcelain, many minerals.

# Ceramic material



## *Polymers:*

- Polymers in the form of thermo-plastics (nylon, polyethylene, polyvinyl chloride, rubber, etc.) consist of molecules that have covalent bonding within each molecule and van der Waals forces between them. Polymers in the form of thermo-sets (e.g., epoxy, phenolics, etc.) consist of a network of covalent bonds.
- They are based on H, C and other non-metallic elements.
- Polymers are amorphous, except for a minority of thermoplastics.
- Due to the kind of bonding, polymers are typically electrical and thermal insulators.
- However, conducting polymers can be obtained by doping, and conducting polymer-matrix composites can be obtained by the use of conducting fillers.
- They decompose at moderate temperatures (100 – 400 C), and are lightweight.

# Polymer material



## *Composite materials:*

- Composite materials are multiphase materials obtained by artificial combination of different materials to attain properties that the individual components cannot attain. E.g. lightweight brake disc obtained by embedding SiC particles in Al-alloy matrix, Reinforced cement concrete, a structural composite obtained by combining cement (the matrix, i.e., the binder, obtained by a reaction known as hydration, between cement and water), sand (fine aggregate), gravel (coarse aggregate), and, thick steel fibers.
- However, there are some natural composites available in nature, for example – wood.
- In general, composites are classified according to their matrix materials. The main classes of composites are
  - **Metal-matrix composites,**
  - **Polymer-matrix composites and**
  - **Ceramic-matrix composites.**

# APPLICATION OF COMPOSITES

The applications of composite materials continue to be of increasing importance due to the industry's need for modern analysis and improved performance



BULLET PROOF VEST



AIRCRAFTS



AUTOMOBILE PARTS



BOATS HULLS



SPORT'S KITS



BUILDING CONSTRUCTION

# **Biomaterials:**

➤ These are any type material that can be used for replacement of damaged or diseased human body parts. Primary requirement of these materials is that they must be biocompatible with body tissues, and must not produce toxic substances.

➤ Other important material factors are:

- Ability to support forces;
- Low friction,
- Wear,
- Density,
- Cost; and
- Reproducibility.



Typical applications involve heart valves, hip joints, dental implants, intraocular lenses.

Examples: **Stainless steel, Co-28Cr-6Mo, Ti-6Al-4V, ultra high molecular weight poly-ethelene, high purity dense Al-oxide, etc.**

## *Advanced Materials*

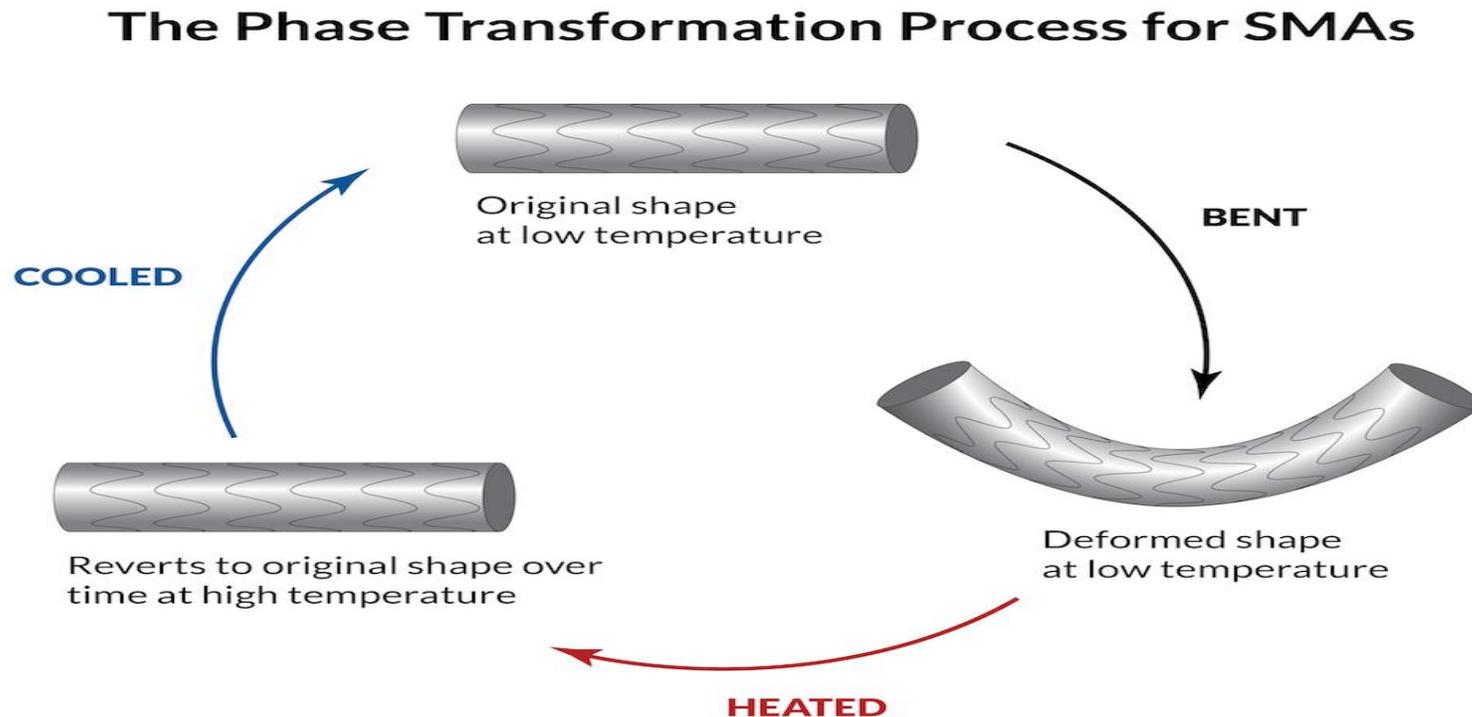
- These are materials used in *High-Tech* devices those operate based on relatively intricate and sophisticated principles (e.g. computers, air/space-crafts, electronic gadgets, etc.).
- These materials are either traditional materials with enhanced properties or newly developed materials with high-performance capabilities. Hence these are relatively expensive.
- Typical applications: Integrated circuits, lasers, Liquid crystal display's (LCDs), fiber optics, thermal protection for space shuttle, etc. Examples: **Metallic foams, inter-metallic compounds, multi-component alloys, magnetic alloys, special ceramics and high temperature materials, etc.**

# *Future Materials*

- Group of new and state-of-the-art materials now being developed, and expected to have significant influence on present-day technologies, especially in the fields of medicine, manufacturing and defense.
- **Smart/Intelligent material** system consists some **type of sensor** (*detects an input*) and an **actuator** (*performs responsive and adaptive function*).
- **Actuators** may be called upon to change shape, position, natural frequency, mechanical characteristics in response to changes in temperature, electric/magnetic fields, moisture, pH, etc.
- **Four types of materials used as actuators:**
  - Shape memory alloys,
  - Piezo-electric ceramics,
  - Magneto-strictive materials,
  - Electro-/Magneto-rheological fluids.

# Shape memory alloys

- Shape memory alloy is an alloy
- SMA is one of the type of smart material
- SMA are materials that remember their original shapes
- If deformed, they recover their original shape upon heating
- Different shapes like bars, wires, plates and rings etc. could be made from SMA.



## ➤ **Materials / Devices used as sensors:**

- **Optical fibers,**
- **Piezo-electric materials,**
- **Micro-electro-mechanical systems (MEMS), etc.**

## **Typical applications:**

- By incorporating sensors, actuators and chip processors into system, researchers are able to stimulate biological human-like behavior; Fibers for bridges, buildings, and wood utility poles;
- They also help in fast moving and accurate robot parts, high speed helicopter rotor blades; Actuators that control chatter in precision machine tools; Small microelectronic circuits in machines ranging from computers to photolithography prints; Health monitoring detecting the success or failure of a product.

## *Modern Materials needs*

➤ Though there has been tremendous progress over the decades in the field of materials science and engineering, innovation of new technologies, and need for better performances of existing technologies demands much more from the materials field. More over it is evident that new materials/technologies are needed to be environmental friendly. Some typical needs, thus, of modern materials needs are listed in the following:

- Engine efficiency increases at high temperatures: requires **high temperature structural materials**
- Use of **nuclear energy requires** solving problem with residues, or advances in nuclear waste processing.
- **Hypersonic flight** requires materials that are light, strong and resist high temperatures.
- **Optical communications** require optical fibers that absorb light negligibly.
- **Civil construction** – materials for unbreakable windows.
- **Structures:** materials that are strong like metals and resist corrosion like plastics.

# MATERIAL SCIENCE AND ENGINEERING



## UNIT 1

# INTRODUCTION TO CRYSTALLOGRAPHY

---

**Dr. SWATI GANGWAR**

**Mr. KAPIL KUMAR**

Department Of Mechanical Engineering, MMMUT Gorakhpur

# Why we study Crystallography?

It is useful for the identification of minerals. The later are chemical substances formed under natural conditions and have crystal forms.



**Crystallography is of major importance to a wide range of scientific disciplines including physics, chemistry, molecular biology, materials science and mineralogy.**

**Study of crystals can provide new chemical information. In laboratories and industry, we can prepare pure chemical substances by crystallization process.**

**It is very useful for solid state studies of materials.**

- **CRYSTALLOGRAPHY** is simply a fancy word meaning "the study of crystals"
- The study of crystalline solids and the principles that govern their growth, external shape, and internal structure
- Crystallography is easily divided into 3 sections
  - geometrical, physical, and chemical.

# ***MATERIALS AND PACKING***

- The materials classified into two categories:

## **Crystalline materials**

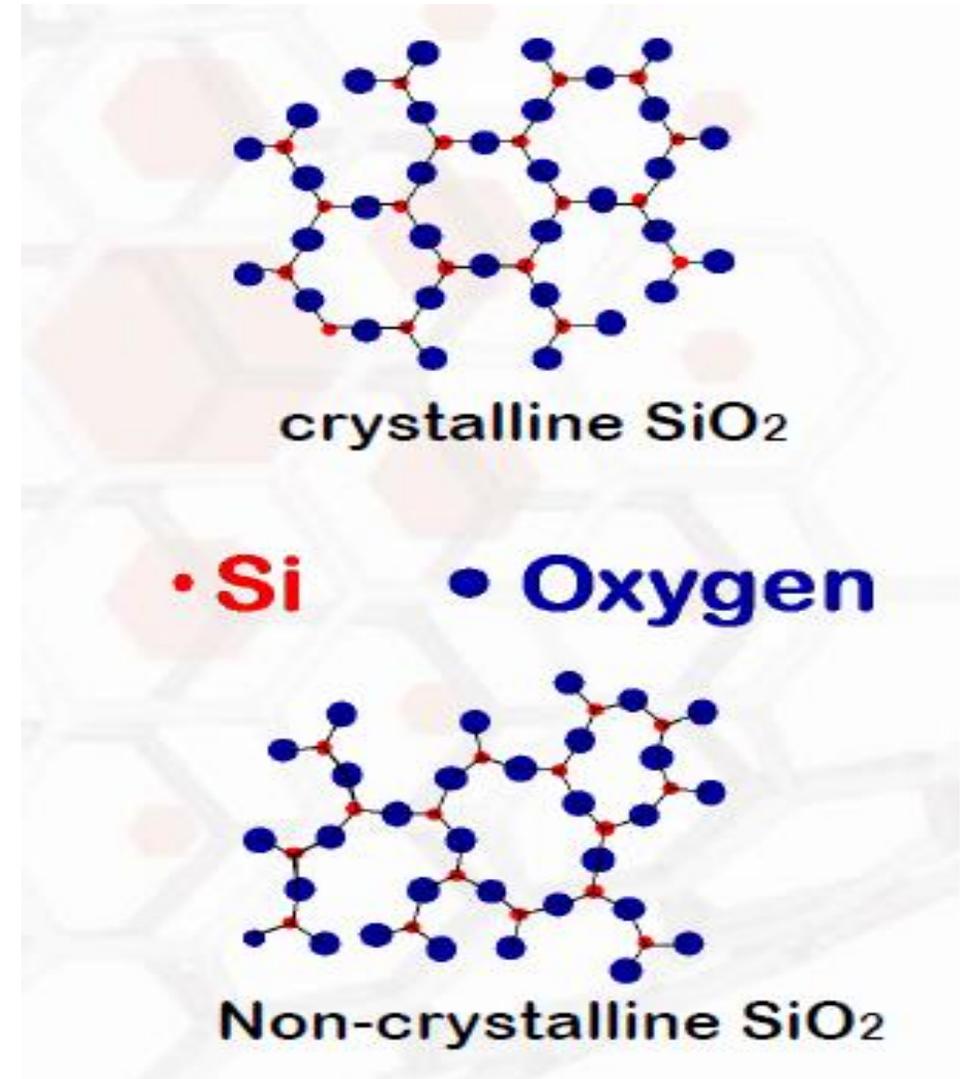
- The atoms are ordered
- Short range and long range order
- Deviations from the perfect order are of importance for the properties of the materials.

Examples: Metals, some ceramics and polymers etc.

## **Amorphous materials/Non-crystalline materials**

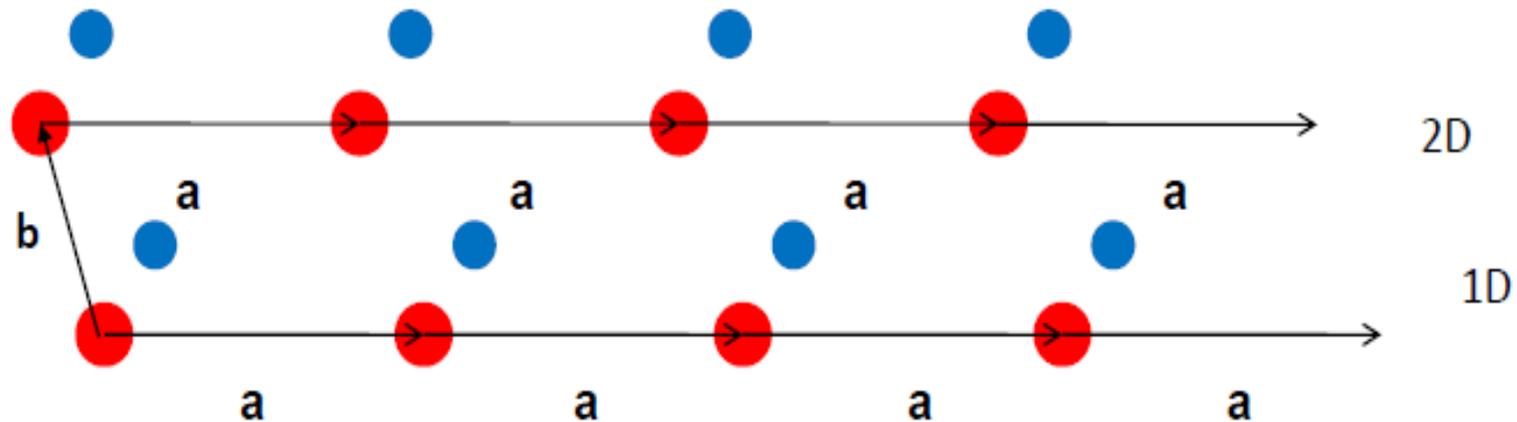
- The atoms are "randomly" distributed in space.
- Not quite true, there is short range order.
- **Complex structures**
- **Rapid cooling**

Examples: Glass, polystyrene etc.



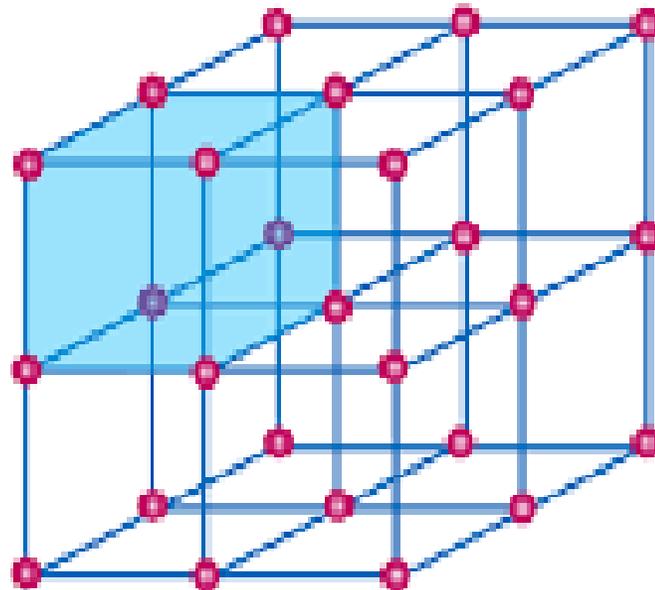
# Introduction to crystallography

- **Crystallography** describes and characterizes the structure of crystals.
- Basic concept is symmetry
- *Translational symmetry*: if you are standing at one point in a crystal, and move a distance (vector)  $a$  the crystal will look exactly the same as where you started.



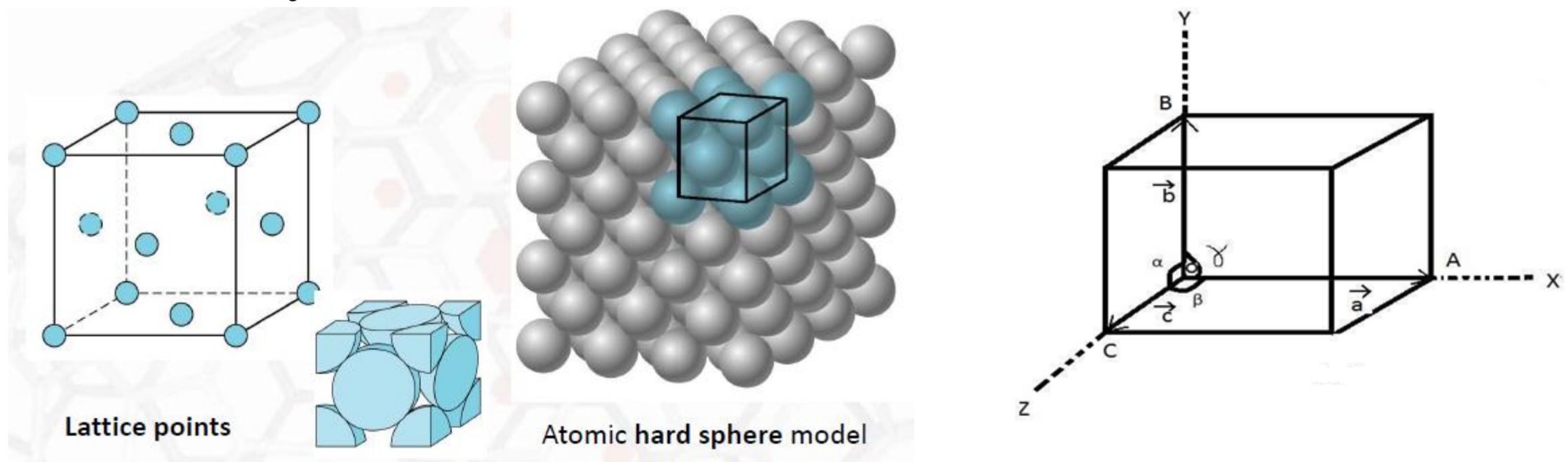
# The lattice

- A periodic pattern of points in space, such that each lattice point has identical surroundings.
- Each of these points represents one or a group of atoms, basis.



# Unit Cell

- Unit cell is the *smallest* unit of volume that permits **identical** cells to be stacked together *to fill all space*.
- By *repeating* the pattern of the unit cell over and over in all directions, the entire **crystal** lattice can be constructed.

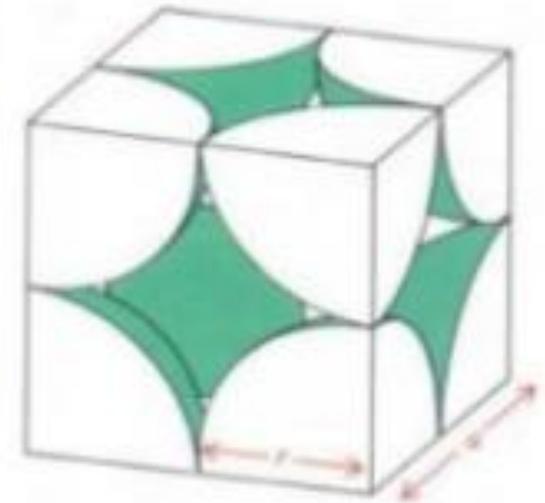
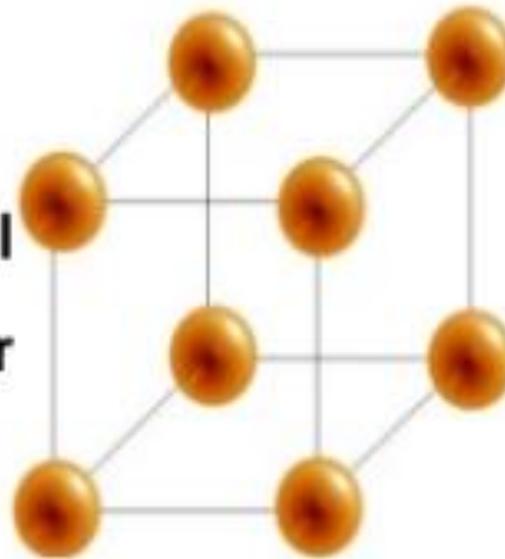


## UNIT CELL TYPES

Primitive lattice (P)  
Centered lattice (I):

- Primitive lattice (P) :

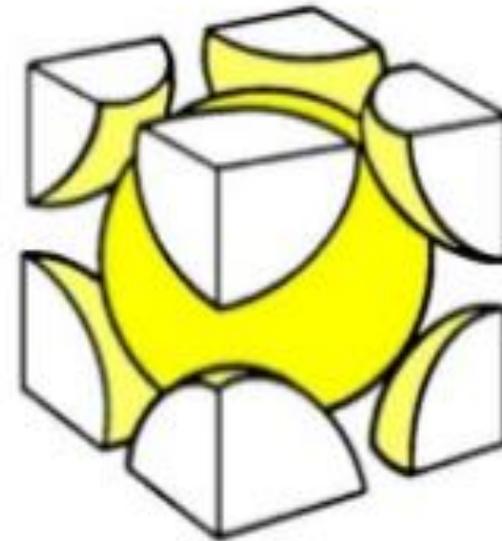
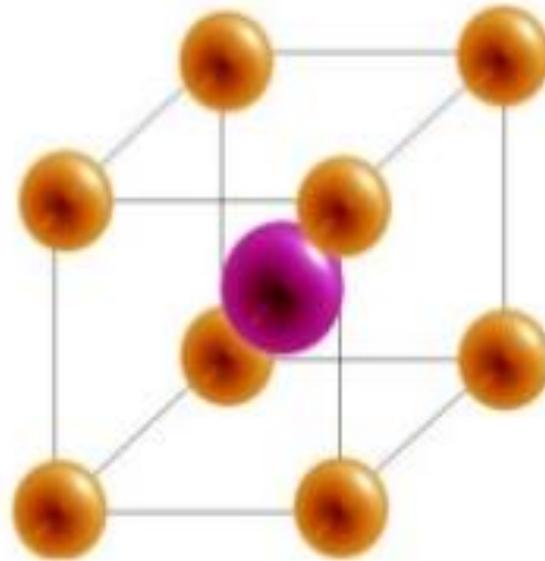
In this lattice the unit cell consists of eight corner atoms.



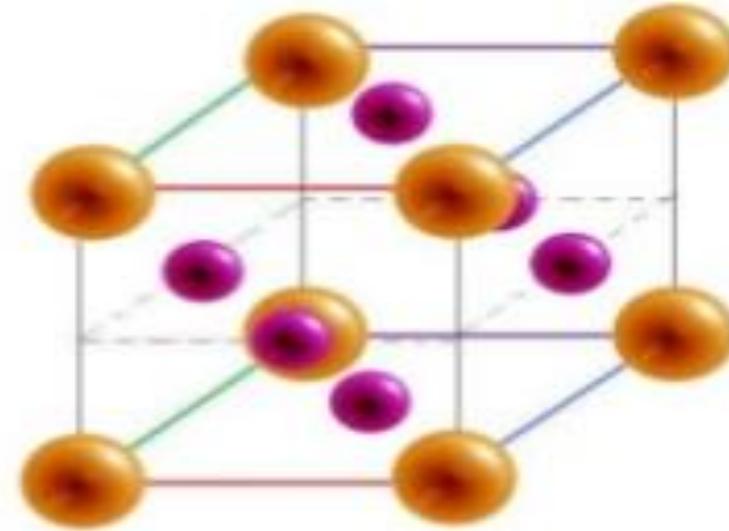
## Centered lattice (I):

- Body Centered Unit Cells
- Face Centered Unit Cells
- End Centered Unit Cells

Body Centered Unit Cells(B)

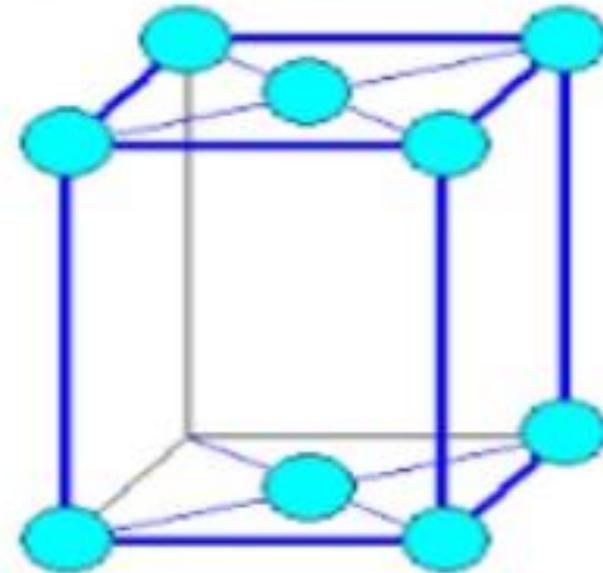


## Face Centered lattice (F):

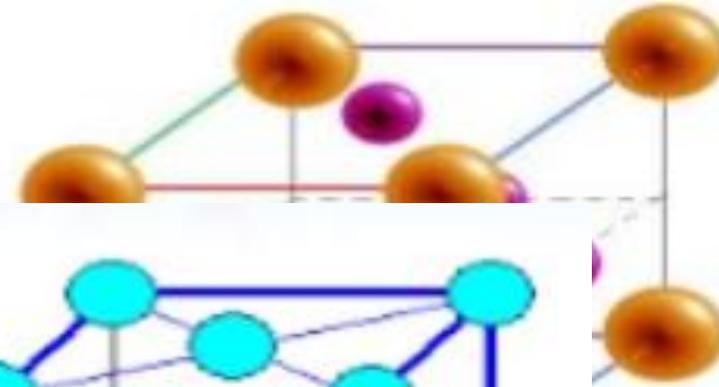


## Base Centered lattice (C):

In this lattice along with the corner atoms, the base and opposite face will have centre atoms

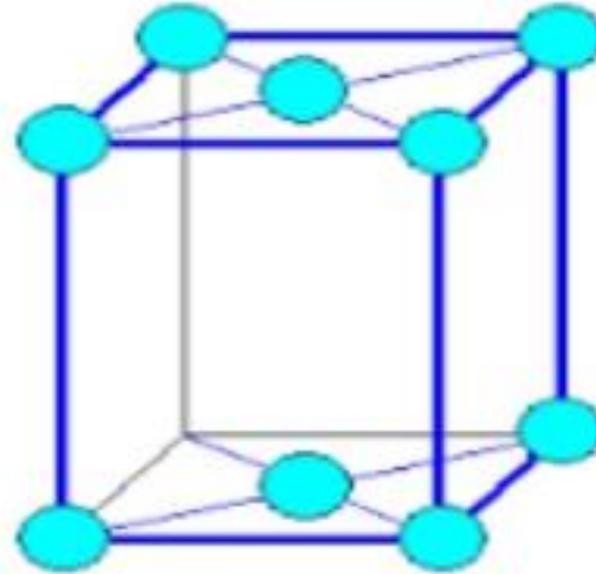


## Face Centered lattice (F):

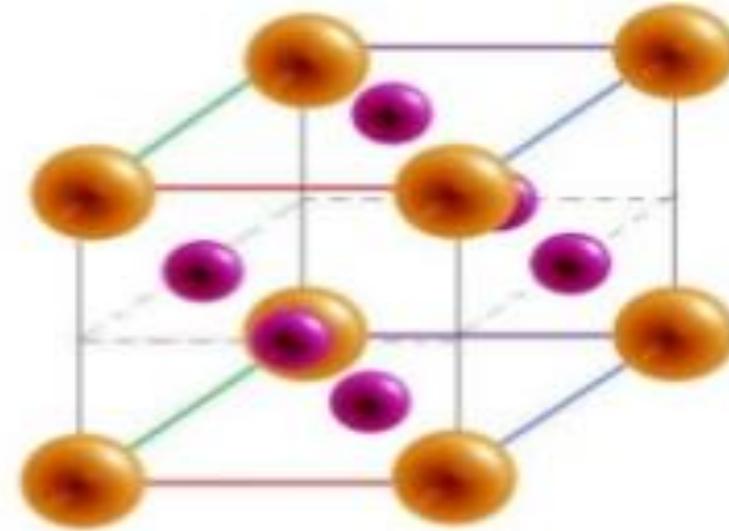


## Base Centered lattice (C):

In this lattice along with the corner atoms, the base and opposite face will have centre atoms

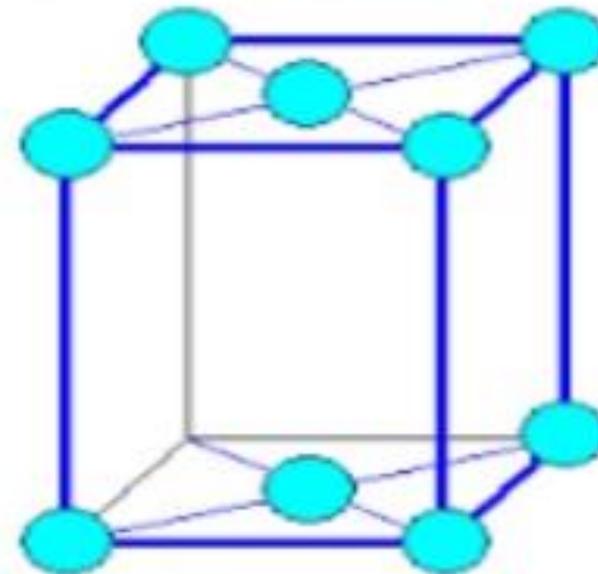


## Face Centered lattice (F):



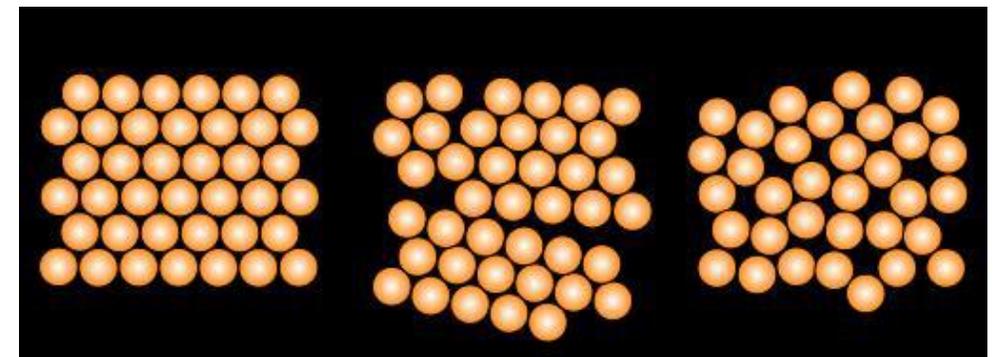
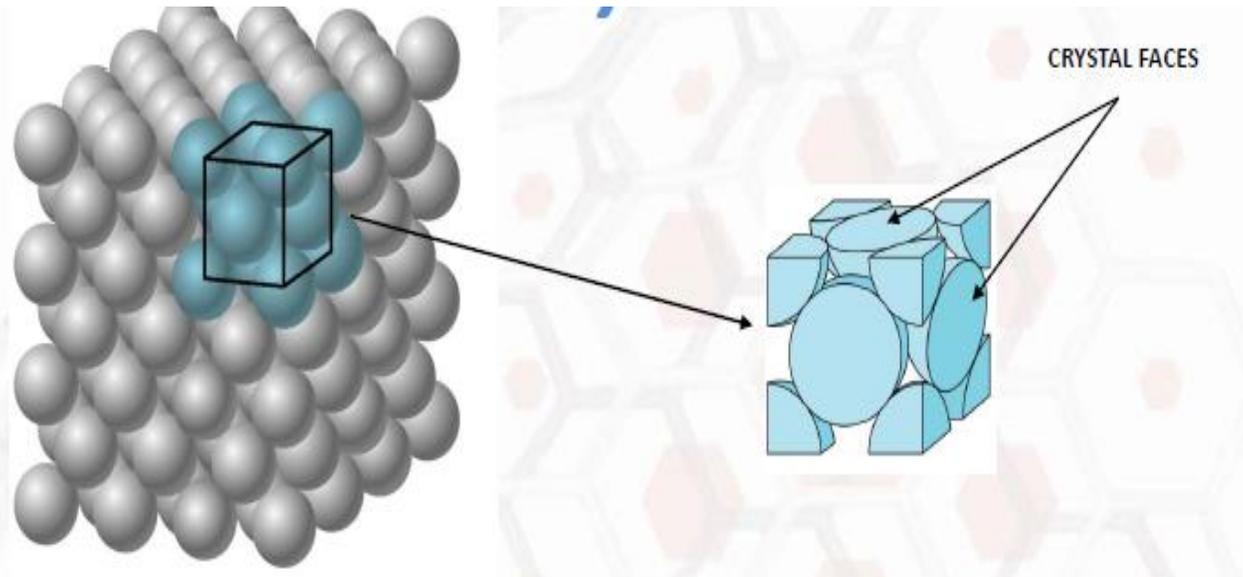
## Base Centered lattice (C):

In this lattice along with the corner atoms, the base and opposite face will have centre atoms



# Crystal

- A **CRYSTAL** is any solid material in which the component atoms are arranged in a *definite pattern* and whose surface regularity reflects its *internal symmetry*.



# Crystal Systems

- Goal is to Quantitatively Describe
- *(a) Shape* and *Size* of the Unit Cell (**point symmetry**).
- *(b) Location* of the *Lattice Points* (**translational symmetry**).
  
- **What we will do ?**
- For *(a)* to specify the **Crystal System** and the **Lattice Parameters**.
- For *(b)* to define the “**Bravais**” **Lattice**.

# The Crystal Systems

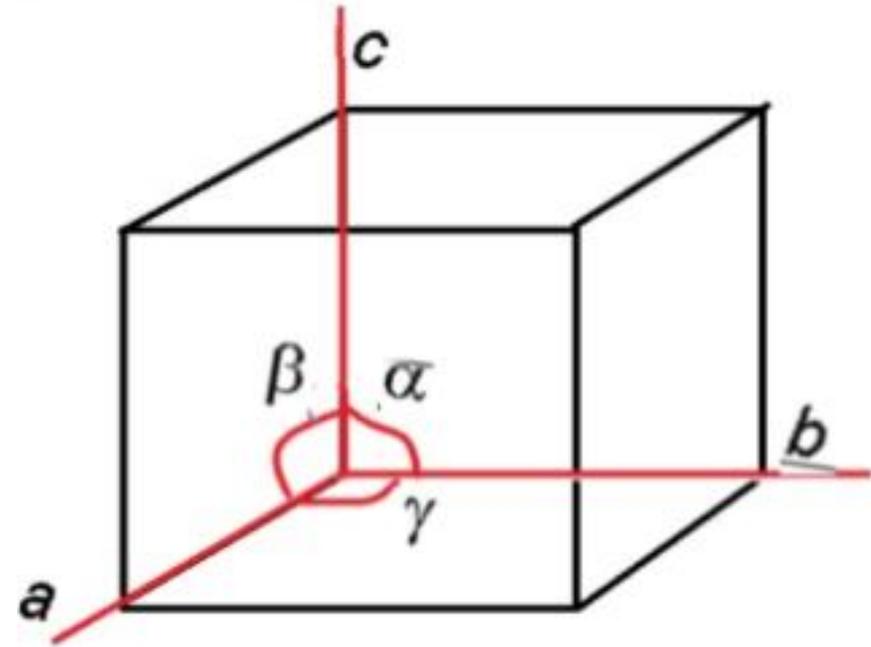
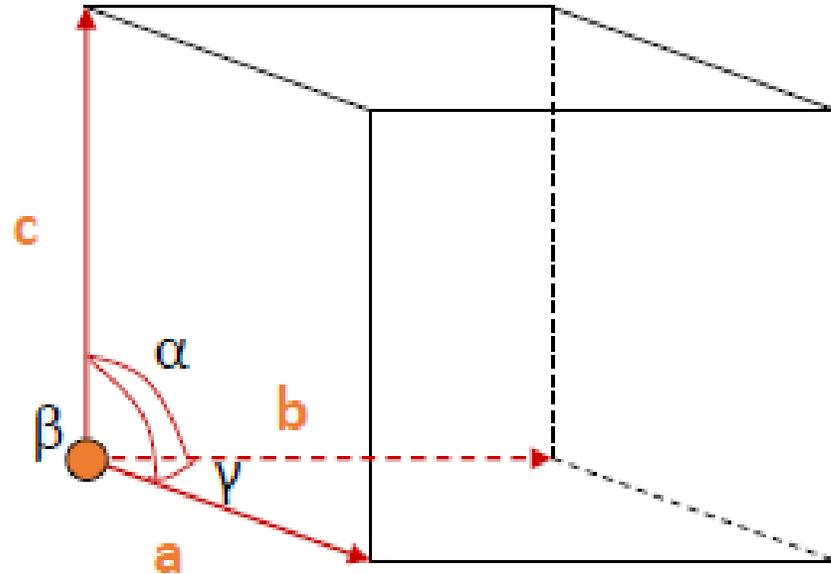
- In turn these symmetry classes, because some of them show similarities among each other, are divided among the different *Crystal Systems*.

## Crystal System

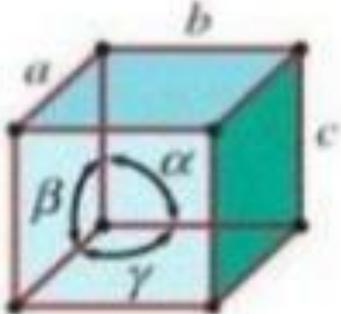
1. The **CUBIC** (also called **Isometric system**)
2. The **TETRAGONAL** system
3. The **HEXAGONAL** system
4. The **ORTHORHOMBIC** system
5. The **MONOCLINIC** system
6. The **TRICLINIC** system
7. The **RHOMBOHEDRAL** System

Every Crystal System involves a number of Crystal Classes.

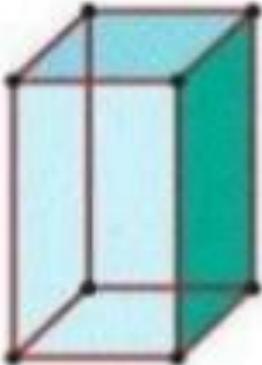
# CRYSTALLOGRAPHIC AXES



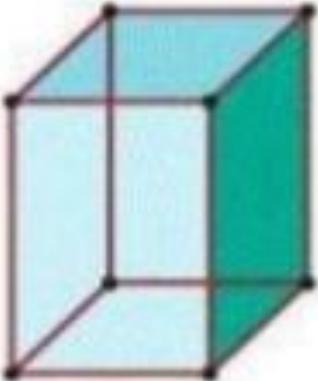
# The Crystal Systems



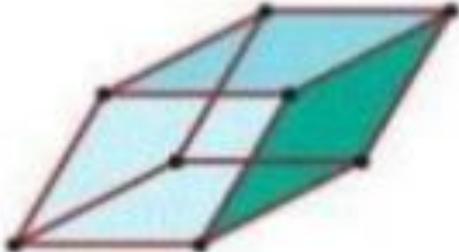
**Simple cubic**  
 $a = b = c$   
 $\alpha = \beta = \gamma = 90^\circ$



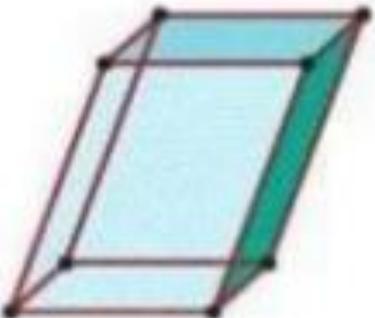
**Tetragonal**  
 $a = b \neq c$   
 $\alpha = \beta = \gamma = 90^\circ$



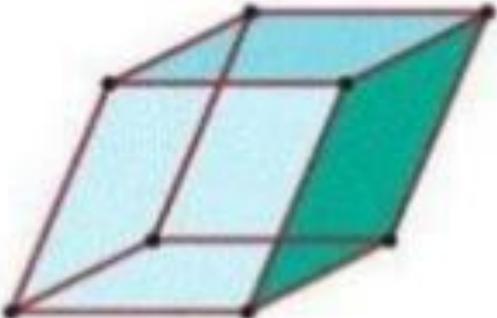
**Orthorhombic**  
 $a \neq b \neq c$   
 $\alpha = \beta = \gamma = 90^\circ$



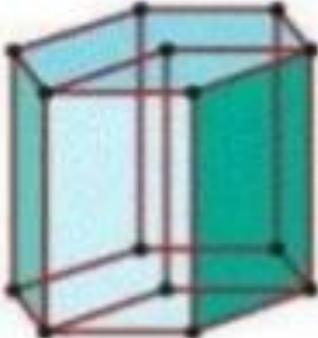
**Rhombohedral**  
 $a = b = c$   
 $\alpha = \beta = \gamma \neq 90^\circ$



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



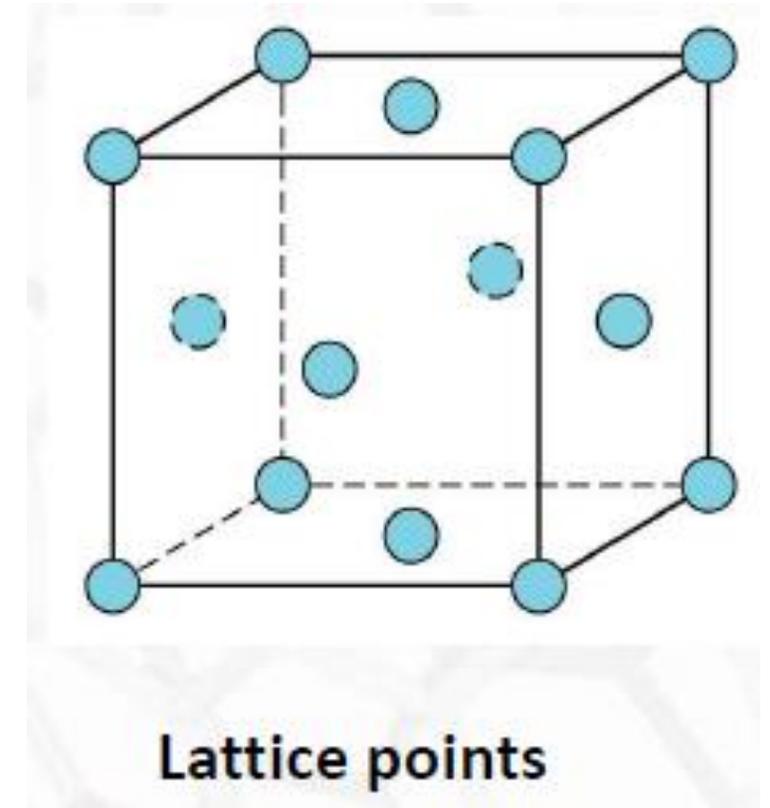
**Triclinic**  
 $a \neq b \neq c$   
 $\alpha \neq \beta \neq \gamma \neq 90^\circ$



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

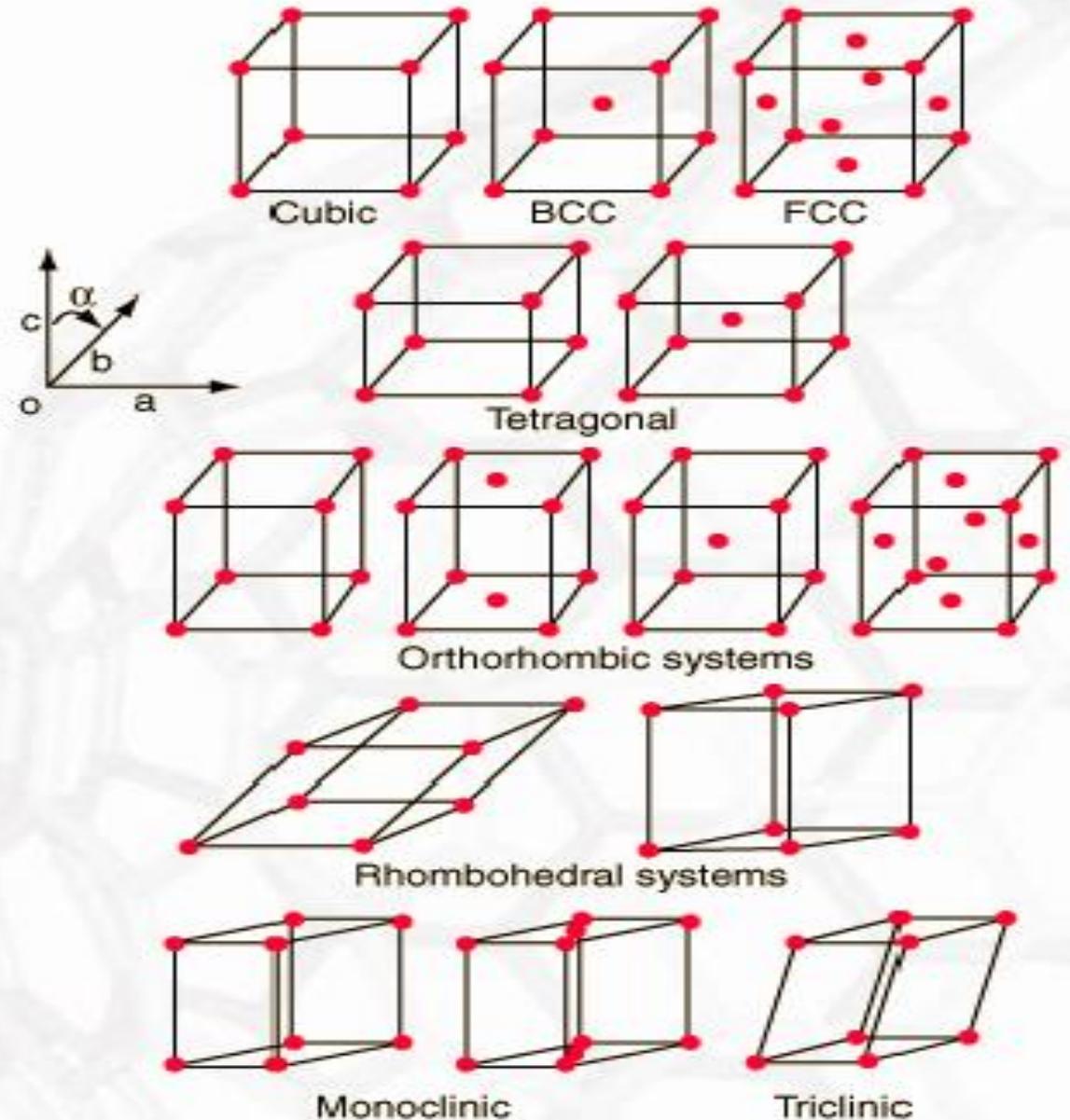
# Bravais Lattices

- By means of unit cells we managed to reduce all possible crystal structures to a relatively small numbers of basic unit cell geometries.
- Now let us consider the issue how atoms (viewed as hard spheres ) can be stacked together *within a given unit cell*.
- **Lattice points** are theoretical points arranged periodically in 3-D space, rather than actual atoms.
- There is a limited number of possibilities, referred to as *Bravais lattice*.



# The 14 Bravais Lattices

- Where Can I Put the Lattice Points?
- The French scientist August Bravais, demonstrated in 1850 that only these **14 types** of unit cells are compatible with the orderly arrangements of atoms found in crystals.
- These three-dimensional configurations of points used to describe the orderly arrangement of atoms in a crystal.
- Each point represents one or more atoms in the actual crystal, and if the points are connected by lines, a crystal lattice is formed.



# MATERIAL SCIENCE AND ENGINEERING



## UNIT 1

# CRYSTAL STRUCTURES

---

**Dr. SWATI GANGWAR**

**Mr. KAPIL KUMAR**

Department Of Mechanical Engineering, MMMUT Gorakhpur

# Crystal Structure

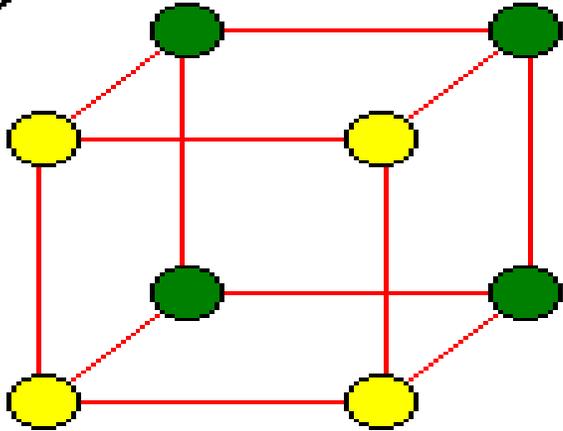
- In crystallography, crystal structure is a description of the ordered arrangement of atoms, ions or molecules in a crystalline material.

## *Metallic Crystals*

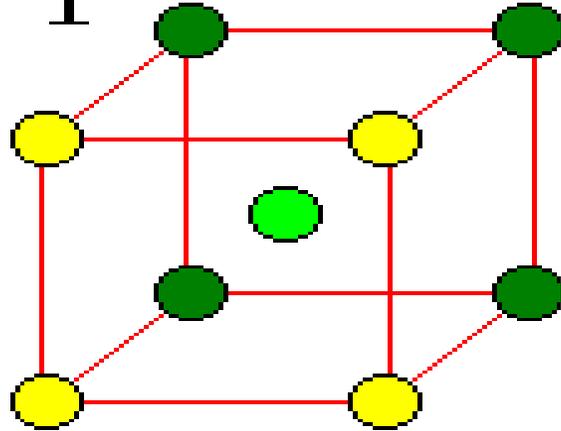
- It tend to be densely packed.
- have several reasons for dense packing:
  - Typically, only one element is present, so all atomic radii are the same.
  - Metallic bonding is not directional.
  - Nearest neighbor distances tend to be small in order to lower bond energy.
- These metallic crystals have the simplest crystal structures. We will look at three such structures...

# *Cubic Unit Cells*

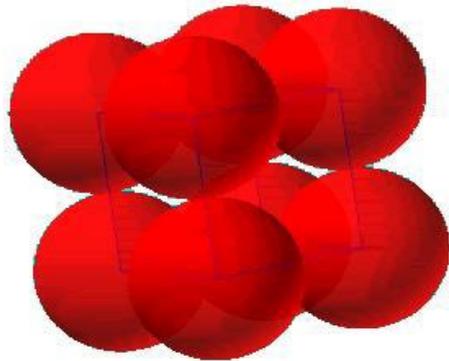
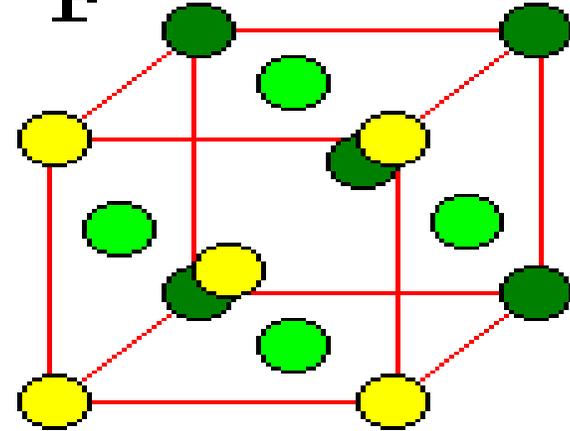
**P**



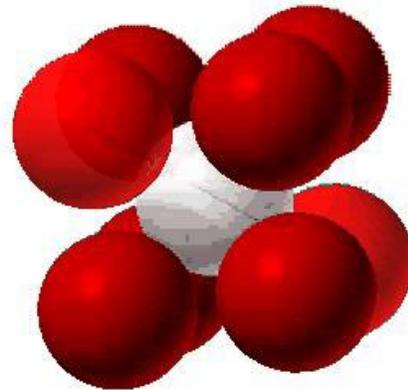
**I**



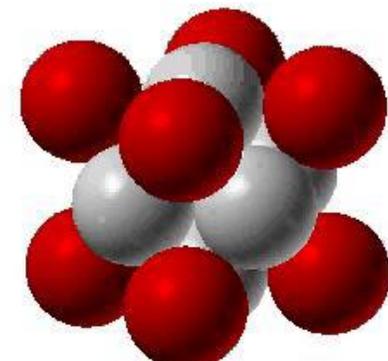
**F**



**SIMPLE CUBIC  
STRUCTURE (SC)**



**BODY CENTERED CUBIC  
STRUCTURE (BCC)**



**FACE CENTERED CUBIC  
STRUCTURE (FCC)**

## Coordination number

- It is defined as the number of nearest neighbors in the unit cell.

## Atomic Packing Factor (APF)

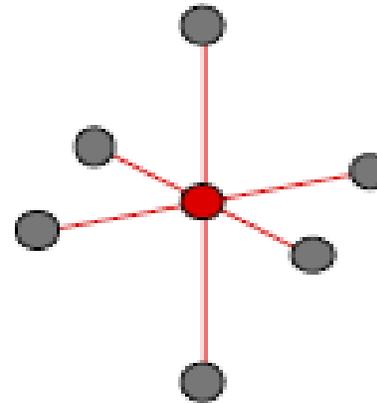
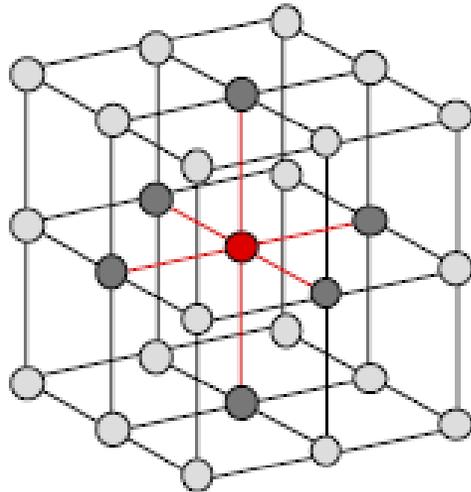
- It can be defined as the ratio between the volume of the basic atoms of the unit cell (which represent the volume of all atoms in one unit cell) to the volume of the unit cell itself.
- For cubic crystals, A.P. F it depends on the radius of atoms and characterization of chemical bonding.

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

\*assume hard spheres

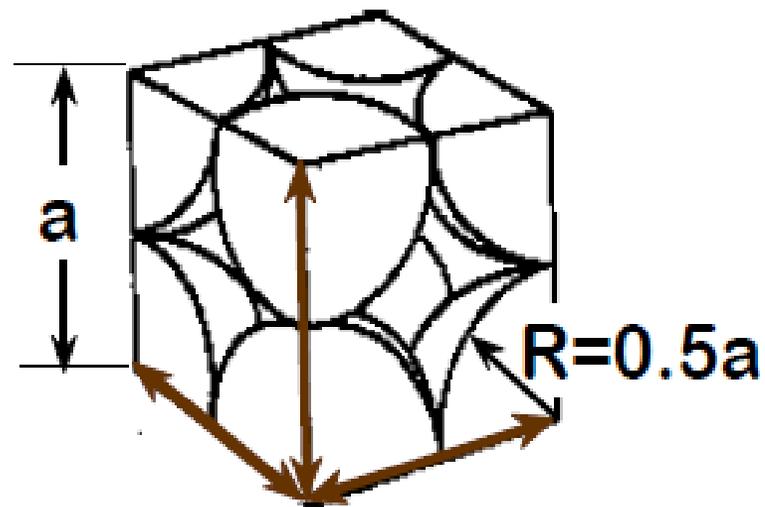
# *Simple Cubic (SC) Structure*

- This structure is rare due to poor packing (only Polonium has this structure).
- Close-packed directions are cube edges.



Coordination number = 6

# Atomic Packing Factor for Simple Cubic



close-packed directions  
contains  $8 \times 1/8 =$   
**1 atom/unit cell**

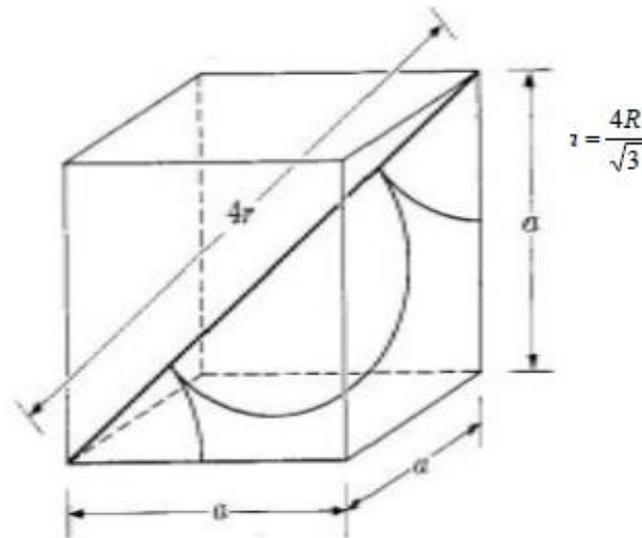
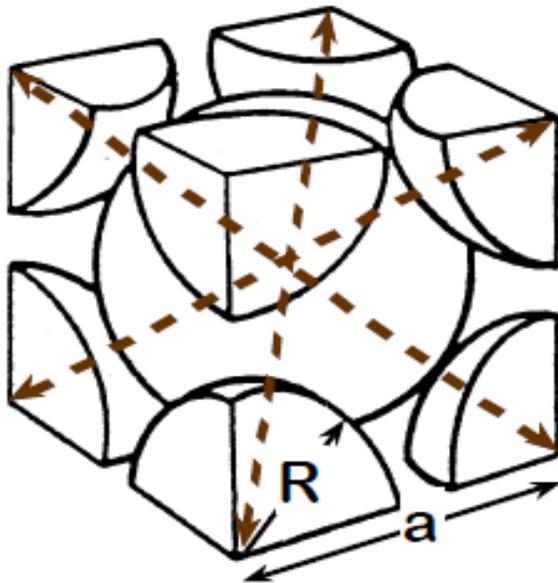
$$APF = \frac{\text{atoms unit cell} \times \text{volume atom}}{\text{volume unit cell}}$$

atoms unit cell → 1      $\frac{4}{3} \pi (0.5a)^3$  ← volume atom  
volume unit cell ←  $a^3$

APF for a simple cubic structure = 0.52

# Body Centered Cubic Structure (BCC)

- Close packed directions are cube diagonals.
- Coordination number = 8
- Close-packed directions: length =  $4R = \sqrt{3}a$
- Unit cell contains:  $1 + 8 \times 1/8 = 2$  atoms/unit cell



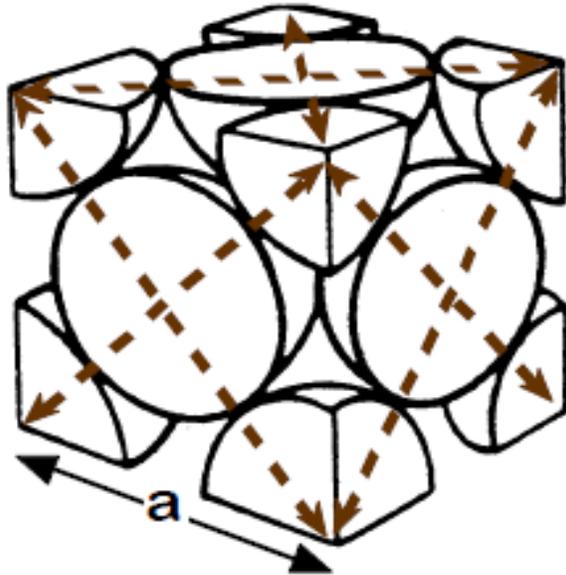
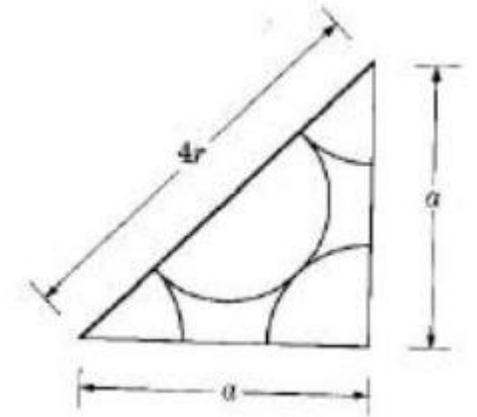
$$\text{APF} = \frac{\text{atoms unit cell} \times \text{volume atom}}{\text{volume unit cell}}$$

$$\text{APF} = \frac{2 \times \frac{4}{3} \pi \left(\frac{\sqrt{3}a}{4}\right)^3}{a^3}$$

- APF for a body-centered cubic structure = 0.68

# Face Centered Cubic Structure (FCC)

- Close packed directions are face diagonals.
- Coordination number = 12
- Close-packed direction length =  $4R = \sqrt{2}a$
- Unit cell contains:  $6 \times 1/2 + 8 \times 1/8 = 4$  atoms/unit cell



$$\text{APF} = \frac{\text{atoms unit cell} \times \text{volume atom}}{\text{volume unit cell}}$$

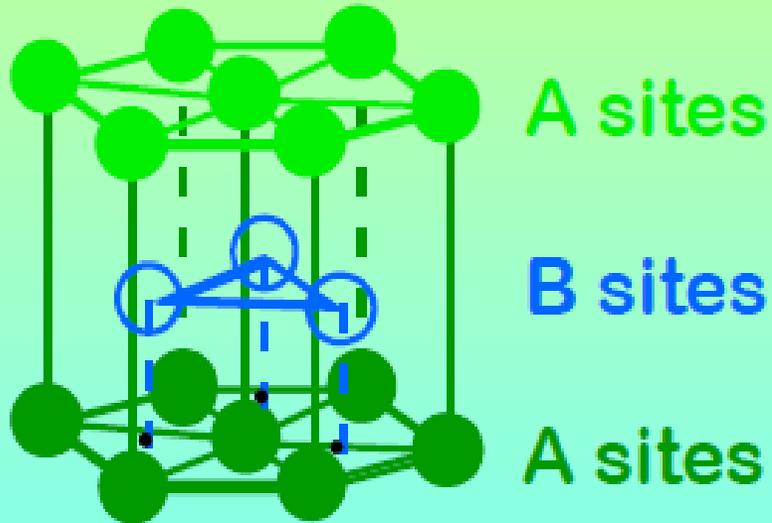
$$\text{APF} = \frac{4 \times \frac{4}{3} \pi (\sqrt{2}a/4)^3}{a^3}$$

- APF for a face-centered cubic structure = 0.74

# *Hexagonal Close-Packed (HCP) Structure*

- Coordination number = 12
- Close-packed direction length =  $2R = a$
- Unit cell contains:  $2 \times 1/2 + 3 + (6 \times 2) \times 1/6 = 6$  atoms/unit cell
- ABAB... Stacking Sequence

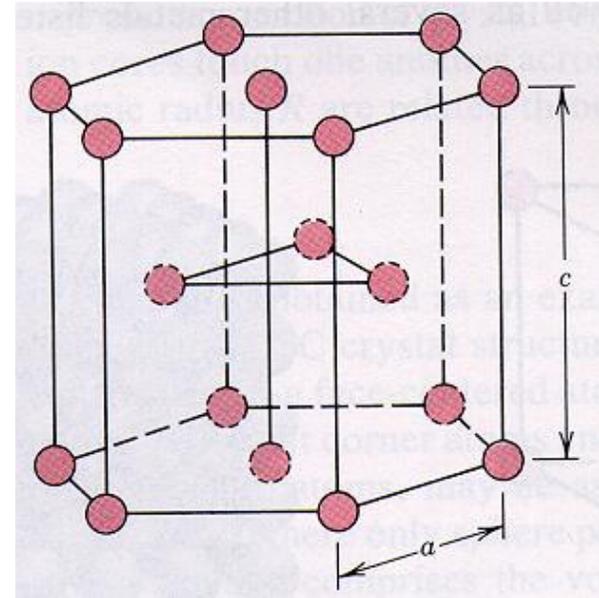
## 3D Projection



## • 2D Projection



- HCP crystal structure contains 6 atoms per unit cell.
- $C = 1.633 a$
- $A = 2r$
- Volume of HCP unit cell = Area of the hexagonal face x height of the hexagon.
- Area of the hexagonal face = area of each triangle x 6

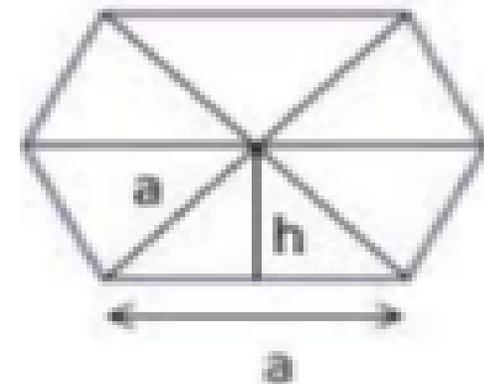


$$\text{Area of triangle} = \frac{bh}{2} = \frac{ah}{2} = \frac{1}{2} a \cdot \frac{a\sqrt{3}}{2}$$

$$\text{Area of hexagon} = 6 \cdot \frac{a^2\sqrt{3}}{4}$$

$$\text{Volume of HCP} = 6 \cdot \frac{a^2\sqrt{3}}{4} \cdot C = 6 \cdot \frac{a^2\sqrt{3}}{4} \cdot 1.633a$$

$$\text{APF} = 6 \cdot \frac{4\pi r^3}{3} / \left( \frac{\sqrt{3}}{4} \cdot 6 \cdot 1.633 \cdot a^3 \right)$$



- APF for a *HCP crystal* structure = 0.74

# *Theoretical Density ( $\rho$ )*

$$\rho = \frac{nA}{V_c N_A}$$

# atoms/unit cell  $\rightarrow$   $n$  Atomic weight (g/mol)  $\rightarrow$   $A$

Volume/unit cell  
( $\text{cm}^3/\text{unit cell}$ )  $\rightarrow$   $V_c$  Avogadro's number  
( $6.023 \times 10^{23}$  atoms/mol)  $\rightarrow$   $N_A$

# Densities of Materials Classes

$$\rho_{\text{metal}} > \rho_{\text{ceramics}} > \rho_{\text{polymers}}$$

Why?

Metals have...

- close-packing (metallic bonding)
- large atomic mass

Ceramics have...

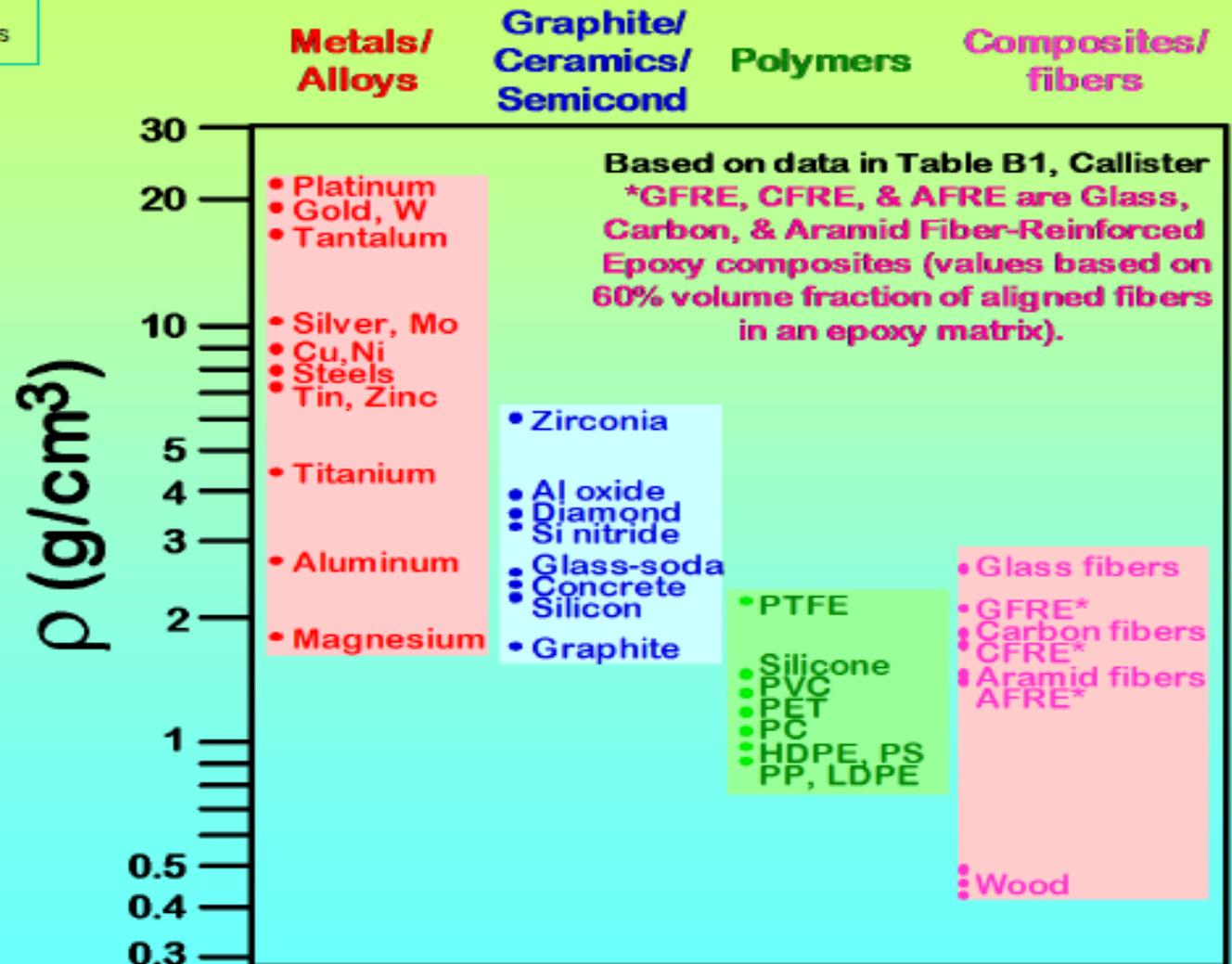
- less dense packing (covalent bonding)
- often lighter elements

Polymers have...

- poor packing (often amorphous)
- lighter elements (C,H,O)

Composites have...

- intermediate values



# Problem 1

- If the atomic radius for Pb= 0.175nm, find the volume of the unit cell.
- Solution: Pb is fcc, hence

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

$$R = 0.175\text{nm}$$

$$a = 0.495 \text{ nm}$$

$$\text{Volume for cubic} = a^3 = 1.21\text{e-}28 \text{ m}^3$$

## Problem 2

Magnesium is hcp with  $c/a = 1.624$ , density =  $1.74 \text{ g/cm}^3$ . Find the atomic radius of magnesium.

Solution: density =  $n \cdot MW / (V_c \cdot NA)$

For hcp  $n = 6$

$$V_c = \frac{3\sqrt{3} a^2 c}{2} = 2.6 \cdot (1.624)a^3 = 4.22a^3$$

$$c = 1.624a$$

$$NA = 6.02 \cdot 10^{23} \text{ atoms/mol}$$

$$MW \text{ magnesium} = 24.3 \text{ g/mol}$$

## Example: Copper

- crystal structure = FCC: 4 atoms/unit cell
- atomic weight = 63.55 g/mol (1 amu = 1 g/mol)
- atomic radius  $R = 0.128 \text{ nm}$  (1 nm =  $10^{-7} \text{ cm}$ )  
 $V_C = a^3$  ; For FCC,  $a = 4R\sqrt{2}$  ;  $V_C = 4.75 \times 10^{-23} \text{ cm}^3$

Result: theoretical  $\rho_{\text{Cu}} = 8.89 \text{ g/cm}^3$

Compare to actual:  $\rho_{\text{Cu}} = 8.94 \text{ g/cm}^3$

# MATERIAL SCIENCE AND ENGINEERING



## UNIT 1

# MILLER INDICES

---

**Dr. SWATI GANGWAR**

**Mr. KAPIL KUMAR**

Department Of Mechanical Engineering, MMMUT Gorakhpur

# Miller Indices

- Miller Indices are used to refer to specific lattice planes of atoms.
- These directions and planes could be in lattices or in crystals.
- These are reciprocals of the fractional intercepts (with fractions cleared) that the plane makes with the crystallographic x, y and z axes of three nonparallel edges of the cubic unit cell.
- The number of indices will match with the dimension of the lattice or the crystal.
- E.g. in 1D there will be 1 index and 2D there will be two indices etc.

# Importance of Miller Indices

In Materials Science it is important to have a notation system for atomic planes since these planes influence

- Optical properties
- Reactivity
- Surface tension
- Dislocations

# Notation Summary

- $(h,k,l)$  represents a point – note the exclusive use of commas
- Negative numbers/directions are denoted with a bar on top of the number
- $[hkl]$  represents a direction
- $\langle hkl \rangle$  represents a family of directions
- $(hkl)$  represents a plane
- $\{hkl\}$  represents a family of planes

# Miller Indices for Planes: Procedure

Choose a plane that does not pass through origin

**Step 1:** Identify the plane intercepts on the x, y and z-axes.

**Step 2:** Specify intercepts in fractional coordinates.

**Step 3:** Take the reciprocals of the fractional intercepts.

**Step 4:** Fractions?

a. If Yes, Clear fractions by multiplying by an integer to determine smallest set of whole numbers, then go to b

b. If No, Place a “bar” over the Negative indices

**Step 5:** Enclose in parenthesis (hkl) where h,k,l are miller indices of cubic crystal plane for x, y and z axes.

**Note:** if the one of axis value was negative then move the center of cubic to negative value direction .

# Miller Indices for Planes: Illustration

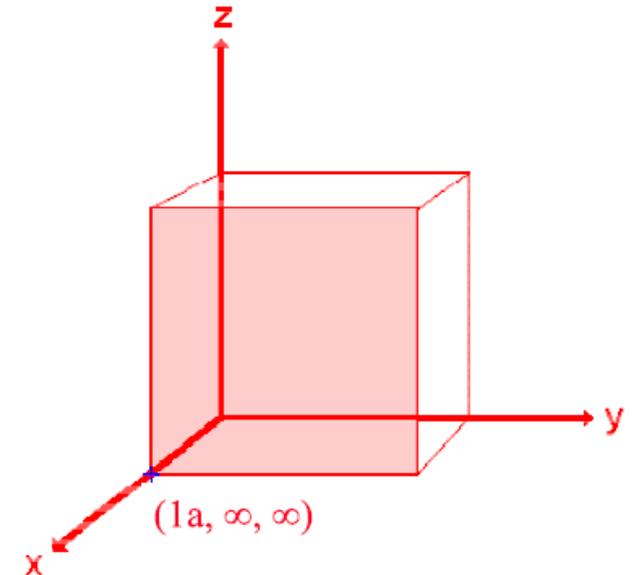
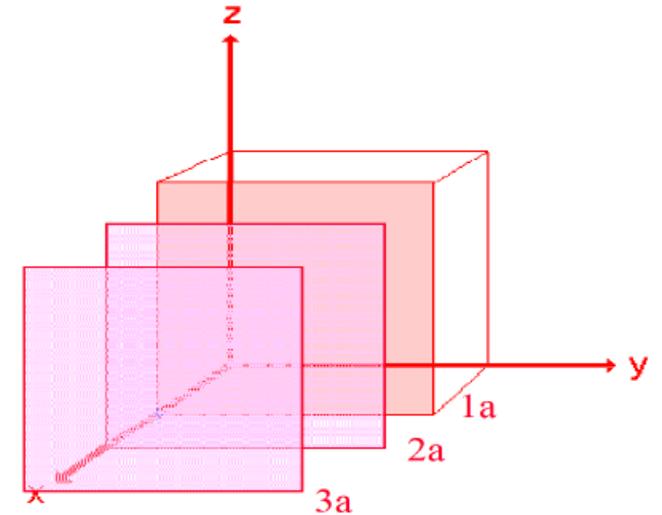
- Consider the plane in pink, which is one of an infinite number of parallel planes each a consistent distance (“a”) away from the origin (purple planes)
- The plane intersects the x-axis at point a. It runs parallel along y and z axes.

$$x = \frac{1}{1} = 1$$

$$y = \frac{1}{0} = \infty$$

$$z = \frac{1}{0} = \infty$$

- Thus, this plane can be designated as  $(1, \infty, \infty)$ .



- Likewise, the **yellow** plane can be designated as  $(\infty, 1, \infty)$ .
- And the **green** plane can be written as  $(\infty, \infty, 1)$ .
- **Miller Indices are the reciprocals of the parameters of each crystal face.**

Thus:

- **Pink Face**

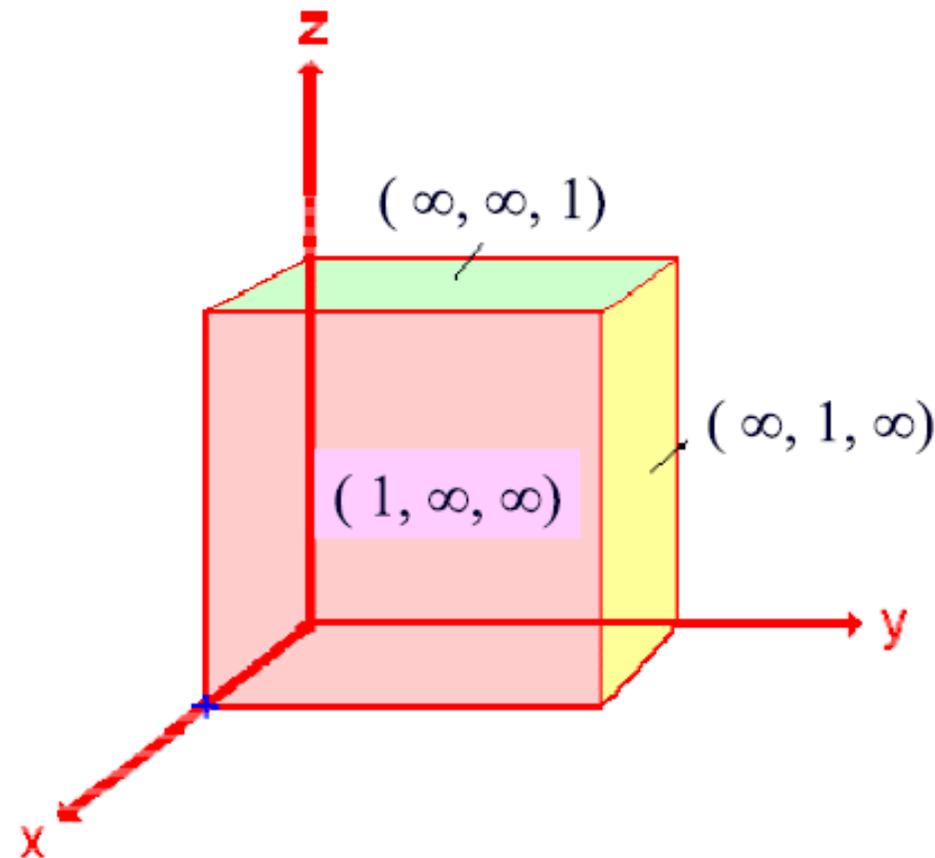
$$= (1/1, 1/\infty, 1/\infty) = \mathbf{(100)}$$

- **Green Face**

$$= (1/\infty, 1/\infty, 1/1) = \mathbf{(001)}$$

- **Yellow Face**

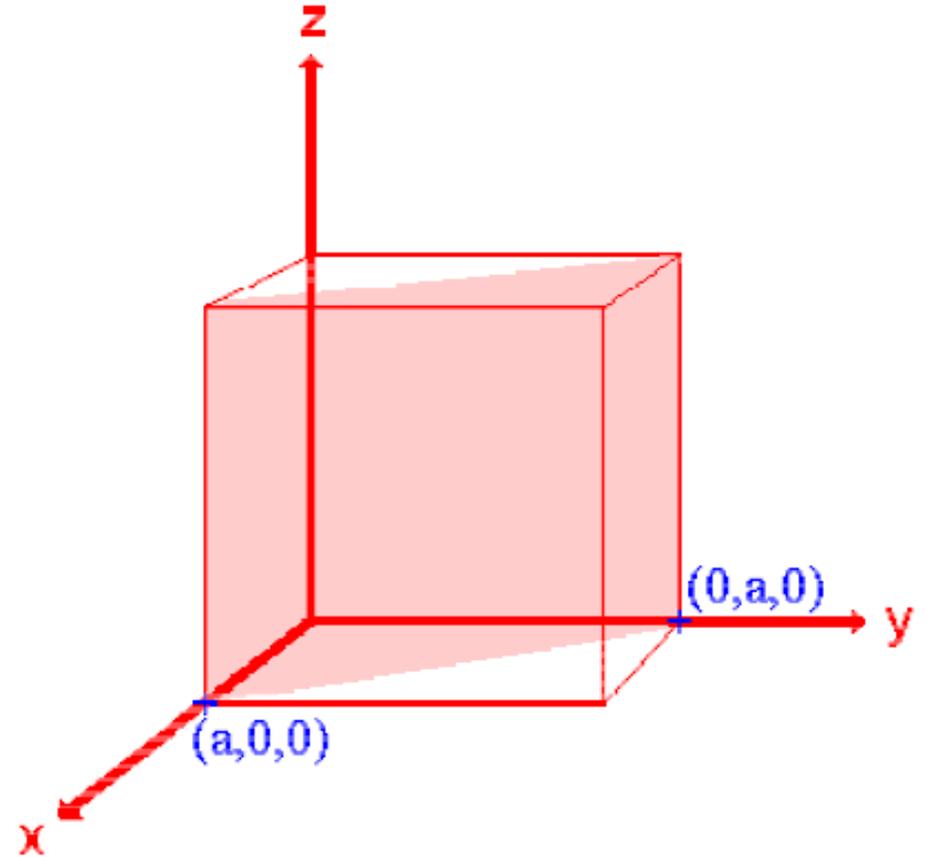
$$= (1/\infty, 1/1, 1/\infty) = \mathbf{(010)}$$



Example 1: What's the Miller Index of this plane?

The plane of interest cuts two of the crystallographic axes.

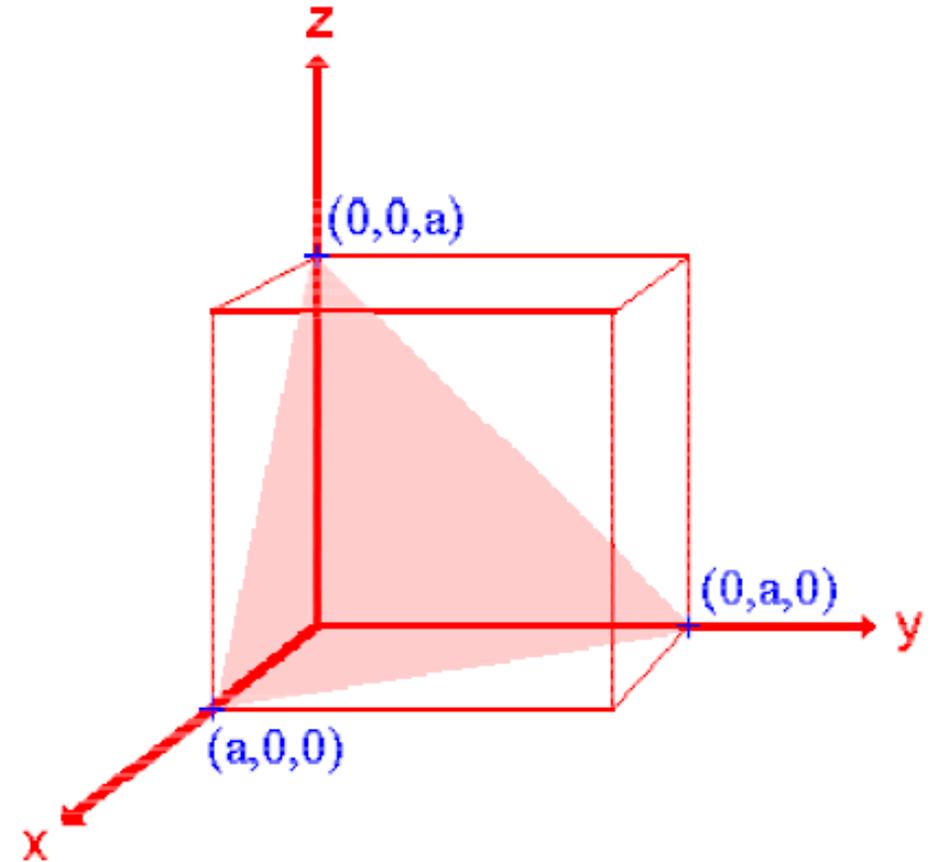
	x (a)	y (b)	z (c)
Intercept on axes	1	1	$\infty$
Reciprocal	1/1	1/1	$1/\infty = 0$
Integer Clear	1	1	0
Miller Indices	<b>(110)</b>		



Example 2: What's the Miller Index of this plane?

This plane cuts all three crystallographic axes.

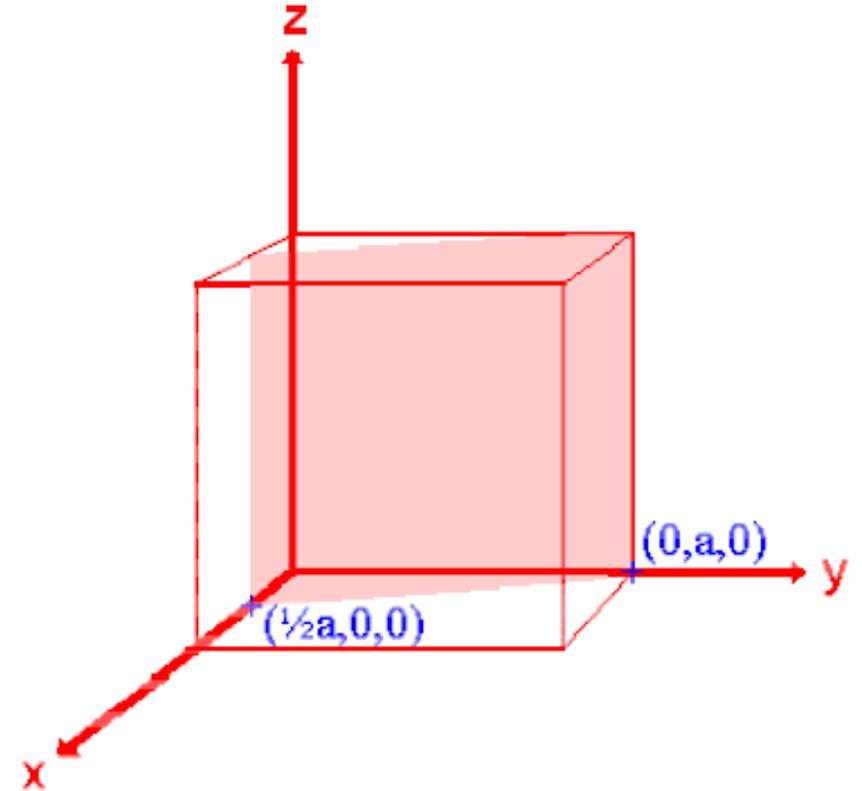
- Intercepts =  $(1,1,1) = (111)$

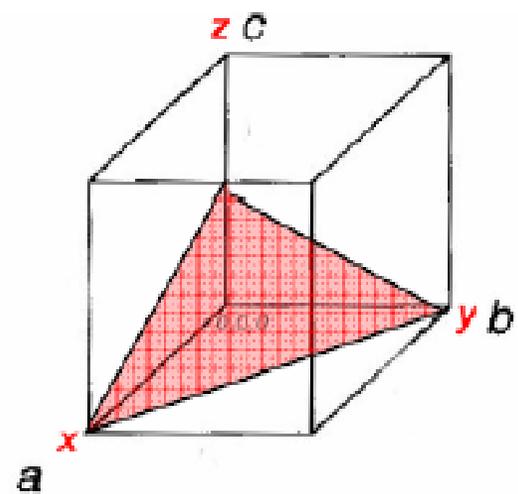


Example 3: What's the Miller Index of this plane?

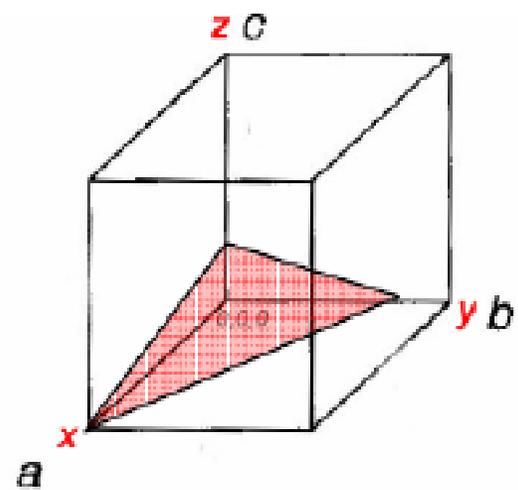
This plane cuts two of the reference axes, but not equidimensionally.

•Intercepts:  $(\frac{1}{2}, 1, 0) = (210)$



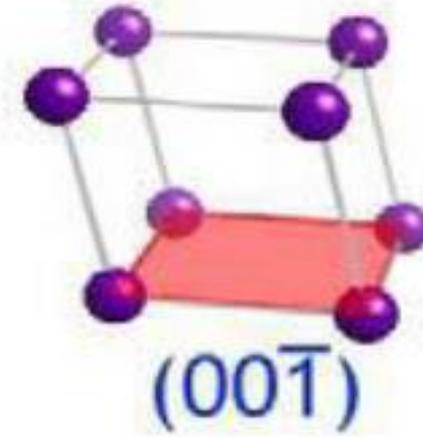
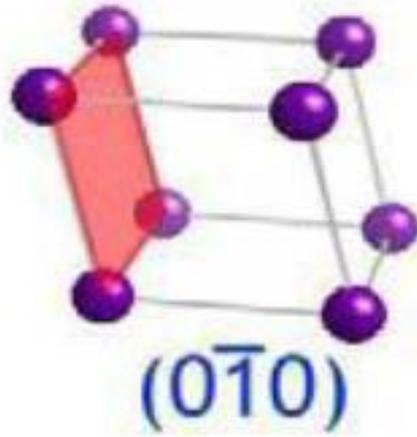
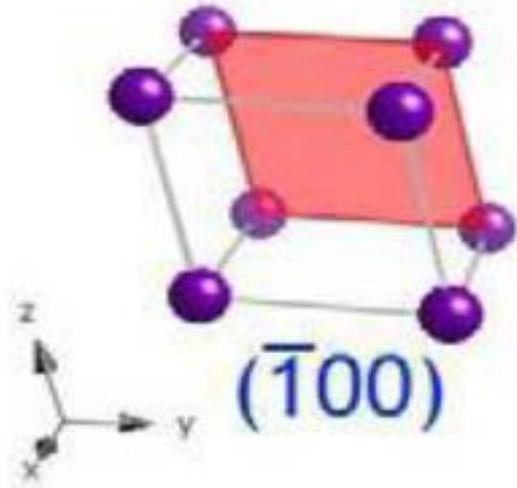
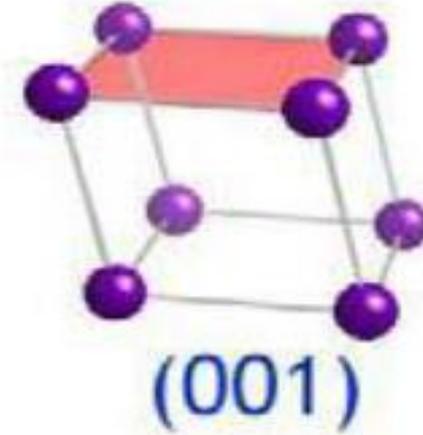
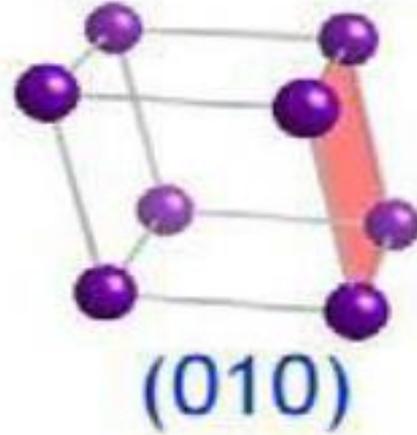
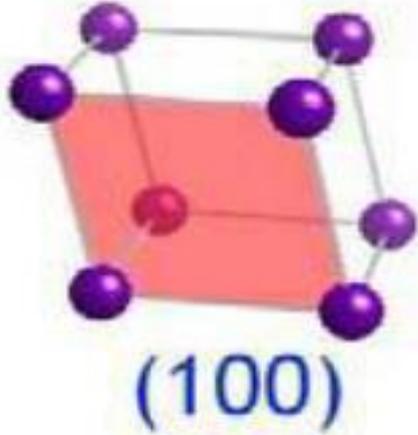


	x (a)	y (b)	z (c)
Intercept on axes	1	1	$\frac{1}{2}$
Reciprocal	1	1	2
Integer Clear	1	1	2
Miller Indices	<b>(112)</b>		

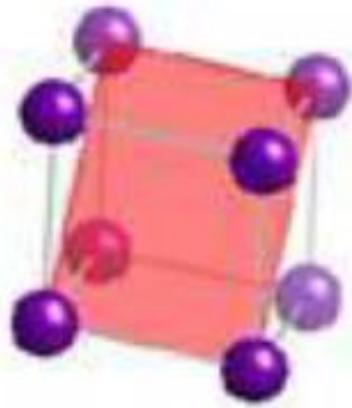


	x (a)	y (b)	z (c)
Intercept on axes	1	$\frac{3}{4}$	$\frac{1}{4}$
Reciprocal	1	$\frac{4}{3}$	4
Integer Clear	3	4	12
Miller Indices	<b>(3 4 12)</b>		

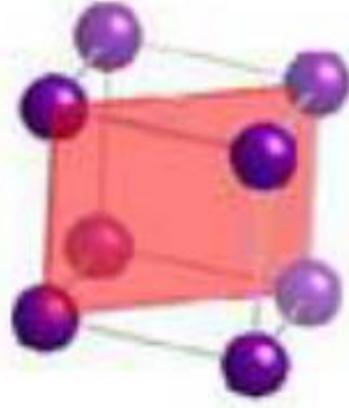
# Miller Indices of different planes:



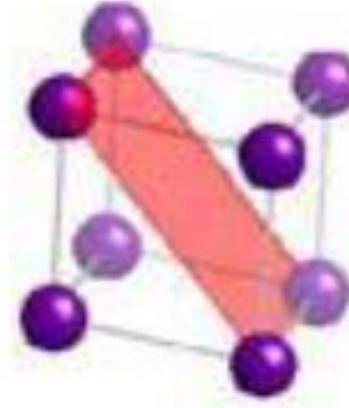
# Miller Indices of different planes:



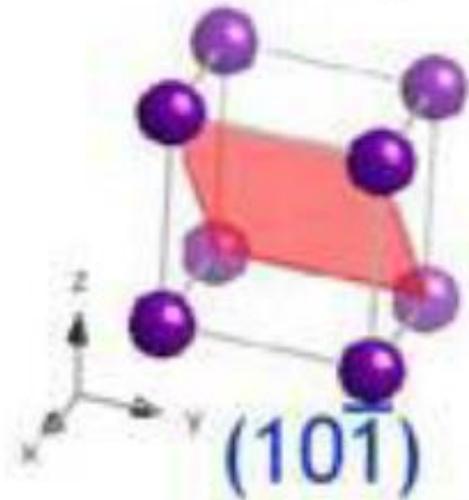
(101)



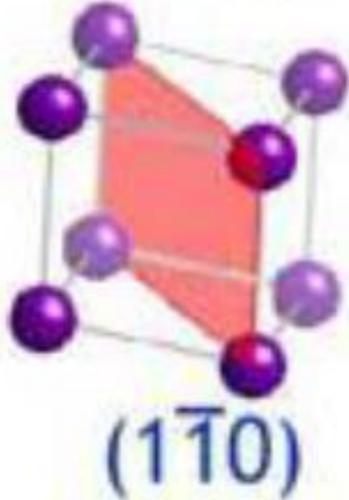
(110)



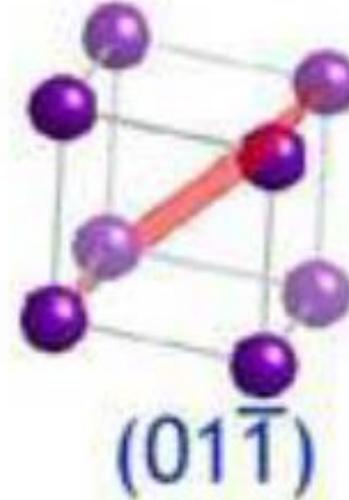
(011)



( $\bar{1}01$ )



( $\bar{1}10$ )



( $0\bar{1}\bar{1}$ )

# Crystallographic Directions

**Step 1:** Identify the plane intercepts on the x, y and z-axes.

**Step 2:** Take the reciprocals of the intercepts. No fraction needed.

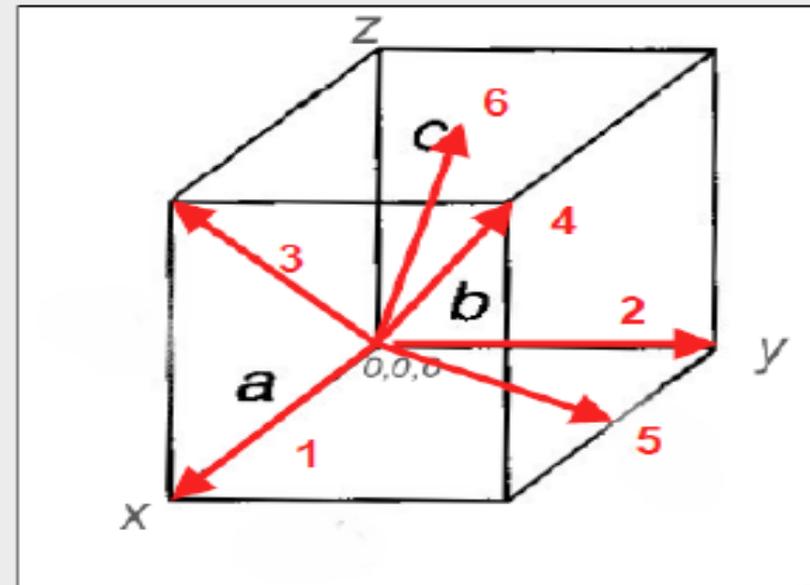
Negative direction has a top bar on the (h k l) value.

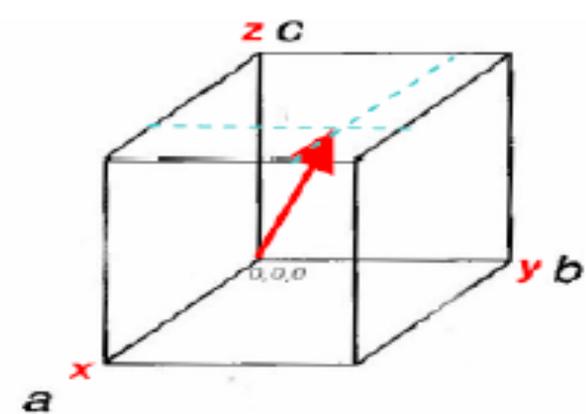
## Based on intersection with the cell boundaries

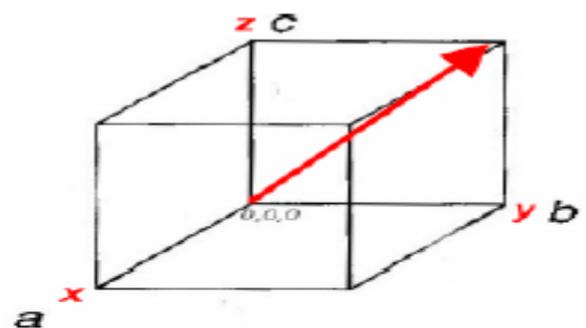
Indicated with square brackets [ h, k, l ]

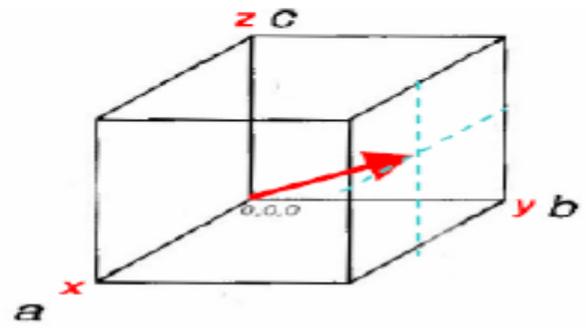
- Direction 1      1, 0, 0 = [100]
- Direction 2      0, 1, 0 = [010]
- Direction 3      1, 0, 1 = [101]
- Direction 4      1, 1, 1 = [111]
- Direction 5       $\frac{1}{2}$ , 1, 0 = [120]
- Direction 6       $\frac{1}{2}$ ,  $\frac{1}{2}$ , 1 = [112]

-- Parallel directions have the same value  
Lowest Integer Value [111] = [222]



		<b>x (a)</b>	<b>y (b)</b>	<b>z (c)</b>
	<b>Point Coordinates</b>	$\frac{3}{4}$	$\frac{3}{4}$	<b>1</b>
	<b>Clear Fractions</b>	<b>3</b>	<b>3</b>	<b>4</b>
	<b>Crystal Direction</b>	<b>[334]</b>		

		<b>x (a)</b>	<b>y (b)</b>	<b>z (c)</b>
	<b>Point Coordinates</b>	<b>0</b>	<b>1</b>	<b>1</b>
	<b>Clear Fractions</b>	<b>0</b>	<b>1</b>	<b>1</b>
	<b>Crystal Direction</b>	<b>[011]</b>		

		<b>x (a)</b>	<b>y (b)</b>	<b>z (c)</b>
	<b>Point Coordinates</b>	$\frac{1}{2}$	<b>1</b>	$\frac{1}{2}$
	<b>Clear Fractions</b>	<b>1</b>	<b>2</b>	<b>1</b>
	<b>Crystal Direction</b>	<b>[121]</b>		

# Inter-planer Distance between parallel planes

- The space lattice consist from many crystal planes which separated by inter-planer smallest distance
- The distance can be calculated by using x- ray diffraction , by using the law below :-

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

- Where  $d_{hkl}$  = interplanar spacing between parallel closest planes with Miller indices  $h$ ,  $k$ , and  $l$
- $a$  = lattice constant (edge of unit cube).
- $h, k, l$  = Miller indices of cubic planes being considered.

# Angles between crystal planes

- The crystal consist many from plane which contact with them in varity angles , The angle between crystal planes (h1 k1 l1) and (h2 k2 l2) can be calculated by using the following equation :-

$$\cos \theta = \frac{h_1 h_2 + k_1 k_2 + l_1 l_2}{\sqrt{(h_1^2 + k_1^2 + l_1^2)} * \sqrt{(h_2^2 + k_2^2 + l_2^2)}}$$

Example :-

Find the angle between the planes  $(1\bar{1}1)$  &  $(111)$ ?

$$\cos \theta = \frac{h_1 h_2 + k_1 k_2 + l_1 l_2}{\sqrt{(h_1^2 + k_1^2 + l_1^2)} * \sqrt{(h_2^2 + k_2^2 + l_2^2)}}$$

$$\cos \theta = \frac{1 + (-1) + 1}{\sqrt{1 + 1 + 1} * \sqrt{1 + 1 + 1}}$$

$$\cos \theta = \frac{1}{3}$$

$$\cos \theta = 0.333$$

$$\cos^{-1} 0.333 = \theta$$

$$\theta = 70.32^\circ$$

### Example 2

Find the interplaner distance for plane (220) , which have FCC Craystal and raidus of atom (1.414 A) ?

Solution:-

The crystal is FCC then

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

$$a = \frac{4(1.414)}{\sqrt{2}} = \frac{4(1.414)}{1.414} = 4 \text{ A}^\circ$$

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$$d_{hkl} = \frac{4}{\sqrt{4 + 4 + 0}} = 1.414 \text{ A}^\circ$$

Example: (H.W)

Copper has an FCC crystal structure and a unit cell with a lattice constant of 0.361 nm.

What is its interplanar spacing  $d_{220}$ ?

# MATERIAL SCIENCE AND ENGINEERING



## UNIT 1

# X-RAY CRYSTALLOGRAPHY

---

**Dr. SWATI GANGWAR**

**Mr. KAPIL KUMAR**

Department Of Mechanical Engineering, MMMUT Gorakhpur

# X-RAY

- X-rays were discovered in 1895 by the German physicist Wilhelm Conrad Röntgen and were so named because their nature was unknown at the time.
- He was awarded the Nobel prize for physics in 1901.



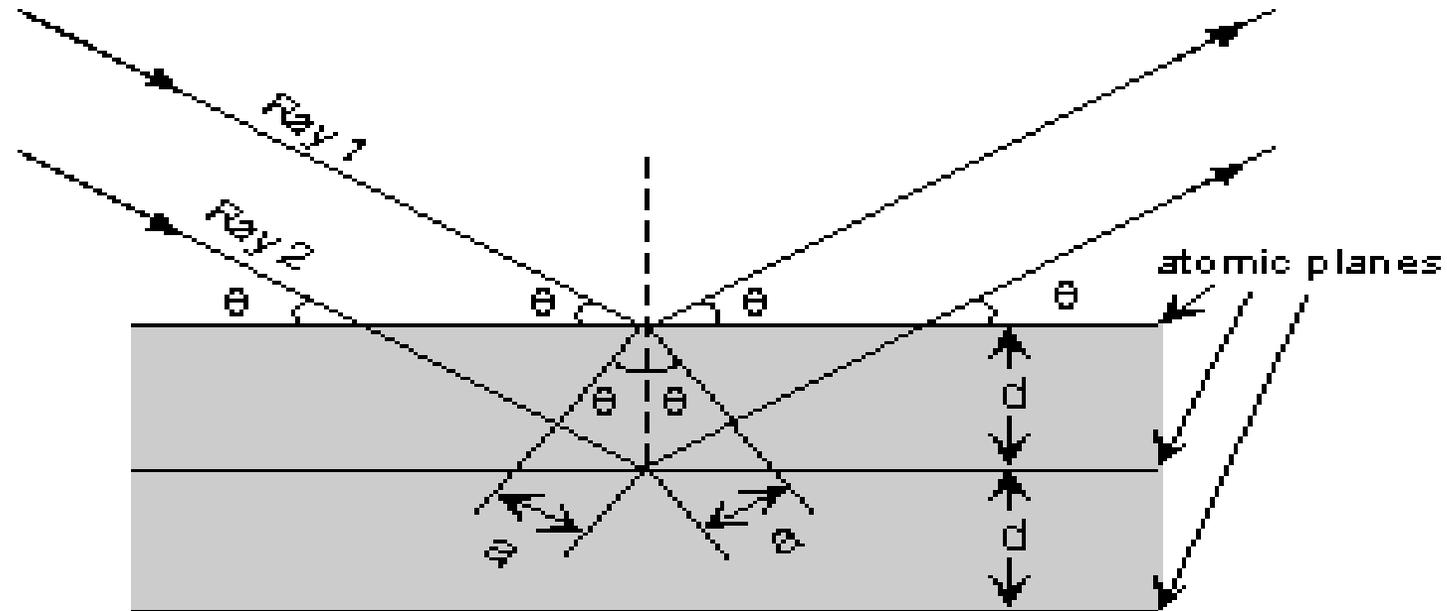
Wilhelm Conrad Röntgen  
(1845-1923)

# FUNDAMENTALS OF DIFFRACTION

- A beam of X-rays consists of a bundle of separate waves, the waves can interact with one another. Such interaction is termed *interference*.
- **If all the waves in the bundle are in phase**, that is their crests and troughs occur at exactly the same position (the same as being an integer number of wavelengths out of phase,  $n\lambda$ ,  $n = 1, 2, 3, 4$ , etc.), the waves will interfere with one another and their amplitudes will add together to produce a resultant wave that is has a **higher amplitude** (the sum of all the waves that are in phase. )

# BRAGG'S LAW

- Two such X-rays are shown here, where the spacing between the atomic planes occurs over the distance,  $d$ .
- Ray 1 reflects off of the upper atomic plane at an angle  $\theta$  equal to its angle of incidence. Similarly, Ray 2 reflects off the lower atomic plane at the same angle  $\theta$ . While Ray 2 is in the crystal, however, it travels a distance of  $2a$  farther than Ray 1.



If this distance  $2a$  is equal to an integral number of wavelengths ( $n\lambda$ ), then Rays 1 and 2 will be in phase on their exit from the crystal and constructive interference will occur. If not destructive interference will occur and the waves will not be as strong as when they entered the crystal.

Condition for constructive interference to occur is

$$n\lambda = 2a$$

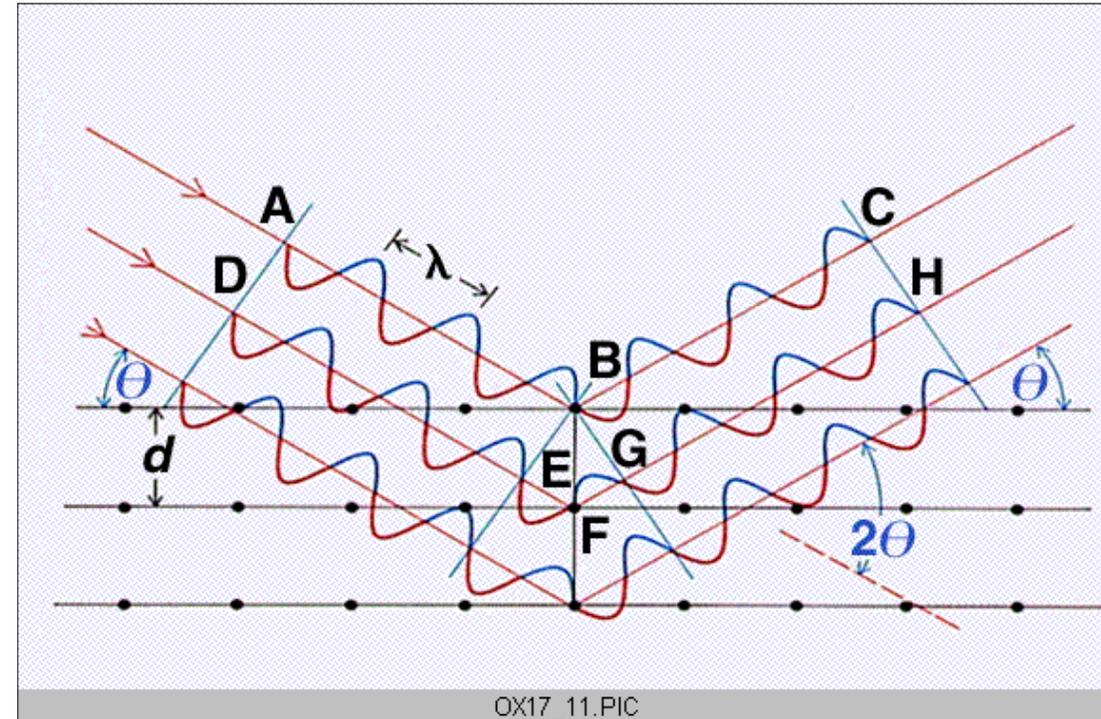
but, from trigonometry, we can figure out what the distance  $2a$  is in terms of the spacing,  $d$ , between the atomic planes.

$$a = d \sin \theta$$

$$\text{or } 2a = 2 d \sin \theta$$

$$\text{thus, } n\lambda = 2d \sin \theta$$

This is known as **Bragg's Law for X-ray diffraction**.



# X RAY CRYSTALLOGRAPHY

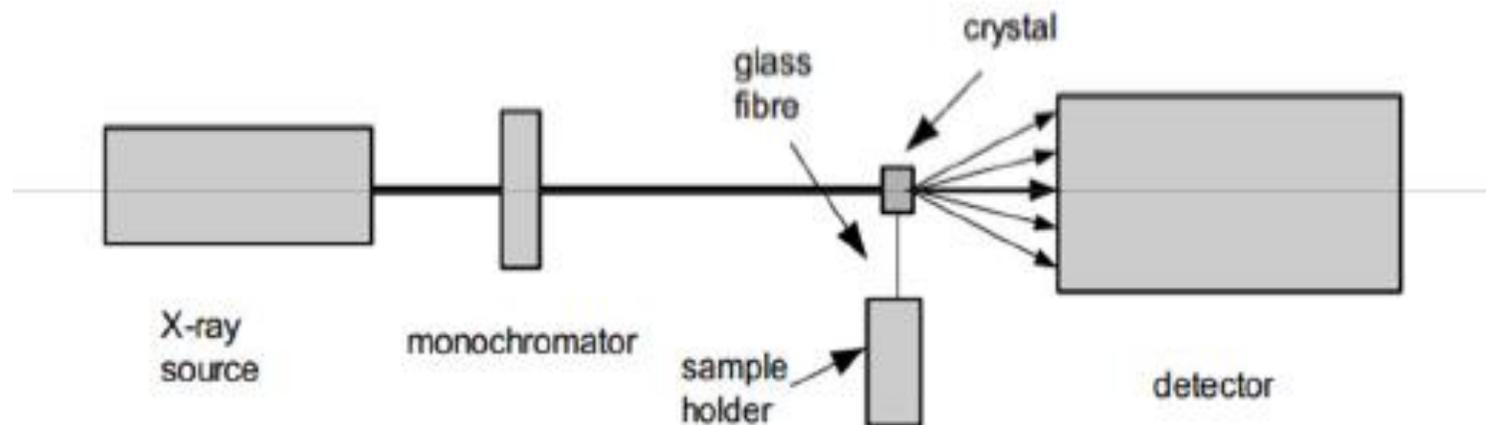
- X-ray crystallography is a **method of determining the arrangement of atoms within a crystal**, in which a beam of X-rays strikes a crystal and causes the beam of light to spread into many specific directions.
- From the **angles and intensities of these diffracted beams**, a crystallographer can **produce a three-dimensional picture of the density of electrons within the crystal**.
- Because X-rays have wavelengths similar to the size of atoms, they are useful to explore within crystals.

# USES

- Used to study many materials which form **crystals like salts, metals, minerals, semiconductors, as well as various inorganic, organic and biological molecules.**
- Determine electron density, the mean positions of the atoms in the crystal their chemical bonds, their disorder and various other information.
- **Size of atoms, the lengths and types of chemical bonds, and the atomic-scale differences** among various materials, especially minerals and alloys. The method also revealed the **structure and function of many biological molecules, including vitamins, drugs, proteins and nucleic acids such as DNA.**
- **Characterizing the atomic structure of new materials** and in discerning materials that appear similar by other experiments.
- X-ray crystal structures can also account for unusual electronic or elastic properties of a material, shed light on chemical interactions and processes, or serve as the basis for designing pharmaceuticals against diseases.

# X-RAY DIFFRACTION

- X-Ray Crystallography uses the uniformity of light diffraction of crystals to determine the structure of a molecule or atom.
- Then they use an X-ray beam to “hit” the crystallized molecule. The electrons surrounding the molecule diffract as the X-rays hit them. This forms a pattern, this type of pattern is called the X-ray diffraction pattern.



# Advantages and disadvantages of X-rays

## Advantages;

- X-ray is the cheapest, the most convenient and widely used method.
- X-rays are not absorbed very much by air, so the specimen need not be in an evacuated chamber.

## Disadvantage;

- They do not interact very strongly with lighter elements.

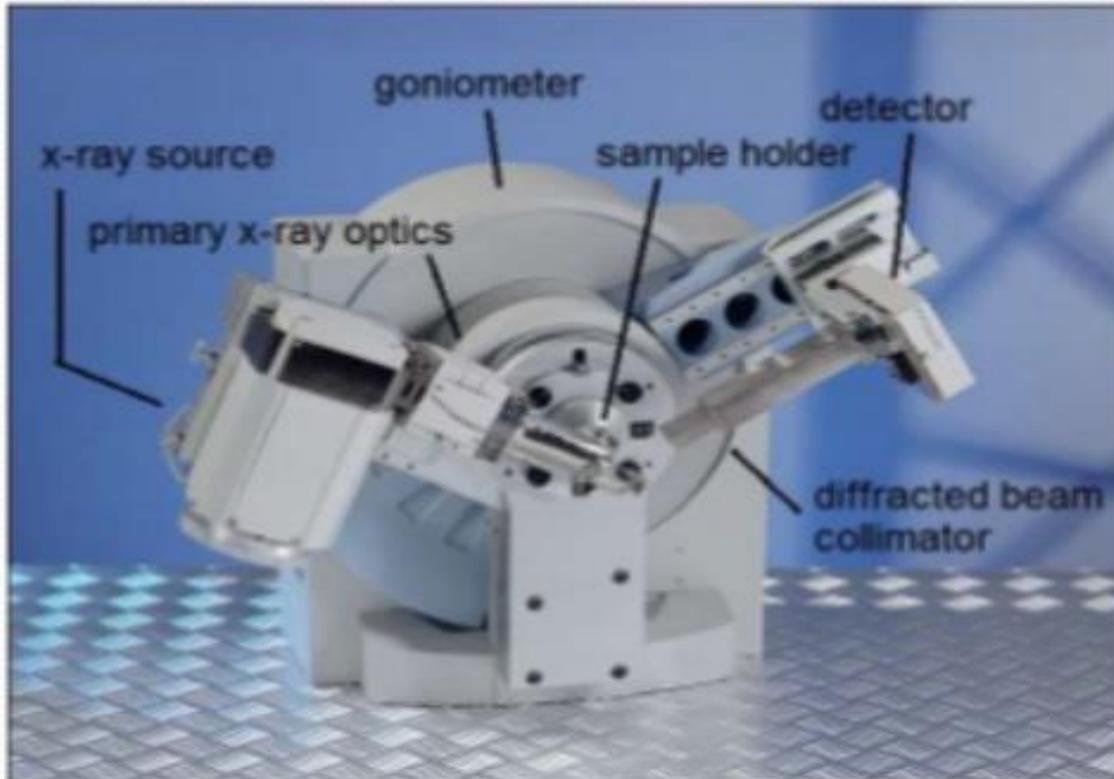
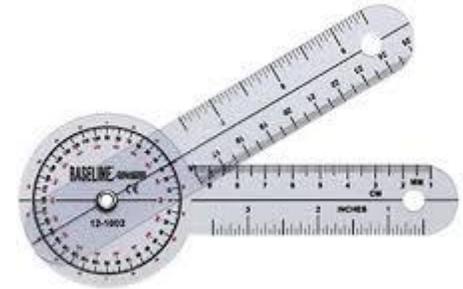
# Application of XRD

XRD is a nondestructive technique. Some of the uses of x-ray diffraction are;

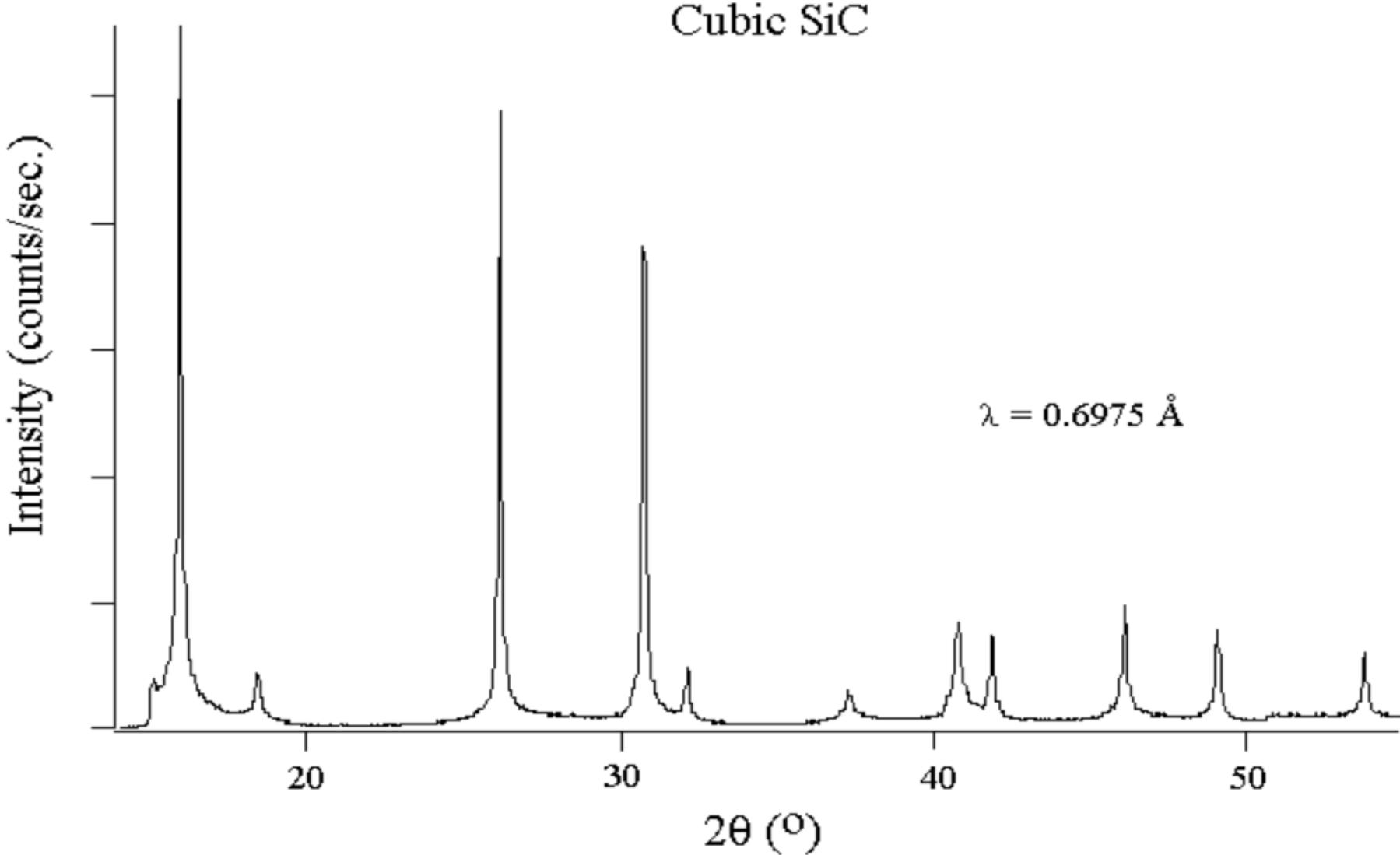
1. Differentiation between crystalline and amorphous materials;
2. Determination of the structure of crystalline materials;
3. Determination of electron distribution within the atoms, and throughout the unit cell;
4. Determination of the orientation of single crystals;
5. Determination of the texture of polygrained materials;

Generally a typical x-ray diffraction contain below parts:

1. Detector
2. X-ray source
3. Crystal on the end of mounting needle
4. Liquid nitrogen steam to keep crystal cold
5. Movable mount to rotate crystal



The following figures show experimental x-ray diffraction patterns of cubic SiC using synchrotron radiation.



# MATERIAL SCIENCE AND ENGINEERING



## UNIT 1

# CRYSTAL IMERFECTIONS

---

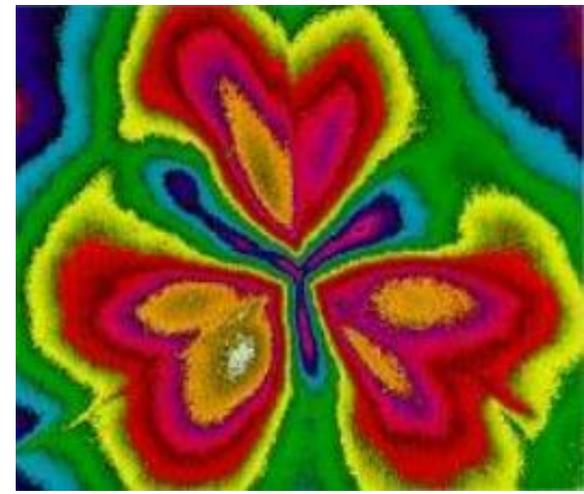
**Dr. SWATI GANGWAR**

**Mr. KAPIL KUMAR**

Department Of Mechanical Engineering, MMMUT Gorakhpur

# Crystal Imperfection or defects

- Any deviation from the perfect atomic arrangement in a crystal is said to contain imperfections or defects.
- A **crystalline defect** is a lattice irregularity having one or more of its dimensions on the order of an atomic dimension.
- A perfect crystal, with every atom of the same type in the correct position, does not exist. There always exist crystalline *defects*.
- Crystal imperfections have strong influence upon many properties of crystals, such as strength, electrical conductivity and hysteresis loss of ferromagnetism.

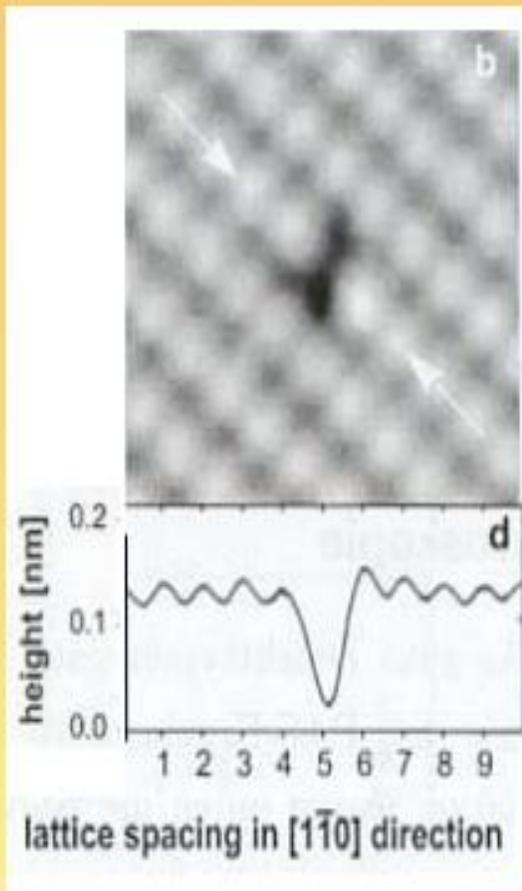


- Adding alloying elements to a metal is one way of introducing a crystal defect. Thus some important properties of crystals are controlled by as much as by imperfections and by the nature of the host crystals.
- The conductivity of some semiconductors is due to entirely trace amount of chemical impurities.
- Atomic diffusion may be accelerated enormously by impurities or imperfections
- Mechanical and plastic properties are usually controlled by imperfections.

# Imperfections in Solids

- The **properties** of materials are profoundly **influenced** by the presence of **imperfections**.
- It is important to have knowledge about the **types of imperfections** that exist and the roles they play in **affecting** the behavior of materials.

## Point defects



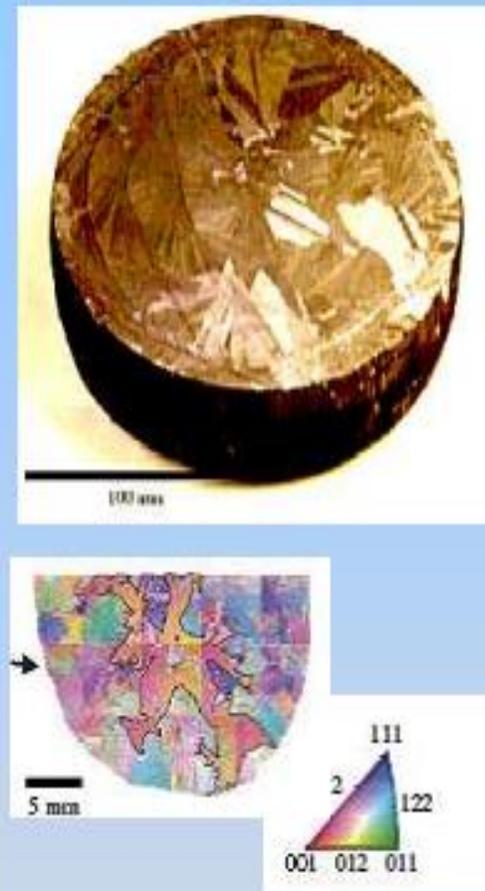
Gebauer 2000

## Dislocations



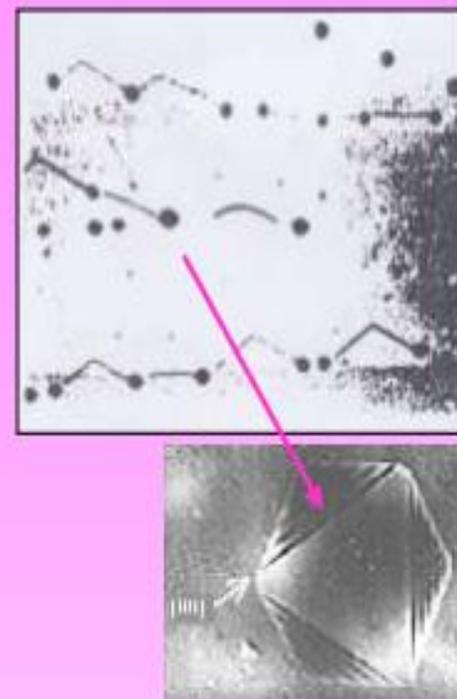
Schröder 1967

## Grain boundaries



Fujiwara 2006

## Inclusions



Hähnert, Rudolph 1993

# Crystal Defects Classification

- For ease of their characterization, defects are classified on the basis of their geometry, which is realistic as defects are disrupted region in a volume of a solid.

## **1. Point defects (Zero Dimension):**

- a. Vacancy
- b. *Interstitial atom or interstitialcy*
- c. Schottky
- d. Frenkel

## **2. Line defects (One Dimension)**

- a. Edge dislocation
- b. Screw dislocation

## **3. Surface defects (Two Dimension)**

- a. Grain boundaries
- b. Tilt boundaries
- c. Twin boundaries

## **4. Volume defects (Three Dimension)**

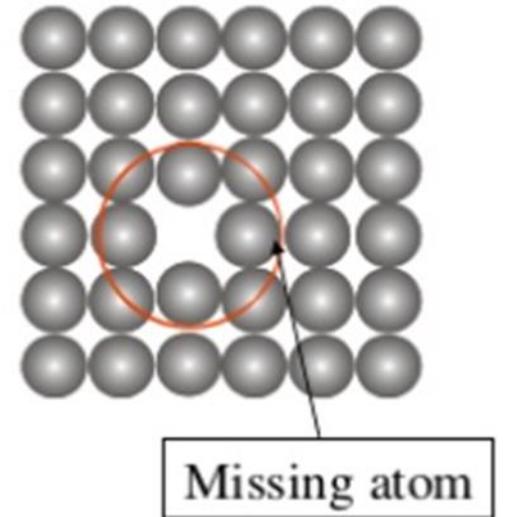
- a. Cracks
- b. Voids
- c. Inclusions

# 1. Point defects

- Point defects, are imperfect point-like regions in the crystal, where an atom is missing or is in an irregular place in the lattice structure.
- Typical size of a point defect is about 1-2 atomic diameters.

## a. Vacancy

- A *vacancy* is a vacant lattice position from where the atom is missing. It is usually created when the solid is formed by cooling the liquid.
- There are other ways of making a vacancy, but they also occur **naturally as a result of thermal excitation**, and these are thermodynamically stable at temperatures greater than zero.



- At equilibrium, the fraction of lattice sites that are vacant at a given temperature ( $T$ ) are:

$$\frac{n}{N} = e^{-Q/kT}$$

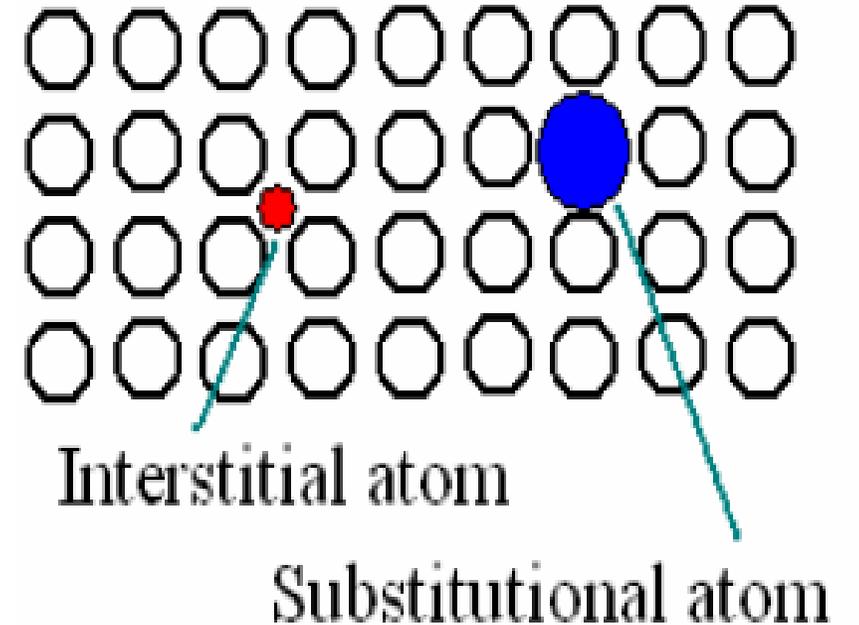
where  $n$  is the number of vacant sites in  $N$  lattice positions,  $k$  is gas or Boltzmann's constant,  $T$  is absolute temperature in kelvins, and  $Q$  is the energy required to move an atom from the interior of a crystal to its surface.

- It is clear from the equation that there is an exponential increase in number of vacancies with temperature.
- When the density of vacancies becomes relatively large, there is a possibility for them to cluster together and form voids.



## ***b. Interstitialcy***

- An *interstitial atom* or *interstitialcy* is an atom that occupies a place outside the normal lattice position.
- It may be the same type of atom as the rest surrounding it (self interstitial) *or* a foreign impurity atom. Interstitialcy is most probable if the atomic packing factor is low.
- Another way an impurity atom can be fitted into a crystal lattice is by substitution. A *substitutional atom* is a foreign atom occupying original lattice position by displacing the parent atom.
- In the case of vacancies and foreign atoms (both interstitial and substitutional), there is a change in the coordination of atoms around the defect. This means that the forces are not balanced in the same way as for other atoms in the solid, which results in lattice distortion around the defect.



# Frenkel defects

- When an ion displaced from a regular position to **an interstitial position creating a vacancy**, the pair of vacancy-interstitial is called *Frenkel defect*. Cations are usually smaller and thus displaced easily than anions.
- Closed packed structures have fewer interstitials and displaced ions than vacancies because additional energy is required to force the atoms into the interstitial positions.

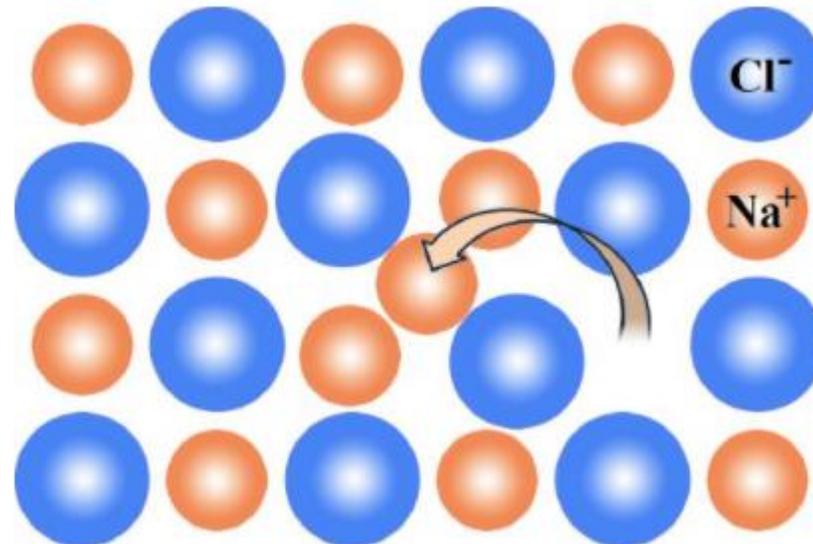


Fig. Frankel defect for NaCl structure

# Schottky Defects

- **A pair of one cation and one anion can be missing** from an ionic crystal, without violating the condition of charge neutrality when the valency of ions is equal. The pair of vacant sites, thus formed, is called *Schottky defect*.

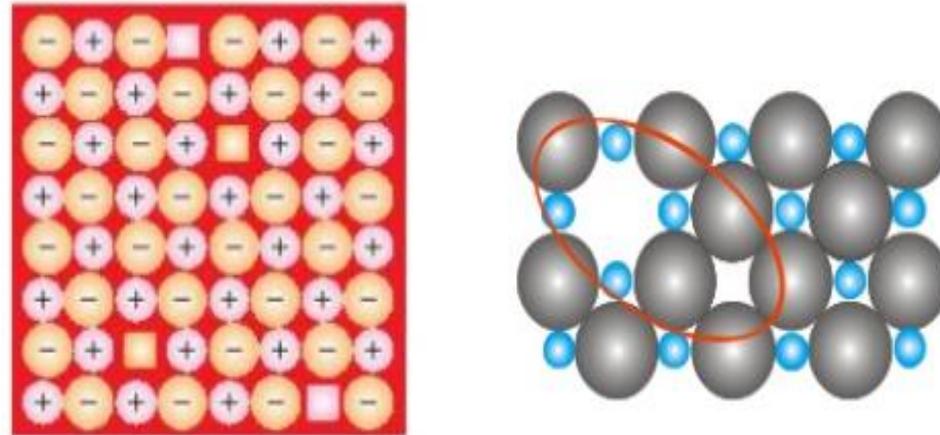


Fig. Schottky Defects

## 2. Line defects or Dislocations

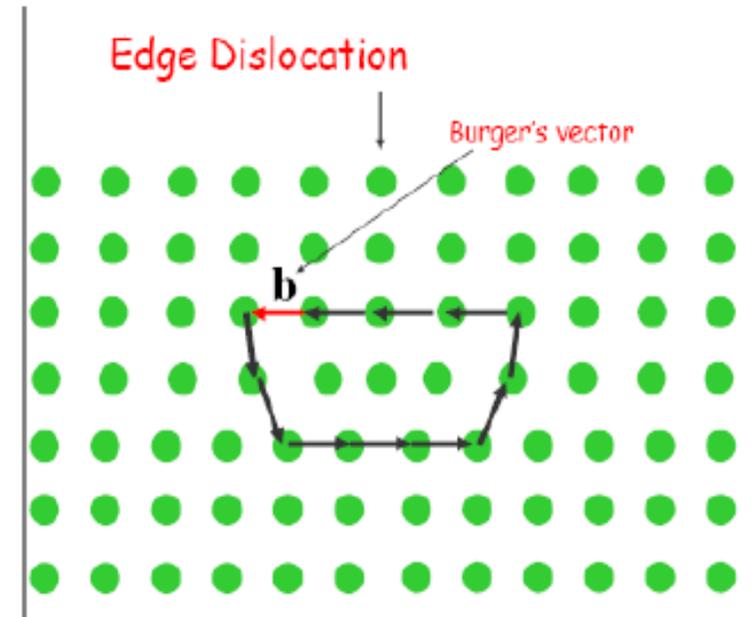
- In **linear defects** groups of atoms are in irregular positions. Linear defects are commonly called dislocations. Any deviation from perfectly periodic arrangement of atoms along a line is called the line imperfection.
- A line defect is a lattice distortion created about a line formed by the solidification process, plastic deformation, vacancy condensation or atomic mismatch in solid solutions.
- The **line imperfection acting as boundary between the slipped and un-slipped region**, lies in the slip plane and is called a dislocation.
- Dislocations are generated and move when a stress is applied. The strength and ductility of metals are controlled by dislocations. They are **characterized by the Burgers vector ( $b$ )**, whose direction and magnitude can be determined by constructing a loop around the disrupted region and noticing the extra inter-atomic spacing needed to close the loop.

Two types of dislocations are distinguished as

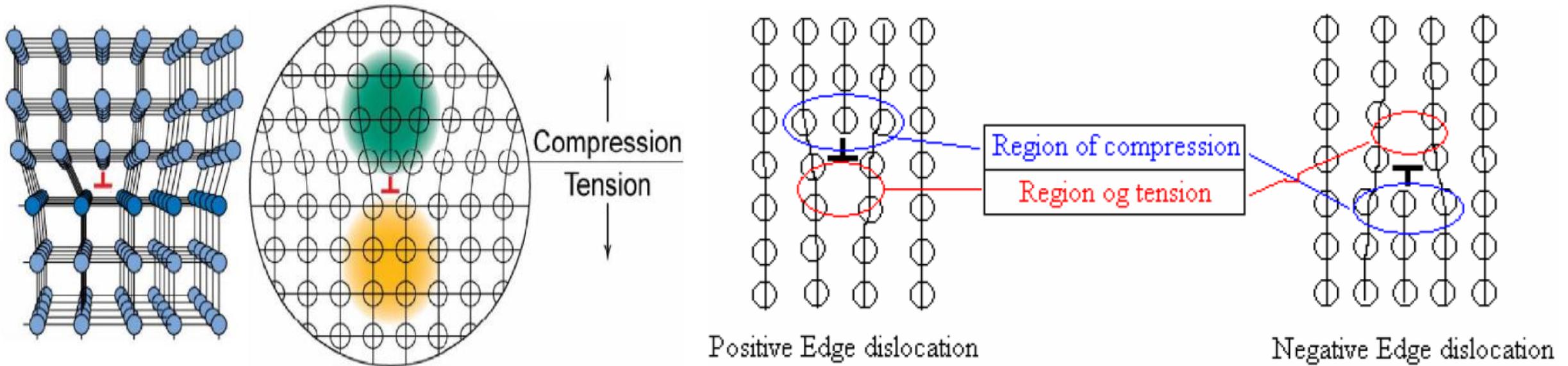
1. Edge dislocations and
2. Screw dislocations.

## 1. *Edge dislocation or Taylor-Orowan dislocation*

- It is characterized by a **Burger's vector** that is **perpendicular to the dislocation line**.
- **Edge dislocation** is , a row of atoms is absent or is displaced by a unit distance within a crystal structure. It may be described as an edge of an extra plane of atoms within a crystal structure. Thus regions of compression and tension are associated with an edge dislocation. Because of extra incomplete plane of atoms, the atoms above the dislocation line are squeezed together and are in state of compression whereas atoms below are pulled apart and experience tensile stresses.



- Edge dislocation is considered *positive* when compressive stresses present above the dislocation line, and is represented by  $\perp$ .
- If the stress state is opposite i.e. compressive stresses exist below the dislocation line, it is considered as **negative edge dislocation**, and represented by  $\top$ . A schematic view of edge dislocations are shown ahead.

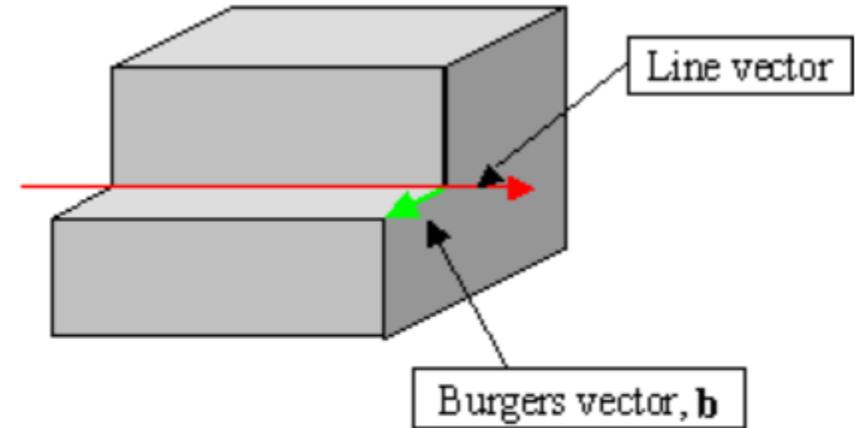


## *Edge dislocations*

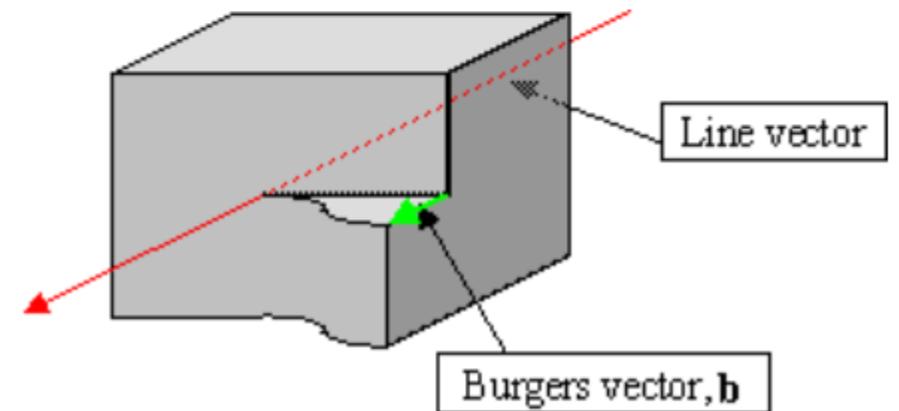
## 2. Screw or Burgers dislocation

- *Screw dislocation* or *Burgers dislocation* has its **dislocation line parallel to the Burger's vector.**
- A screw dislocation is like a spiral ramp with a imperfection line down its axis.
- **Screw dislocations result when displacing planes relative to each other through shear.**
- Shear stresses are associated with the atoms adjacent to the screw dislocation; therefore extra energy is involved as it is in the case of edge dislocations.

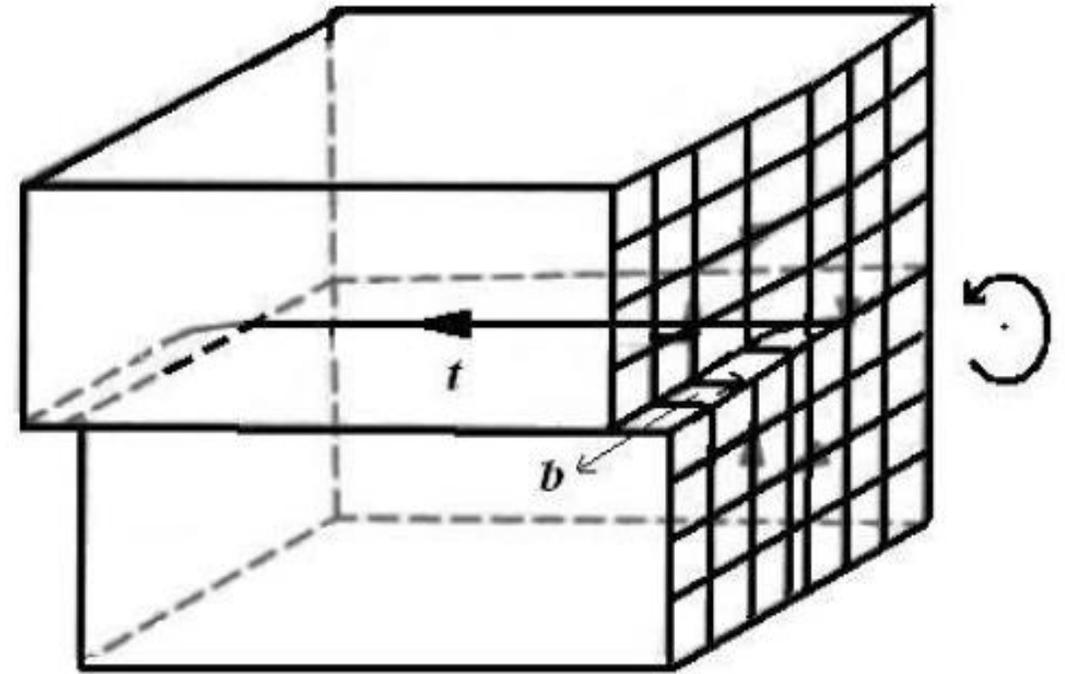
Burgers vector for Line Dislocation.



Burgers vector for Screw Dislocation



- Screw dislocation is considered **positive** if **Burger's vector and  $t$ -vector** or **parallel**, and vice versa. ( $t$ -vector – an unit vector representing the direction of the dislocation line).
- A positive screw dislocation is represented by 
- a dot surrounded by circular direction in clock-wise direction”,
- whereas the negative screw dislocation is represented by  a dot surrounded by a circular direction in anti-clock-wise direction”.



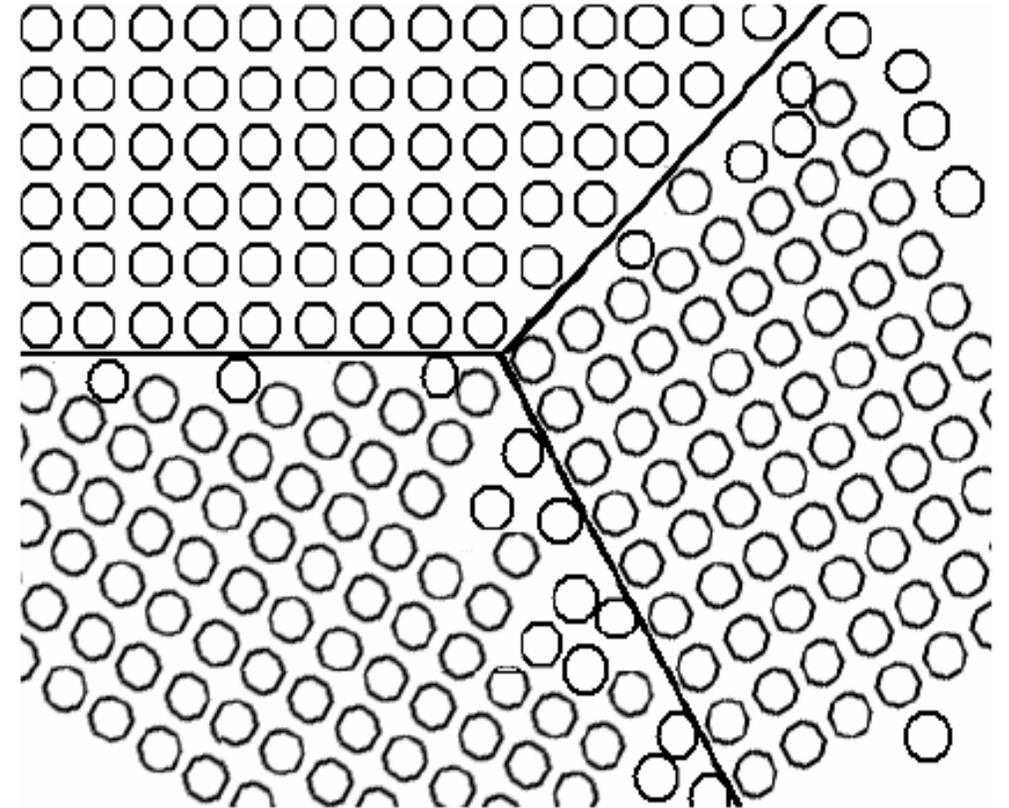
*Negative screw dislocation*

### 3. Surface defects

- These defects can be defined as boundaries that have two dimensional imperfections in crystalline solids, and have different crystal structures and/or crystallographic orientations on either side of them. They refer to the regions of distortions that lie about a surface having thickness of a few atomic diameters.
- These imperfections are not thermodynamically stable, rather they are meta-stable imperfections. They arise from the clustering of line defects into a plane.

## a. Grain boundaries

- Crystalline solids are, usually, made of number of grains separated by grain boundaries. **Grain boundaries** are several atoms distances wide, and there is **mismatch of orientation of grains** on either side of the boundary as shown in *figure*.
- When this **misalignment** is slight, on the order of few degrees ( $< 10^\circ$ ), it is called ***low angle grain boundary***. These boundaries can be described in terms of aligned dislocation arrays.



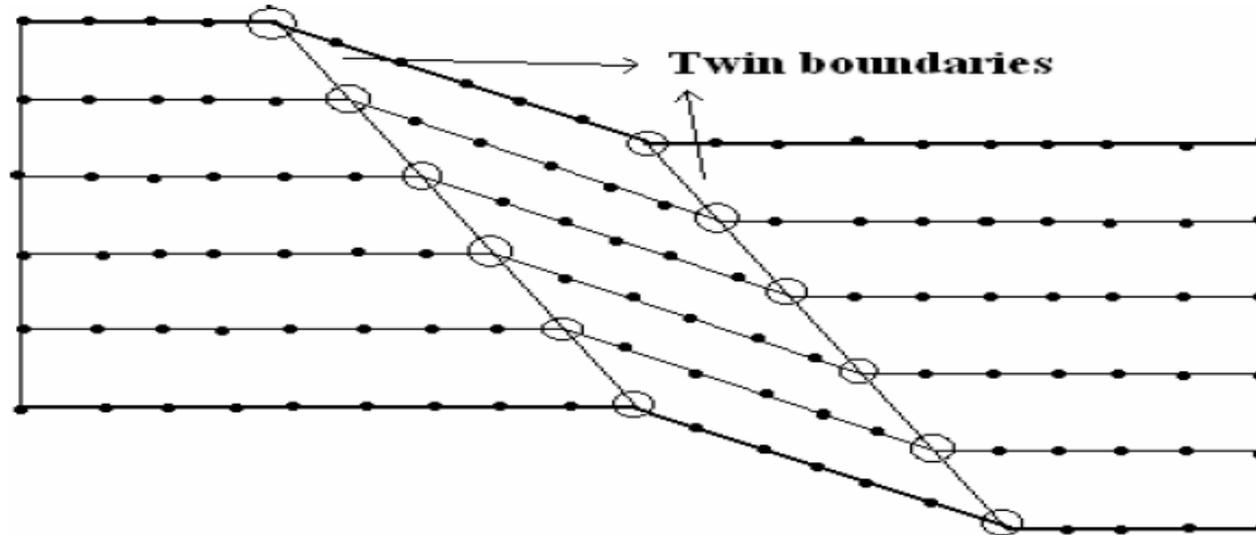
*Schematic presentation of grain boundaries*

# Tilt boundaries

- If the low grain boundary is formed by edge dislocations, it is called *tilt boundary*, and
- *twist boundary* if formed of screw dislocations.
- Both tilt and twist boundaries are planar surface imperfections in contrast to high angle grain boundaries.
- For *high angle grain boundaries*, degree of disorientation is of large range ( $> 15^\circ$ ).
- Grain boundaries are chemically more reactive because of grain boundary energy. In spite of disordered orientation of atoms at grain boundaries, polycrystalline solids are still very strong as cohesive forces present within and across the boundary.

# *Twin boundaries*

- It is a special type of grain boundary across which there is **specific mirror lattice symmetry**. Twin boundaries occur in pairs such that the orientation change introduced by one boundary is restored by the other (*figure*).
- **The region between the pair of boundaries is called the twinned region.**
- Twins which form during the process of recrystallization are called *annealing twins*, whereas *deformation twins* form during plastic deformation.
- Annealing twins are typically found in metals that have FCC crystal structure while mechanical/deformation twins are observed in BCC and HCP metals.



# ***Bulk or Volume defects***

- Volume defects as name suggests are **defects in 3-dimensions**.
- These **include pores, cracks, foreign inclusions and other phases**.
- These defects are normally **introduced during processing and fabrication steps**. All these defects are capable of acting as stress raisers, and thus **deleterious to parent metal's mechanical behavior**.
- However, in some cases foreign particles are added purposefully to strengthen the parent material. The procedure is called dispersion hardening where foreign particles act as obstacles to movement of dislocations, which facilitates plastic deformation.
- The second-phase particles act in two distinct ways
  - **particles are either may be cut by the dislocations or**
  - **the particles resist cutting and dislocations are forced to bypass them.**
- Strengthening due to ordered particles is responsible for the good high-temperature strength on many super-alloys.