



ORISSA SCHOOL OF MINING ENGINEERING,  
KEONJHAR

ଓଡିଶା ଖଣି ସାନ୍ତ୍ରୀକ ବିଦ୍ୟାଳୟ, କେଉଁଝର

GOVERNMENT OF ODISHA | ଓଡିଶା ସରକାର

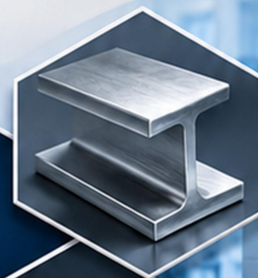
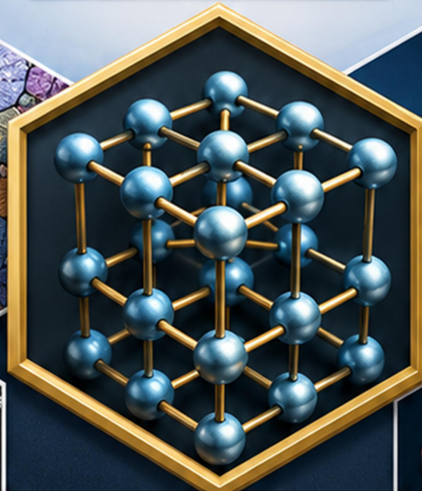
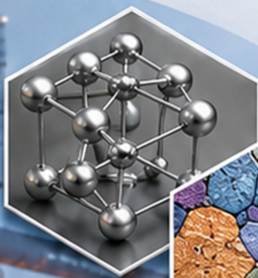


— LECTURE NOTE ON —

# INTRODUCTION TO MATERIALS ENGINEERING

SUBJECT CODE:  
**MTPC201 (Th1)**

SEMESTER - 3<sup>rd</sup>



DEPARTMENT OF  
**METALLURGY**

— ORISSA SCHOOL OF MINING ENGINEERING, KEONJHAR —



— PREPARED BY —  
**TUSHAR K. PATTANAYAK**

Sr Lect, Metallurgical Engineering  
OSME Keonjhar

## Lecture-1

### UNIT–1: INTRODUCTION TO MATERIALS ENGINEERING

#### Chapter–1: Introduction to Materials Engineering

**Course:** MTPC201 – Introduction to Materials Engineering

**Semester:** 3rd Semester Diploma in Metallurgical Engineering

**Reference Books:** William D. Callister, V. Raghavan, Sidney H. Avner, Van Vlack, W.F. Smith, Rollason. The topics are aligned with your syllabus.

#### Chapter Learning Outcomes

After studying this chapter, students will be able to:

1. Define Materials Engineering.
2. Explain the historical development of engineering materials.
3. Describe the scope of Materials Engineering.
4. Explain the Processing–Structure–Properties–Performance (PSPP) relationship.
5. Understand the role of a materials engineer in modern industries.

#### 1.1 Introduction

Every object around us is made of one or more materials. The chair on which we sit, the mobile phone we use, the car we travel in, the bridge we cross, and even the artificial heart valve used in medicine are all made from carefully selected engineering materials.

The success of an engineering product depends not only on its design but also on the proper selection of materials. An unsuitable material may lead to premature failure, corrosion, excessive weight, or high manufacturing cost.

Therefore, understanding the properties and behaviour of materials is one of the most important aspects of engineering.

#### 1.2 What is a Material?

A **material** is any substance used to manufacture engineering products or structures.

Examples include:

| <b>Material</b> | <b>Common Applications</b> |
|-----------------|----------------------------|
|-----------------|----------------------------|

|       |                                 |
|-------|---------------------------------|
| Steel | Buildings, bridges, automobiles |
|-------|---------------------------------|

|           |                         |
|-----------|-------------------------|
| Aluminium | Aircraft, beverage cans |
|-----------|-------------------------|

|        |                  |
|--------|------------------|
| Copper | Electrical wires |
|--------|------------------|



## **Material    Common Applications**

Glass        Windows, optical fibres

Plastic      Packaging, electrical insulation

Rubber      Tyres, seals

Ceramic     Tiles, cutting tools

Composite   Aircraft wings, wind turbine blades

### **1.3 What is Materials Engineering?**

#### **Definition**

**Materials Engineering** is the branch of engineering that deals with the **selection, processing, characterization, improvement, and application of engineering materials** to meet specific service requirements.

It combines the principles of **physics, chemistry, mathematics, metallurgy, and mechanical engineering** to develop materials with desired properties.

#### **Simple Definition (Exam)**

**Materials Engineering is the science and engineering of studying, selecting, processing, and improving materials for engineering applications.**

### **1.4 Why Do We Study Materials Engineering?**

The choice of material determines:

- Strength
- Weight
- Cost
- Durability
- Corrosion resistance
- Electrical conductivity
- Thermal conductivity
- Service life
- Safety

#### **Example 1**

Aircraft are manufactured using **aluminium and titanium alloys** because they are lightweight and strong.

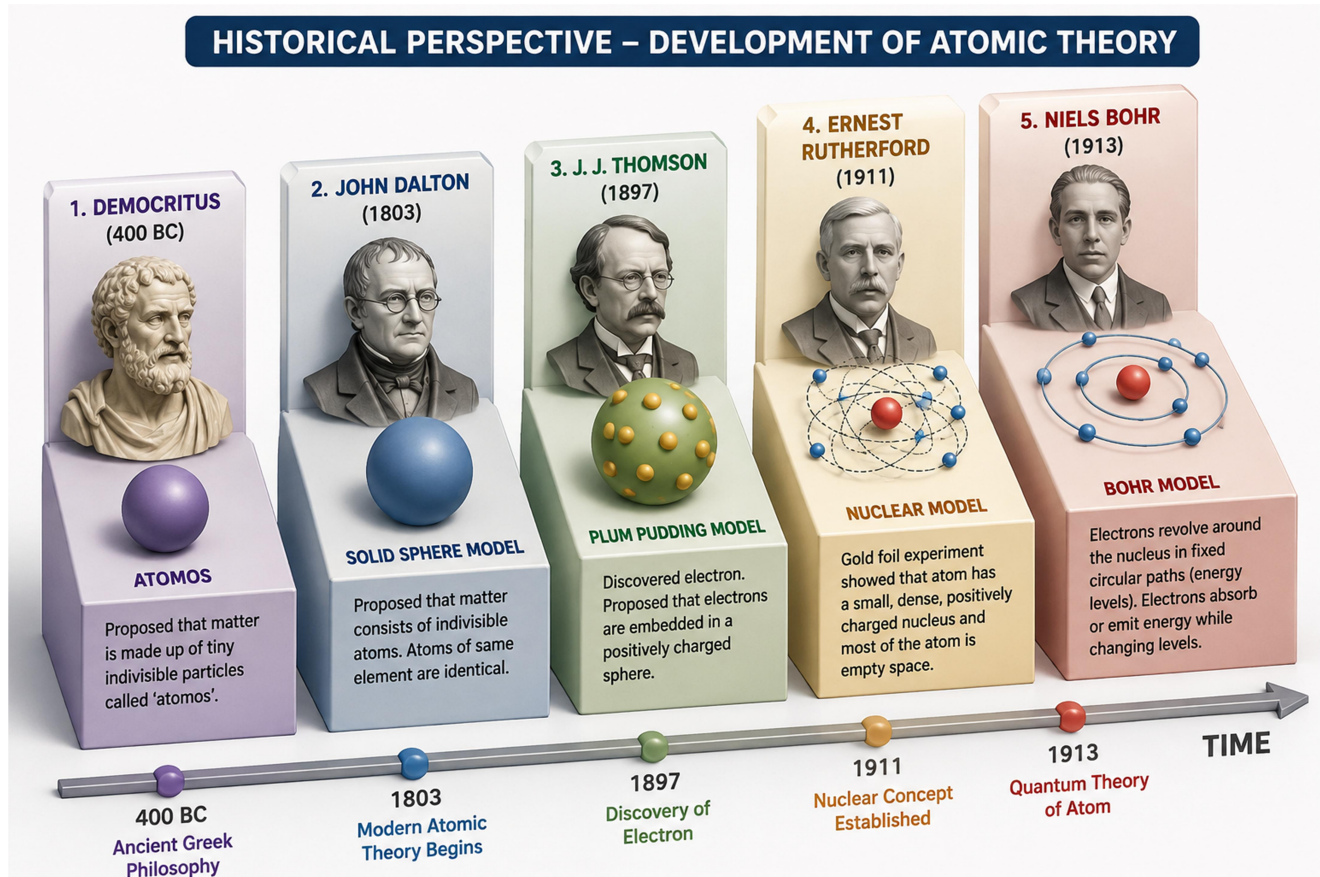
## Example 2

Electrical transmission cables are made of **aluminium** because it is lightweight, corrosion-resistant, and has good electrical conductivity.

## Example 3

Artificial hip joints are made from **titanium alloys** because they are biocompatible and corrosion-resistant.

## 1.5 Historical Perspective of Materials



The history of civilization is closely linked with the development of materials.

### (A) Stone Age (≈2.5 million BC – 3000 BC)

The earliest humans used naturally available materials.

#### Materials Used

- Stone
- Wood
- Bone
- Animal horns

#### Applications

- Hunting tools



- Weapons
- Houses
- Fire-making tools

### **Limitations**

- Brittle
- Difficult to shape
- Heavy

### **(B) Bronze Age (≈3300 BC – 1200 BC)**

Humans discovered alloying.

Bronze = Copper + Tin

### **Advantages**

- Stronger than copper
- Better wear resistance
- Better corrosion resistance

### **Applications**

- Swords
- Spears
- Statues
- Coins

### **(C) Iron Age (≈1200 BC onwards)**

Iron gradually replaced bronze because it was stronger and more abundant.

### **Applications**

- Agricultural tools
- Weapons
- Bridges
- Household tools

### **Importance**

Iron transformed agriculture, construction, and transportation.

### **(D) Steel Age**

The discovery that adding carbon to iron produces steel revolutionized engineering.

### **Advantages**

- High strength
- High toughness
- Good machinability
- Heat treatable
- Economical

### **Applications**

- Railways
- Buildings
- Pressure vessels
- Automobiles
- Ships

### **(E) Polymer Age**

The twentieth century witnessed rapid development of synthetic polymers.

Examples:

- PVC
- Nylon
- Bakelite
- Polyethylene

### **Applications**

- Packaging
- Pipes
- Electrical insulation
- Household products

### **(F) Semiconductor Age**

The invention of semiconductor materials transformed electronics.

Examples

- Silicon

- Germanium

#### Applications

- Computers
- Mobile phones
- Integrated circuits
- Solar cells

### **(G) Advanced Materials Age**

Modern engineering increasingly uses advanced materials.

#### Examples

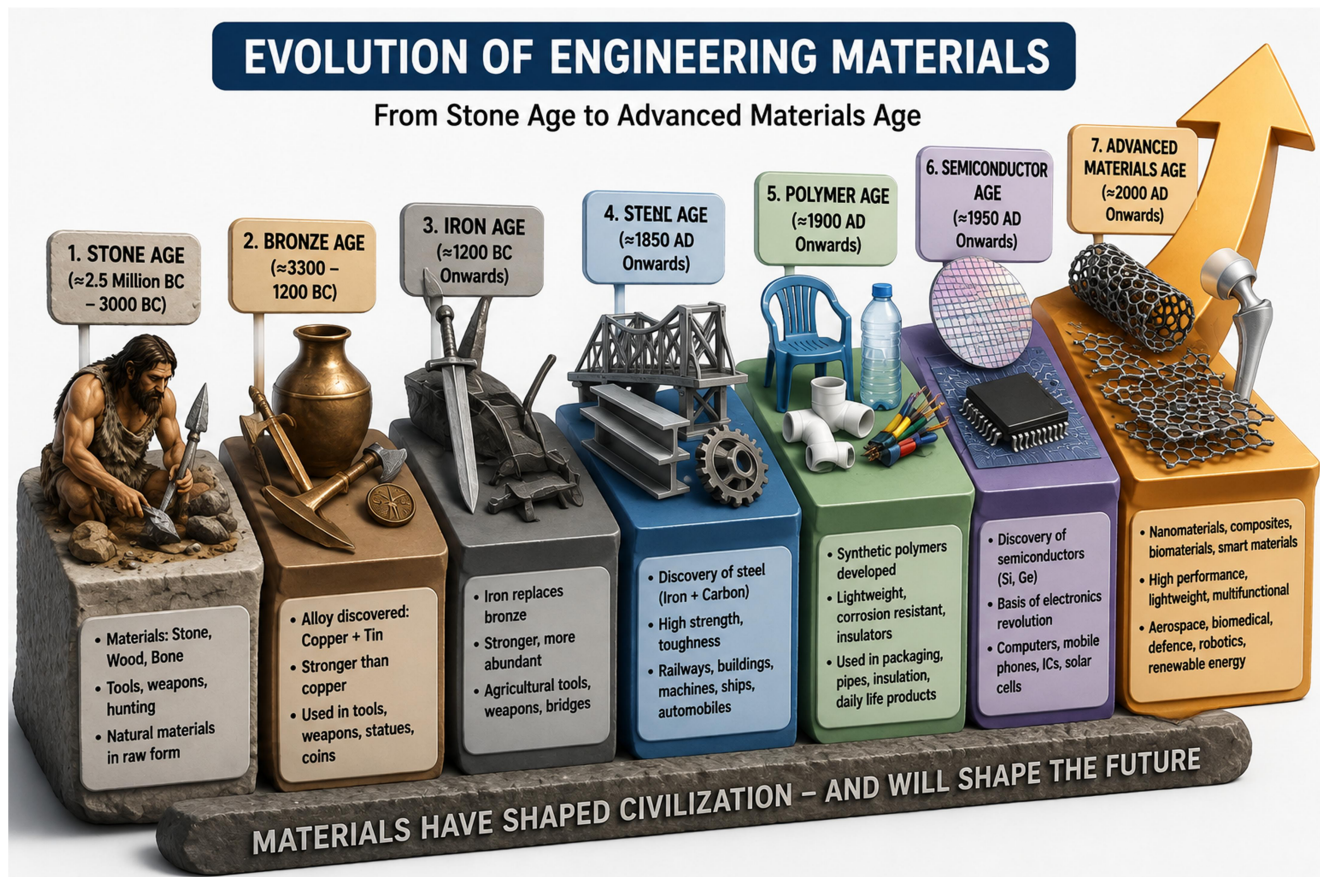
- Carbon fibre composites
- Graphene
- Carbon nanotubes
- Biomaterials
- Shape memory alloys
- Smart materials
- Nanomaterials

#### Applications

- Aerospace
- Biomedical engineering
- Defence
- Electric vehicles
- Renewable energy
- Robotics



## Evolution of Engineering Materials



### 1.6 Scope of Materials Engineering

Materials Engineering has applications in almost every engineering discipline.

#### Major Areas

##### Aerospace Engineering

Materials:

- Titanium alloys
- Aluminium alloys
- Carbon fibre composites

Applications:

- Aircraft
- Rockets
- Satellites

##### Automobile Engineering

Materials:

- Steel
- Aluminium
- Magnesium alloys
- Polymers

Applications:

- Engine
- Chassis
- Body panels

### **Biomedical Engineering**

Materials:

- Titanium
- Stainless steel
- Ceramics
- Polymers

Applications:

- Bone implants
- Dental implants
- Artificial joints

### **Electrical Engineering**

Materials:

- Copper
- Aluminium
- Silicon

Applications:

- Transformers
- Motors
- Wires
- Semiconductors

## **Civil Engineering**

Materials:

- Steel
- Cement
- Concrete
- Glass

Applications:

- Buildings
- Bridges
- Dams

## **Metallurgical Engineering**

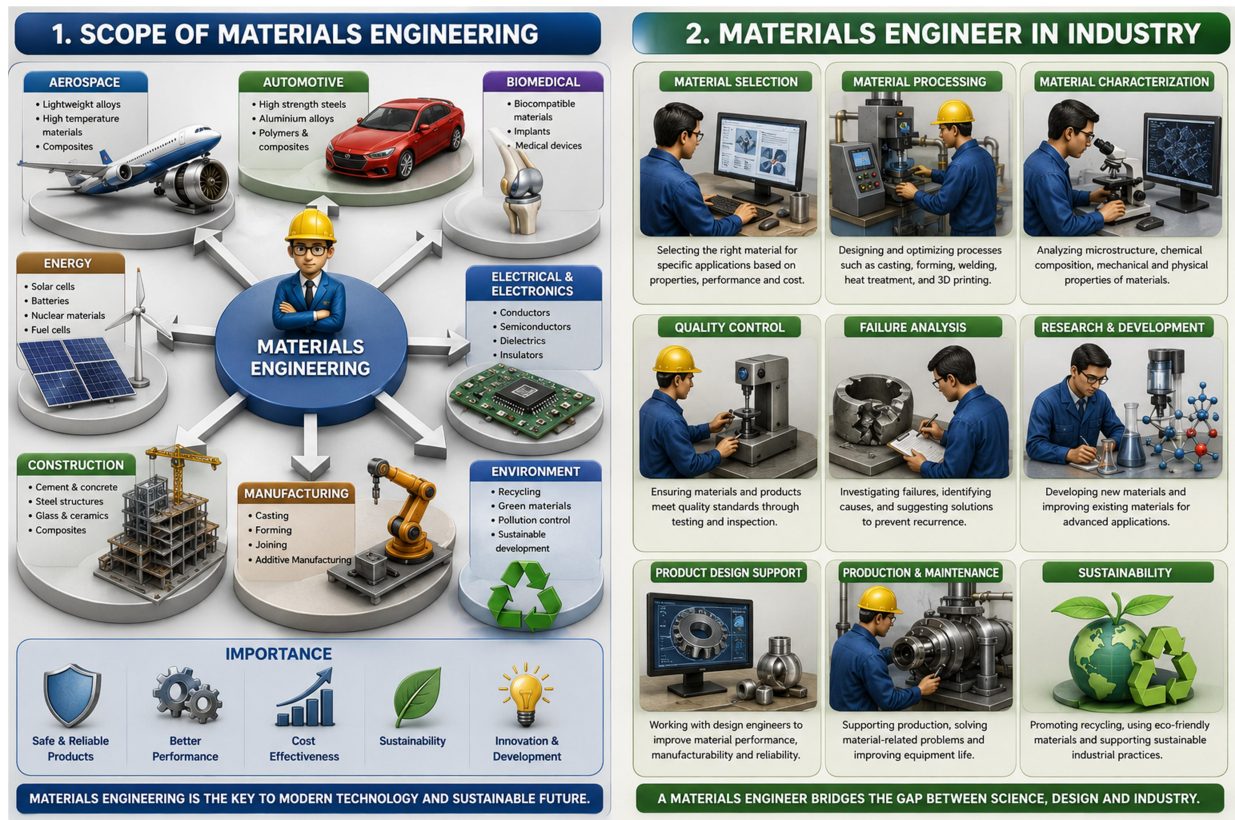
Materials engineers work in:

- Steel plants
- Aluminium plants
- Copper smelters
- Foundries
- Heat treatment industries
- Rolling mills
- Quality control laboratories

### **1.7 Role of a Materials Engineer**

A Materials Engineer:

- Selects suitable materials.
- Designs new alloys and composites.
- Improves manufacturing processes.
- Investigates component failures.
- Performs quality control.
- Conducts material testing.
- Develops environmentally sustainable materials.
- Supports recycling and circular economy practices.



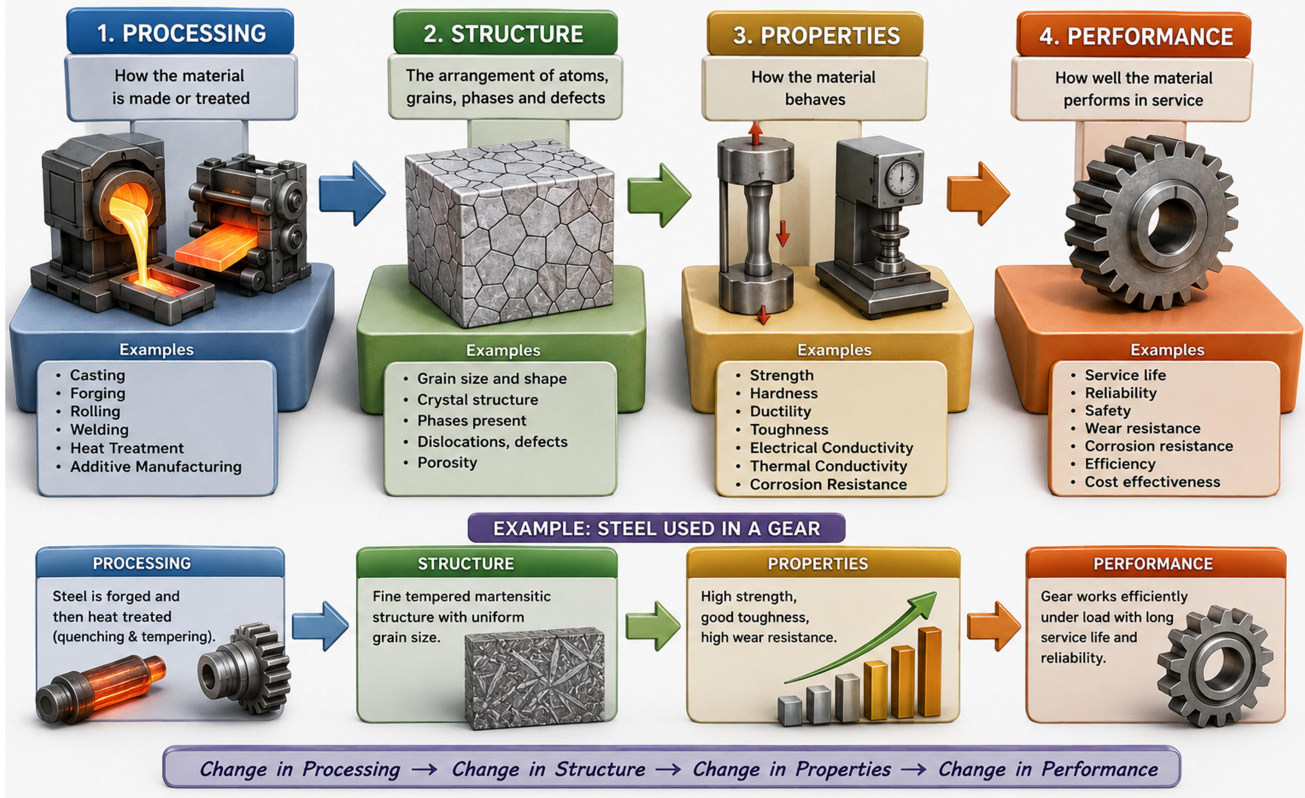
### 1.8 Processing–Structure–Properties–Performance (PSPP) Correlation

One of the most important concepts in Materials Engineering is the relationship between **Processing**, **Structure**, **Properties**, and **Performance**.

#### Flow Diagram



# PROCESSING – STRUCTURE – PROPERTIES – PERFORMANCE RELATIONSHIP



## 1. Processing

Processing refers to the manufacturing method used to produce a material or component.

Examples:

- Casting
- Forging
- Rolling
- Welding
- Heat treatment
- Powder metallurgy
- Additive manufacturing (3D printing)

## 2. Structure

Structure refers to the arrangement of atoms, grains, phases, and defects within a material.

Structures are studied at different scales:

- Atomic structure
- Crystal structure

- Microstructure
- Macrostructure

### **3. Properties**

Properties describe how a material behaves.

Examples:

- Strength
- Hardness
- Ductility
- Toughness
- Electrical conductivity
- Thermal conductivity
- Corrosion resistance

### **4. Performance**

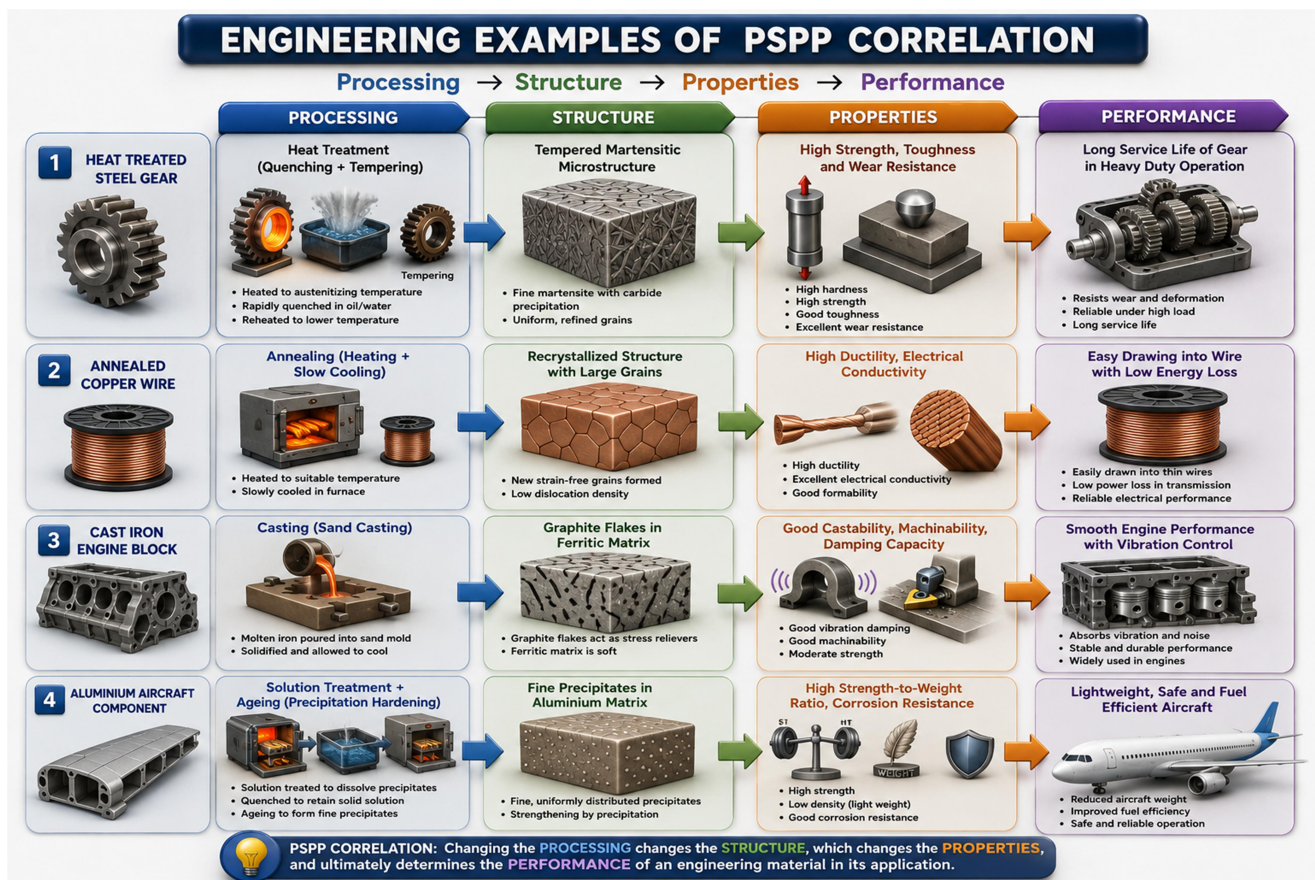
Performance refers to how well a material functions in its intended service environment.

Examples:

- Service life
- Reliability
- Safety
- Efficiency
- Wear resistance

### **Engineering Example**





### Heat treatment of steel

- **Processing:** Heat treatment (quenching and tempering)
- **Structure:** Martensitic microstructure
- **Properties:** High hardness and strength
- **Performance:** Improved wear resistance in gears and cutting tools

This example shows that modifying the **processing** changes the **structure**, which alters the **properties** and ultimately improves the **performance** of the engineering component.

### Key Points to Remember

- Materials are the foundation of all engineering products.
- Human civilization has progressed through the development of new materials.
- Proper material selection improves safety, performance, and economy.
- Materials Engineering integrates science with manufacturing and design.
- The PSPP relationship is a fundamental concept in Materials Engineering.

### Frequently Asked Viva Questions

1. Define Materials Engineering.

2. What is an engineering material?
3. Why is steel widely used in engineering?
4. Name four advanced engineering materials.
5. What is the scope of Materials Engineering?
6. What are the four components of the PSPP relationship?
7. Why is material selection important in engineering design?
8. Give two examples of engineering applications of composites.

### **Examination Questions**

#### **Short Questions (2 Marks)**

1. Define Materials Engineering.
2. State the importance of material selection.
3. What is the Stone Age?
4. Name four advanced materials.
5. What is meant by processing?

#### **Long Questions (10 Marks)**

1. Explain the historical development of engineering materials with suitable examples.
2. Discuss the scope of Materials Engineering in modern industries.
3. Explain the Processing–Structure–Properties–Performance (PSPP) relationship with a neat diagram and suitable engineering examples.

### **Lecture-3**

#### **UNIT–1: INTRODUCTION TO MATERIALS ENGINEERING**

##### **Chapter–2: Atomic Structure**

**Course:** MTPC201 – Introduction to Materials Engineering

**Semester:** 3rd Semester Diploma in Metallurgical Engineering

**Syllabus Covered:** Fundamental concepts on atoms. This chapter expands that syllabus topic using standard references such as Callister, V. Raghavan, Van Vlack, W.F. Smith, Avner, and Rollason.

##### **Chapter Learning Outcomes**

After studying this chapter, students will be able to:

- Explain the structure of an atom.
- Identify subatomic particles and their properties.

- Define atomic number, mass number, isotopes, and ions.
- Explain electron shells and electronic configuration.
- Understand the importance of valence electrons in engineering materials.
- Relate atomic structure to material properties.

## 2.1 Introduction

Everything in the universe is made of **matter**, and matter is composed of tiny particles called **atoms**.

Atoms are the fundamental building blocks of all engineering materials, including metals, ceramics, polymers, semiconductors, and composites.

Although atoms are extremely small, their arrangement and interactions determine the strength, hardness, electrical conductivity, corrosion resistance, and other properties of materials.

## 2.2 What is an Atom?

### Definition

An **atom** is the smallest unit of an element that retains the chemical properties of that element.

Examples:

- An iron atom retains the properties of iron.
- A copper atom retains the properties of copper.

Atoms combine to form molecules and solids.

# FUNDAMENTAL CONCEPTS ON ATOMS

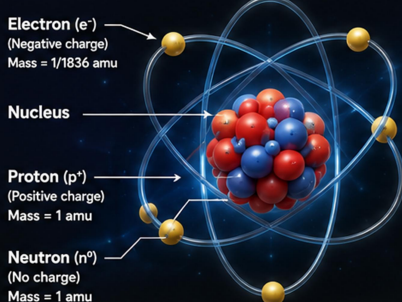
## 1. WHAT IS AN ATOM?

An atom is the smallest particle of an element that retains the chemical properties of that element.



Made up of tiny particles

## 2. STRUCTURE OF AN ATOM



### KEY POINTS

- Nucleus is at the centre.
- Protons and neutrons are in the nucleus.
- Electrons revolve around the nucleus in fixed energy levels called shells.

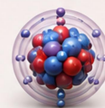
## 3. SUBATOMIC PARTICLES

| Particle | Symbol | Charge | Relative Mass | Location       |
|----------|--------|--------|---------------|----------------|
| Proton   | $p^+$  | +1     | 1 amu         | Nucleus        |
| Neutron  | $n^0$  | 0      | 1 amu         | Nucleus        |
| Electron | $e^-$  | -1     | $1/1836$ amu  | Around nucleus |

## 4. ATOMIC NUMBER (Z)

Number of protons in the nucleus.  
(= Number of electrons in a neutral atom)

Example: Sodium (Na)  
**Z = 11**



11 Protons  
11 Electrons

## 5. MASS NUMBER (A)

Total number of protons and neutrons in the nucleus.  
( $A = Z + N$ )

Example: Carbon-12  
**A = 12**



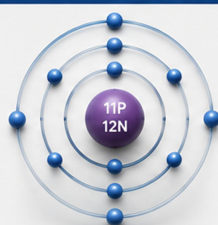
Z = 6 (Protons)  
N = 6 (Neutrons)  
A = 12

## 6. ELECTRONIC CONFIGURATION

Electrons are arranged in shells around the nucleus.

| Shell                 | Symbol | Maximum Electrons |
|-----------------------|--------|-------------------|
| 1 <sup>st</sup> Shell | K      | 2                 |
| 2 <sup>nd</sup> Shell | L      | 8                 |
| 3 <sup>rd</sup> Shell | M      | 18                |
| 4 <sup>th</sup> Shell | N      | 32                |

## 7. EXAMPLE: SODIUM (Na) – Z = 11



Electronic configuration  
**2, 8, 1**

**K shell = 2 electrons**

**L shell = 8 electrons**

**M shell = 1 electron**

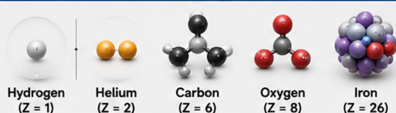
**Valence electrons = 1**  
(outermost shell electrons)

## 9. ATOMS TEND TO BECOME STABLE

Atoms gain, lose or share electrons to attain a stable configuration (octet rule – 8 electrons in outer shell, except H and He have 2).



## EXAMPLES OF ATOMS



## 8. VALENCE ELECTRONS

Electrons present in the outermost shell are called valence electrons. They are responsible for chemical bonding and properties of elements.



Valence  $e^- = 1$



Valence  $e^- = 2$



Valence  $e^- = 3$



Valence  $e^- = 6$

## 10. IMPORTANCE

- Basis for understanding bonding between atoms.
- Determines physical and chemical properties of materials.
- Helps in studying crystal structure, defects and material behaviour.
- Essential for selecting and designing engineering materials.

## 2.3 Historical Development of Atomic Theory

### (A) Democritus (400 BC)

- Proposed that matter consists of tiny indivisible particles called **atomos**.
- This idea was philosophical and lacked experimental proof.

### (B) John Dalton (1808)

#### Dalton's Atomic Theory

1. Matter consists of tiny indivisible atoms.
2. All atoms of the same element are identical.
3. Atoms cannot be created or destroyed during chemical reactions.
4. Compounds are formed by the combination of atoms in fixed proportions.

#### Limitations

- Could not explain isotopes.
- Could not explain ions.
- Did not describe internal atomic structure.

### (C) J. J. Thomson (1897)

- Discovered the **electron** using cathode ray experiments.
- Proposed the **Plum Pudding Model**, where electrons were embedded in a positively charged sphere.

### **Limitation**

Could not explain the scattering of alpha particles.

### **(D) Rutherford (1911)**

- Conducted the famous **Gold Foil Experiment**.
- Concluded that:
  - Most of the atom is empty space.
  - Positive charge is concentrated in a tiny nucleus.
  - Electrons revolve around the nucleus.

### **(E) Niels Bohr (1913)**

- Proposed that electrons move in fixed circular orbits (energy levels).
- Electrons absorb or emit energy when they move between energy levels.

Although modern atomic theory is based on quantum mechanics, Bohr's model remains useful for introducing atomic structure.

## **2.4 Structure of an Atom**

An atom consists of:

1. **Nucleus**
2. **Electrons**

### **Nucleus**

The nucleus is located at the centre of the atom and contains:

- Protons
- Neutrons

The nucleus contains almost all the mass of the atom.

### **Electrons**

Electrons revolve around the nucleus in discrete energy levels (shells).

### **Simple Diagram**

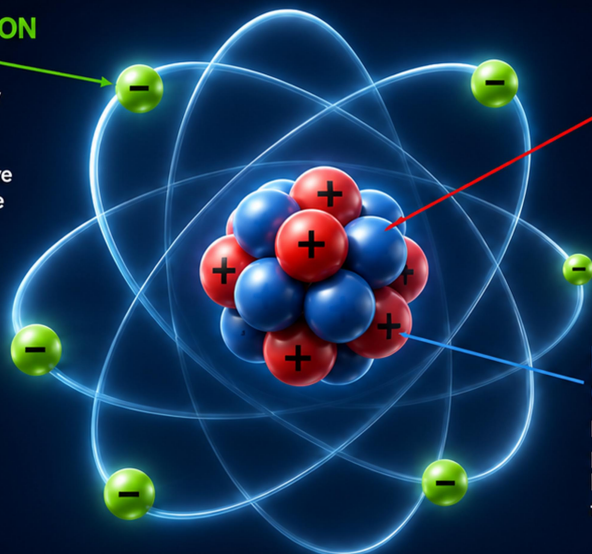


# STRUCTURE OF AN ATOM

An atom is the basic building block of matter.

## ELECTRON ( $e^-$ )

Negatively charged particles that revolve around the nucleus in specific energy levels or shells.



## PROTON ( $p^+$ )

Positively charged particles located in the nucleus.

## NEUTRON ( $n^0$ )

Neutral particles located in the nucleus.

## KEY FEATURES

- An atom consists of a tiny, dense **nucleus** at the center.
- Electrons** revolve around the nucleus in fixed energy levels (shells).
- The atom is mostly **empty space**.
- In a neutral atom, number of **protons** = number of **electrons**.

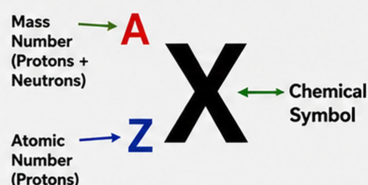
## CHARGE AND MASS

- Proton charge = +1
- Neutron charge = 0
- Electron charge = -1
- Proton mass  $\approx 1$  u
- Neutron mass  $\approx 1$  u
- Electron mass  $\approx 1/1836$  u  
(u = unified atomic mass unit)

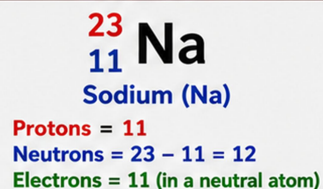
## ATOMIC COMPOSITION

| Particle           | Charge | Relative Mass      | Location               |
|--------------------|--------|--------------------|------------------------|
| Proton ( $p^+$ )   | +1     | 1 u                | Nucleus                |
| Neutron ( $n^0$ )  | 0      | 1 u                | Nucleus                |
| Electron ( $e^-$ ) | -1     | $\frac{1}{1836}$ u | Energy Levels (Shells) |

## ATOMIC NOTATION



## EXAMPLE



**IN SIMPLE WORDS:** The **nucleus (protons + neutrons)** is the heart of the atom, and **electrons** move around it in shells like planets around the sun.

## 2.5 Subatomic Particles

Particle   Symbol   Charge   Relative Mass   Location

|          |       |    |              |                |
|----------|-------|----|--------------|----------------|
| Proton   | $p^+$ | +1 | 1 amu        | Nucleus        |
| Neutron  | $n^0$ | 0  | 1 amu        | Nucleus        |
| Electron | $e^-$ | -1 | $1/1836$ amu | Around nucleus |

### Proton

- Positively charged particle.
- Determines the identity of an element.

Example:

Hydrogen  $\rightarrow$  1 proton

Carbon  $\rightarrow$  6 protons

Iron  $\rightarrow$  26 protons

## Neutron

- Electrically neutral.
- Contributes to atomic mass.
- Helps stabilize the nucleus.

## Electron

- Negatively charged particle.
- Responsible for:
  - Chemical bonding
  - Electrical conductivity
  - Thermal conductivity

The number and arrangement of electrons greatly influence the properties of engineering materials.

## 2.6 Atomic Number (Z)

### Definition

The **atomic number** is the number of protons present in the nucleus of an atom.

Atomic Number (Z) = Number of Protons

Example:

- Carbon = 6
- Aluminium = 13
- Iron = 26
- Copper = 29

For a neutral atom:

**Number of protons = Number of electrons**

## 2.7 Mass Number (A)

### Definition

The **mass number** is the total number of protons and neutrons present in the nucleus.

$$A = Z + N$$

where:

- A = Mass number
- Z = Atomic number

- N = Number of neutrons

### Example

Iron:

- Protons = 26
- Neutrons = 30

Mass Number

$$= 26 + 30$$

$$= 56$$

### 2.8 Atomic Notation

Atoms are represented as:

Atoms are represented as:



Example:



where:

- Fe = Iron
- 26 = Atomic number
- 56 = Mass number

## Lecture-4

### 2.9 Electron Shells (Bohr Model)

Electrons occupy specific shells around the nucleus.

| Shell  | Symbol | Maximum Electrons |
|--------|--------|-------------------|
| First  | K      | 2                 |
| Second | L      | 8                 |
| Third  | M      | 18                |
| Fourth | N      | 32                |

Electrons occupy lower-energy shells before higher-energy shells.

## 2.10 Electronic Configuration

### Definition

Electronic configuration is the arrangement of electrons in different shells and subshells.

### Examples

Hydrogen (1)

1

Helium (2)

2

Lithium (3)

2,1

Carbon (6)

2,4

Oxygen (8)

2,6

Sodium (11)

2,8,1

Aluminium (13)

2,8,3

Iron (26)

2,8,14,2 (Bohr shell representation)

## 2.11 Valence Electrons

### Definition

Electrons present in the **outermost shell** are called **valence electrons**.

They are responsible for:

- Chemical bonding
- Electrical conductivity
- Mechanical properties
- Corrosion behaviour

### Examples

| Element | Valence Electrons |
|---------|-------------------|
|---------|-------------------|

|        |   |
|--------|---|
| Sodium | 1 |
|--------|---|

|           |   |
|-----------|---|
| Magnesium | 2 |
|-----------|---|

|           |   |
|-----------|---|
| Aluminium | 3 |
|-----------|---|

|        |   |
|--------|---|
| Carbon | 4 |
|--------|---|

|        |   |
|--------|---|
| Oxygen | 6 |
|--------|---|

## 2.12 Isotopes

### Definition

Atoms of the same element having the same atomic number but different mass numbers are called **isotopes**.

Example:

Hydrogen

- Protium
- Deuterium
- Tritium

All have one proton but different numbers of neutrons.

### Applications

- Medical diagnosis
- Radiography
- Nuclear reactors
- Scientific research

## 2.13 Ions

### Definition

An atom that gains or loses electrons becomes an **ion**.

### Cation

Formed by losing electrons.

Example:

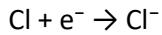




## **Anion**

Formed by gaining electrons.

Example:



Ions play an essential role in ionic bonding, discussed in the next chapter.

## **2.14 Importance of Atomic Structure in Materials Engineering**

Understanding atomic structure helps engineers:

- Select suitable materials.
- Understand bonding.
- Predict mechanical properties.
- Explain electrical conductivity.
- Explain corrosion behaviour.
- Develop new alloys and advanced materials.

### **Key Points to Remember**

- The atom is the basic unit of an element.
- The nucleus contains protons and neutrons.
- Electrons occupy discrete energy levels.
- Atomic number equals the number of protons.
- Mass number equals protons plus neutrons.
- Valence electrons determine chemical bonding and many material properties.
- Isotopes differ only in the number of neutrons.
- Ions are formed by the gain or loss of electrons.

### **Frequently Asked Viva Questions**

1. Define an atom.
2. Name the three subatomic particles.
3. What is the charge on an electron?
4. Define atomic number.
5. Define mass number.
6. What are valence electrons?

7. What are isotopes? Give one example.
8. Differentiate between a cation and an anion.
9. Why are valence electrons important in Materials Engineering?
10. State one limitation of Dalton's atomic theory.

### **Examination Questions**

#### **Short Questions (2 Marks)**

1. Define atomic number.
2. Define mass number.
3. What is an isotope?
4. What is an ion?
5. What are valence electrons?

#### **Long Questions (10 Marks)**

1. Explain the structure of an atom with a neat labelled diagram.
2. Discuss the historical development of atomic theory from Dalton to Bohr.
3. Explain atomic number, mass number, isotopes, ions, and electronic configuration with suitable examples.

### **Lecture-5**

#### **UNIT–1: INTRODUCTION TO MATERIALS ENGINEERING**

##### **Chapter–3: Bonding Forces and Energies**

**Course:** MTPC201 – Introduction to Materials Engineering

**Semester:** 3rd Semester Diploma in Metallurgical Engineering

**Syllabus Covered:** Bonding Forces and Energies. The topic is expanded from your syllabus using standard materials science references (Callister, V. Raghavan, Van Vlack, W.F. Smith, Rollason, and Avner).

#### **Chapter Learning Outcomes**

After studying this chapter, students should be able to:

- Explain why atoms form bonds.
- Define interatomic forces.
- Differentiate between attractive and repulsive forces.
- Explain bond energy and equilibrium bond distance.
- Interpret the potential energy curve.

- Relate bond strength to engineering properties.

### 3.1 Introduction

In nature, atoms rarely exist alone. They tend to combine with other atoms to form molecules or solids because a bonded state has **lower energy and greater stability** than isolated atoms.

For example:

- Two hydrogen atoms combine to form  $H_2$ .
- Iron atoms bond together to form metallic iron.
- Sodium and chlorine combine to form sodium chloride (NaCl).

The force that holds atoms together is called an **interatomic bonding force**.

### 3.2 Why Do Atoms Form Bonds?

Atoms form bonds to achieve a **stable electronic configuration**, usually by completing their outermost (valence) electron shell.

A bonded atom has:

- Lower potential energy
- Greater stability
- Lower tendency to react

**Remember:**

**Nature always favors the lowest energy state.**

### 3.3 Interatomic Forces

Interatomic forces are the forces acting between neighbouring atoms.

They are of two types:

1. Attractive forces
2. Repulsive forces

#### (A) Attractive Force

Attractive forces pull atoms toward each other.

They arise due to:

- Attraction between positively charged nuclei and negatively charged electrons.

When atoms are far apart, attractive forces dominate.

#### (B) Repulsive Force

Repulsive forces push atoms away from each other.

They arise due to:

- Repulsion between electron clouds.
- Repulsion between positively charged nuclei when atoms come very close.

At very short distances, repulsive forces become very large.

### **3.4 Balance Between Attractive and Repulsive Forces**

The actual distance between two bonded atoms is determined by the balance between these forces.

- If atoms are too far apart → attractive force dominates.
- If atoms are too close → repulsive force dominates.
- At one particular distance, the two forces are equal.

This distance is called the **equilibrium bond distance**.

### **3.5 Equilibrium Bond Distance**

#### **Definition**

The equilibrium bond distance is the distance between the centres of two bonded atoms at which the attractive and repulsive forces balance each other.

At this distance:

- Net force = 0
- Potential energy is minimum
- The bond is most stable

**Symbol:** (  $r_0$  )

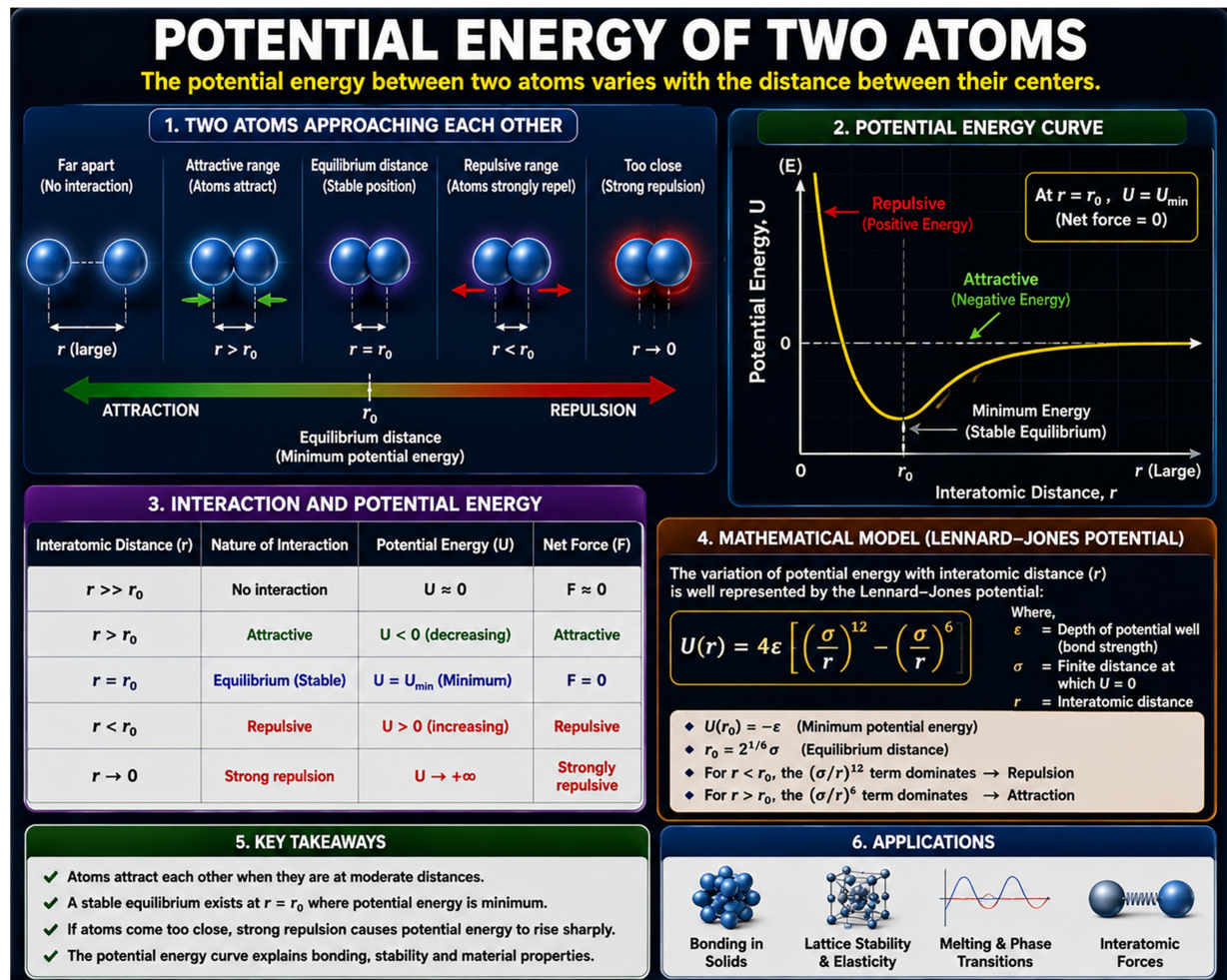
### **3.6 Potential Energy of Two Atoms**

Potential energy changes as the distance between atoms changes.

- Far apart → Potential energy is high.
- Moving closer → Potential energy decreases.
- At equilibrium distance → Potential energy is minimum.
- Closer than equilibrium → Potential energy rises sharply because of repulsion.

This variation is represented by the **Potential Energy Curve**.

## 3.7 Potential Energy Curve



## 3.8 Bond Energy

## Definition

**Bond energy** is the amount of energy required to separate two bonded atoms completely to an infinite distance.

It is also the energy released when a bond is formed.

## Units

- kJ/mol
- eV/atom

## Significance of Bond Energy

A material with **high bond energy** generally has:

- High melting point

- High hardness
- High elastic modulus
- Better thermal stability

A material with **low bond energy** generally has:

- Lower melting point
- Softer structure
- Lower stiffness

### 3.9 Relationship Between Bond Energy and Material Properties

| High Bond Energy         | Low Bond Energy        |
|--------------------------|------------------------|
| High melting point       | Low melting point      |
| High hardness            | Soft material          |
| High strength            | Lower strength         |
| High elastic modulus     | Low elastic modulus    |
| Better thermal stability | Poor thermal stability |

### 3.10 Bond Length

#### Definition

Bond length is the equilibrium distance between the nuclei of two bonded atoms.

Examples:

- Carbon–Carbon bond  $\approx 0.154$  nm
- Hydrogen molecule  $\approx 0.074$  nm

A shorter bond generally indicates a stronger bond.

### 3.11 Bond Stiffness

Bond stiffness measures the resistance of a bond to stretching or compression.

Materials with stiff bonds exhibit:

- High Young's modulus
- Small elastic deformation

Example:

- Diamond has very stiff covalent bonds.



- Rubber has flexible molecular bonds.

### **3.12 Effect of Bonding on Engineering Materials**

The nature of bonding strongly influences material properties.

#### **Mechanical Properties**

- Strength
- Hardness
- Elasticity
- Ductility

#### **Thermal Properties**

- Melting point
- Thermal conductivity
- Thermal expansion

#### **Electrical Properties**

- Conductivity
- Resistivity

#### **Chemical Properties**

- Corrosion resistance
- Chemical stability

### **3.13 Engineering Examples**

#### **Example 1: Diamond**

- Strong covalent bonding
- Very high bond energy
- Extremely hard
- High melting point

Applications:

- Cutting tools
- Abrasives

#### **Example 2: Copper**

- Metallic bonding

- Free electrons
- Excellent electrical conductivity
- Good ductility

Applications:

- Electrical wires
- Heat exchangers

### **Example 3: Sodium Chloride**

- Ionic bonding
- High melting point
- Hard but brittle

Applications:

- Chemical industry
- Food preservation

### **Example 4: Polyethylene**

- Weak secondary bonding between polymer chains
- Flexible
- Low melting point
- Lightweight

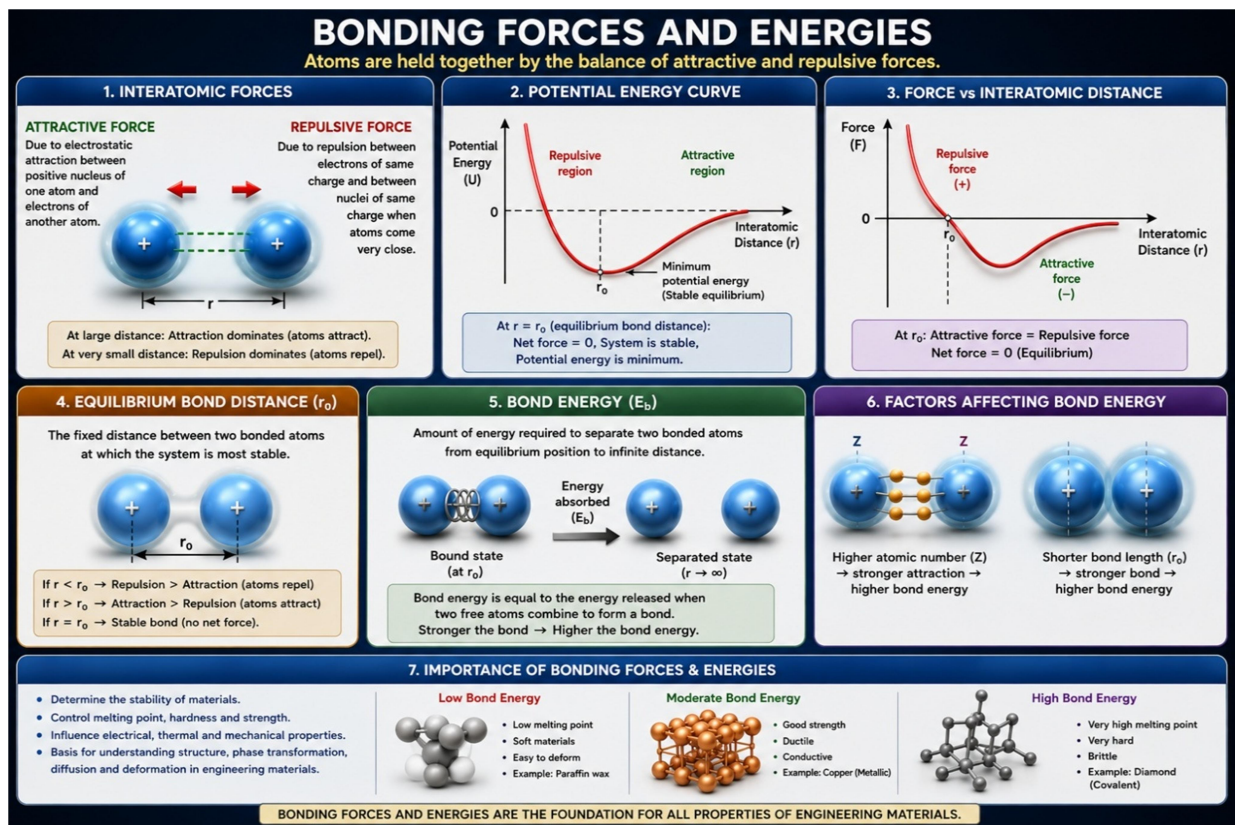
Applications:

- Packaging
- Containers

## **3.14 Importance of Bonding in Metallurgy**

A metallurgical engineer studies bonding because it helps to:

- Select suitable engineering materials.
- Predict material behaviour.
- Design stronger alloys.
- Improve heat treatment processes.
- Develop advanced materials for aerospace, biomedical, and energy applications.



8. Why does diamond have very high hardness?
9. What is the significance of the potential energy curve?
10. How does bonding influence material properties?

#### **Examination Questions**

##### **Short Questions (2 Marks)**

1. Define bond energy.
2. What is equilibrium bond distance?
3. Name the two interatomic forces.
4. Define bond length.
5. State one effect of strong bonding on material properties.

##### **Long Questions (10 Marks)**

1. Explain the attractive and repulsive interatomic forces with a neat potential energy curve.
2. Describe bond energy, bond length, and equilibrium bond distance. Discuss their influence on engineering material properties.
3. Explain how bonding affects the mechanical, thermal, electrical, and chemical behaviour of engineering materials

### **Lecture-7**

#### **UNIT-1: INTRODUCTION TO MATERIALS ENGINEERING**

##### **Chapter-4: Interatomic Bonds**

**Course:** MTPC201 – Introduction to Materials Engineering

**Semester:** 3rd Semester Diploma in Metallurgical Engineering

**Syllabus Covered:** Interatomic Bonds – Covalent Bond, Metallic Bond, Ionic Bond, Hydrogen Bond and Van der Waals Bond. The content below expands these syllabus topics using standard references such as Callister, V. Raghavan, Van Vlack, W.F. Smith, Avner, and Rollason.

##### **Chapter Learning Outcomes**

After studying this chapter, students will be able to:

- Define interatomic bonding.
- Explain why atoms form different types of bonds.
- Describe ionic, covalent, metallic, hydrogen, and van der Waals bonds.
- Compare different types of bonds.

- Relate bond type to engineering properties and applications.

#### 4.1 Introduction to Interatomic Bonds

Atoms rarely exist independently. To attain a **stable, low-energy electronic configuration**, they combine with other atoms. The attractive force that holds atoms together is called an **interatomic bond**.

The type of bond determines many engineering properties such as:

- Strength
- Hardness
- Ductility
- Melting point
- Electrical conductivity
- Thermal conductivity
- Corrosion resistance

Hence, understanding bonding is essential for selecting engineering materials.

#### 4.2 Classification of Interatomic Bonds

Interatomic bonds are broadly classified into:

##### Primary (Strong) Bonds

1. Ionic Bond
2. Covalent Bond
3. Metallic Bond

##### Secondary (Weak) Bonds

4. Hydrogen Bond
5. Van der Waals Bond

#### 4.3 Ionic Bond

##### Definition

An **ionic bond** is formed by the complete transfer of one or more valence electrons from one atom to another, resulting in oppositely charged ions that attract each other through electrostatic forces.

It usually forms between a **metal** and a **non-metal**.

##### Formation of Sodium Chloride (NaCl)

Sodium (Na) has one valence electron.

Electronic configuration:

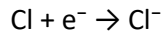
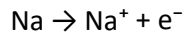
- Na = 2, 8, 1

Chlorine (Cl) has seven valence electrons.

Electronic configuration:

- Cl = 2, 8, 7

Sodium transfers one electron to chlorine:



The electrostatic attraction between  $\text{Na}^+$  and  $\text{Cl}^-$  forms an ionic bond.

### **Characteristics of Ionic Bond**

- Strong bond
- Non-directional
- High melting point
- High boiling point
- Hard
- Brittle
- Poor conductor in solid state
- Good conductor in molten or aqueous state

### **Examples**

- Sodium chloride (NaCl)
- Magnesium oxide (MgO)
- Calcium fluoride ( $\text{CaF}_2$ )

### **Engineering Applications**

- Refractory materials
- Electrical insulators
- Ceramic products
- Furnace linings

## **4.4 Covalent Bond**

### **Definition**

A **covalent bond** is formed when two atoms share one or more pairs of valence electrons.

It generally occurs between **non-metal atoms**.

### **Formation of Hydrogen Molecule**

Each hydrogen atom has one electron.

Two hydrogen atoms share their electrons:



Each atom achieves a stable electron configuration.

### **Characteristics**

- Very strong bond
- Directional bond
- High hardness
- High melting point
- Poor electrical conductivity (except graphite)
- Excellent chemical stability

### **Examples**

- Diamond (Carbon)
- Silicon
- Germanium
- Hydrogen molecule
- Oxygen molecule

### **Engineering Applications**

- Cutting tools (Diamond)
- Semiconductor devices (Silicon)
- Solar cells
- Electronic chips

## **4.5 Metallic Bond**

### **Definition**

A **metallic bond** is formed when positively charged metal ions are held together by a "sea" of freely moving (delocalized) electrons.



## **Electron Sea Model**

Metal atoms release their outermost electrons.

These electrons move freely throughout the metal crystal.

The attraction between positive metal ions and free electrons creates the metallic bond.

## **Characteristics**

- Excellent electrical conductivity
- High thermal conductivity
- Ductile
- Malleable
- Lustrous
- Moderate to high strength
- Non-directional bond

## **Examples**

- Iron
- Copper
- Aluminium
- Nickel
- Gold
- Silver

## **Engineering Applications**

- Electrical wires
- Structural components
- Heat exchangers
- Machine parts
- Railway tracks

### 4.6 Hydrogen Bond

#### Definition

A **hydrogen bond** is a weak secondary bond formed between a hydrogen atom already covalently bonded to a highly electronegative atom (such as oxygen, nitrogen, or fluorine) and another electronegative atom.

#### Characteristics

- Stronger than van der Waals forces
- Weaker than primary bonds
- Directional
- Increases boiling point
- Improves molecular stability

#### Examples

- Water ( $\text{H}_2\text{O}$ )
- Ice
- DNA
- Proteins

#### Importance

Hydrogen bonding is responsible for:

- High boiling point of water
- Strength of biological molecules
- Stability of polymers such as nylon

### 4.7 Van der Waals Bond

#### Definition

Van der Waals bonds are weak attractive forces between neutral atoms or molecules caused by temporary or induced dipoles.

#### Characteristics

- Weakest type of interatomic bond
- Acts over short distances
- Easily broken

- Responsible for intermolecular attraction

### Examples

- Solid argon
- Solid nitrogen
- Paraffin wax
- Polymer chains

### Importance

Van der Waals forces influence:

- Polymer flexibility
- Adhesion
- Surface interactions
- Molecular packing

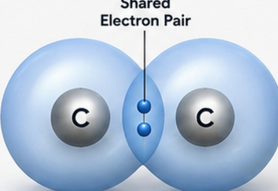
## 4.8 Comparison of Different Bonds

| Property                | Ionic           | Covalent    | Metallic         | Hydrogen           | Van der Waals     |
|-------------------------|-----------------|-------------|------------------|--------------------|-------------------|
| Bond strength           | High            | Very High   | Moderate to High | Moderate           | Very Low          |
| Electron behavior       | Transfer        | Sharing     | Delocalized      | Partial attraction | Temporary dipoles |
| Directionality          | Non-directional | Directional | Non-directional  | Directional        | Non-directional   |
| Electrical conductivity | Poor (solid)    | Poor        | Excellent        | Poor               | Poor              |
| Ductility               | Poor            | Poor        | Excellent        | Poor               | Poor              |

| Property      | Ionic | Covalent  | Metallic         | Hydrogen | Van der Waals |
|---------------|-------|-----------|------------------|----------|---------------|
| Melting point | High  | Very High | Moderate to High | Moderate | Low           |
| Examples      | NaCl  | Diamond   | Copper           | Water    | Paraffin      |

### Types of Interatomic Bonds (3D Illustrations)

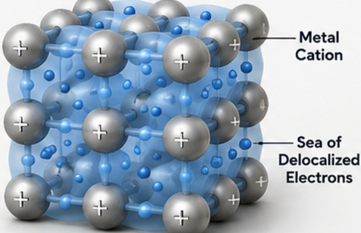
#### 1. COVALENT BOND



Example:  $\text{H}_2$  Molecule  
 $\text{H} - \text{H}$

- Atoms share one or more pairs of electrons.
- Strong and directional bond.
- Usually between non-metal atoms.
- Example: Diamond (C), SiC, Si, Ge.

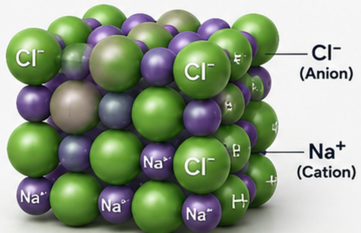
#### 2. METALLIC BOND



Example: Copper (Cu)

- Metal cations held together by delocalized electrons.
- Non-directional bond.
- Good electrical and thermal conductivity.
- Examples: Cu, Al, Fe, Ni, Ag.

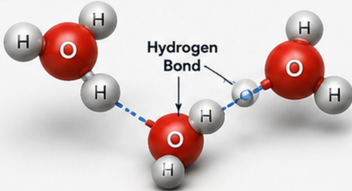
#### 3. IONIC BOND



Example: Sodium Chloride (NaCl)

- Complete transfer of electrons from one atom to another.
- Electrostatic attraction holds ions together.
- High melting point, brittle.
- Examples: NaCl, MgO,  $\text{CaF}_2$ .

#### 4. HYDROGEN BOND



Example: Between Water Molecules ( $\text{H}_2\text{O}$ )

- Attraction between H (covalently bonded to N, O, or F) and a lone pair of another N, O, or F atom.
- Stronger than van der Waals forces but weaker than covalent bonds.
- Responsible for high boiling point of water, DNA structure, protein stability.

#### 5. VAN DER WAALS BOND



Example: Between Two Non-polar Molecules

- Weakest type of bonding.
- Caused by temporary dipoles induced in atoms or molecules.
- Present in non-polar molecules.
- Examples: Noble gases (Ar, Ne), Paraffin wax, Polymers.

## 4.9 Bonding and Material Properties

The type of bonding controls many engineering properties.

| Bond Type | Typical Properties                            |
|-----------|-----------------------------------------------|
| Ionic     | Hard, brittle, high melting point             |
| Covalent  | Very hard, chemically stable                  |
| Metallic  | Ductile, conductive, malleable                |
| Hydrogen  | Influences boiling point and polymer strength |

| <b>Bond Type</b> | <b>Typical Properties</b>         |
|------------------|-----------------------------------|
| Van der Waals    | Soft, flexible, low melting point |

#### **4.10 Engineering Examples**

##### **Diamond**

- Bond: Covalent
- Property: Extremely hard
- Use: Cutting tools

##### **Copper**

- Bond: Metallic
- Property: Excellent electrical conductivity
- Use: Electrical cables

##### **Sodium Chloride**

- Bond: Ionic
- Property: Hard and brittle
- Use: Ceramic and chemical industries

##### **Nylon**

- Bond: Hydrogen bonding between polymer chains
- Property: Good strength
- Use: Textile fibres and gears

##### **Polyethylene**

- Bond: Van der Waals forces between chains
- Property: Flexible and lightweight
- Use: Packaging materials

#### **Key Points to Remember**

- Atoms bond to achieve a stable electronic configuration.
- Primary bonds (ionic, covalent, metallic) are strong and determine the basic structure of materials.
- Secondary bonds (hydrogen and van der Waals) are weaker but significantly affect the behaviour of polymers, liquids, and biological materials.
- Metallic bonding explains why metals are good conductors and can be shaped easily.

- Covalent bonding gives materials high hardness and chemical stability.
- Ionic bonding results in hard but brittle materials with high melting points.

### **Viva Questions**

1. Define an interatomic bond.
2. Differentiate between primary and secondary bonds.
3. Explain the formation of an ionic bond with an example.
4. Why are metals good conductors of electricity?
5. What is a covalent bond? Give two examples.
6. What is a hydrogen bond?
7. Define van der Waals forces.
8. Why is diamond harder than graphite?
9. Why are ionic solids brittle?
10. Which type of bond is present in copper and why does it make copper ductile?

### **Examination Questions**

#### **Short Questions (2 Marks)**

1. Define an ionic bond.
2. Define a covalent bond.
3. What is a metallic bond?
4. Define a hydrogen bond.
5. State two characteristics of van der Waals forces.

#### **Long Questions (10 Marks)**

1. Explain the formation, characteristics, and applications of ionic, covalent, and metallic bonds with suitable examples.
2. Compare primary and secondary bonds. Discuss how different bond types influence the properties of engineering materials.
3. Explain hydrogen bonding and van der Waals bonding. Discuss their importance in polymers and biological materials.

### **Unit–1 Summary**

After completing Unit 1, students should understand:

- The evolution and scope of Materials Engineering.

- The relationship between **Processing–Structure–Properties–Performance (PSPP)**.
- The basic structure of atoms and the role of valence electrons.
- Bonding forces, bond energy, and equilibrium bond distance.
- The five major interatomic bonds and how they govern the properties and applications of engineering materials.

## **Lecture-9**

### **UNIT–1: INTRODUCTION TO MATERIALS ENGINEERING**

#### **Chapter–2: Fundamental Concepts on Atoms, Bonding Forces and Energies**

**Course:** MTPC201 – Introduction to Materials Engineering

**Semester:** 3rd Semester Diploma in Metallurgical Engineering

**Syllabus Covered:** Fundamental Concepts on Atoms; Bonding Forces and Energies. This note is aligned with your uploaded syllabus and expanded using standard references such as William D. Callister, V. Raghavan, Van Vlack, W.F. Smith, Sidney H. Avner, and E.C. Rollason.

#### **Learning Outcomes**

After studying this chapter, students will be able to:

- Explain the basic structure of an atom.
- Describe protons, neutrons, and electrons.
- Understand atomic number, mass number, and electronic configuration.
- Explain valence electrons and their importance.
- Describe attractive and repulsive bonding forces.
- Explain bond energy and equilibrium bond distance.
- Relate bonding forces to the engineering properties of materials.

#### **1. Introduction**

All engineering materials are made up of tiny particles called **atoms**. The arrangement of atoms and the forces acting between them determine the properties of materials such as strength, hardness, electrical conductivity, corrosion resistance, and melting point.

For example:

- Diamond is extremely hard because of strong atomic bonding.
- Copper conducts electricity because of metallic bonding.
- Glass is brittle because of its atomic arrangement.

Thus, understanding atoms and bonding is the first step in learning Materials Engineering.

## 2. What is an Atom?

### Definition

An **atom** is the smallest particle of an element that retains the chemical properties of that element.

Every material consists of millions of atoms arranged in a definite manner.

Examples:

- Iron consists of iron atoms.
- Copper consists of copper atoms.
- Aluminium consists of aluminium atoms.

## 3. Structure of an Atom

An atom has two main parts:

### (A) Nucleus

The nucleus is the central part of an atom.

It contains:

- Protons
- Neutrons

The nucleus contains almost all the mass of the atom.

### (B) Extra-Nuclear Region

Electrons revolve around the nucleus in fixed energy levels (shells).

Electrons are responsible for:

- Chemical bonding
- Electrical conductivity
- Thermal conductivity

### Subatomic Particles

| Particle | Symbol         | Charge | Relative Mass | Location           |
|----------|----------------|--------|---------------|--------------------|
| Proton   | p <sup>+</sup> | +1     | 1 amu         | Nucleus            |
| Neutron  | n <sup>0</sup> | 0      | 1 amu         | Nucleus            |
| Electron | e <sup>-</sup> | -1     | 1/1836 amu    | Around the nucleus |

## 4. Atomic Number (Z)



The **atomic number** is the number of protons present in the nucleus.

Atomic Number (Z) = Number of Protons

Example:

Iron

Atomic number = **26**

Therefore,

- Protons = 26
- Electrons = 26 (neutral atom)

### 5. Mass Number (A)

The **mass number** is the total number of protons and neutrons.

Mass Number (A) = Protons + Neutrons

Example:

Carbon

Protons = 6

Neutrons = 6

Mass Number

= 6 + 6

= **12**

### 6. Electronic Configuration

Electrons are arranged in different energy shells around the nucleus.

Maximum number of electrons:

| Shell  | Symbol | Maximum Electrons |
|--------|--------|-------------------|
| First  | K      | 2                 |
| Second | L      | 8                 |
| Third  | M      | 18                |
| Fourth | N      | 32                |

#### Example

Sodium (Atomic Number = 11)

Electronic configuration:

**2, 8, 1**

## **7. Valence Electrons**

The electrons present in the outermost shell are called **valence electrons**.

These electrons determine:

- Chemical bonding
- Reactivity
- Electrical properties
- Mechanical behaviour

### **Examples**

| <b>Element</b> | <b>Valence Electrons</b> |
|----------------|--------------------------|
| Sodium         | 1                        |
| Magnesium      | 2                        |
| Aluminium      | 3                        |
| Carbon         | 4                        |
| Oxygen         | 6                        |

## **8. Why Do Atoms Form Bonds?**

Atoms combine with each other to achieve a **stable electronic configuration**.

According to the **Octet Rule**, atoms tend to attain **eight electrons in their outermost shell** (except hydrogen and helium, which follow the duplet rule).

When atoms bond:

- Their energy decreases.
- Their stability increases.

### **Remember:**

Nature always favors the **lowest energy state**.

## **9. Interatomic Forces**

Atoms attract and repel each other due to electrostatic interactions.

Two forces act simultaneously between atoms.

### **(A) Attractive Force**

The attractive force is caused by the attraction between:

- Positive nucleus of one atom
- Negative electrons of another atom

This force pulls atoms together.

### **(B) Repulsive Force**

The repulsive force arises due to:

- Electron–electron repulsion
- Nucleus–nucleus repulsion

This force pushes atoms apart when they come very close.

## **10. Equilibrium Bond Distance**

When atoms approach each other:

- Attractive forces increase.
- Repulsive forces also increase.

At one particular distance:

- Attractive force = Repulsive force
- Net force = Zero

This distance is called the **equilibrium bond distance** ( $(r_0)$ ).

At this point:

- The bond is most stable.
- Potential energy is minimum.

## **11. Potential Energy Curve**

The relationship between potential energy and interatomic distance is shown by the **potential energy curve**.

**Interpretation:**

- Left of  $(r_0)$ : Repulsive forces dominate.
- Right of  $(r_0)$ : Attractive forces dominate.
- At  $(r_0)$ : Stable equilibrium and minimum potential energy.

## **12. Bond Energy**

**Definition**

**Bond energy** is the amount of energy required to separate two bonded atoms completely.

It is also equal to the energy released when the bond is formed.

#### **Units**

- kJ/mol
- eV/atom

### **13. Significance of Bond Energy**

#### **High Bond Energy**

Results in:

- High melting point
- High hardness
- High elastic modulus
- Better thermal stability

#### **Low Bond Energy**

Results in:

- Soft materials
- Lower melting point
- Lower stiffness
- Easier deformation

### **14. Relationship Between Bonding and Material Properties**

| <b>Bond Characteristic</b> | <b>Effect on Material</b>    |
|----------------------------|------------------------------|
| Strong bond                | High strength                |
| Strong bond                | High hardness                |
| Strong bond                | High melting point           |
| Weak bond                  | Softness                     |
| Weak bond                  | Low melting point            |
| Strong metallic bond       | High electrical conductivity |

### **15. Engineering Examples**

#### **Diamond**

- Strong covalent bonding
- Very high bond energy
- Extremely hard
- Used in cutting tools

### **Copper**

- Metallic bonding
- Free electrons
- Excellent electrical conductivity
- Used in electrical wiring

### **Sodium Chloride**

- Ionic bonding
- Hard but brittle
- Used in chemical and ceramic industries

### **Polyethylene**

- Weak van der Waals forces between polymer chains
- Flexible
- Lightweight
- Used in packaging

## **16. Importance of Atomic Structure and Bonding in Materials Engineering**

Understanding atomic structure and bonding enables engineers to:

- Select suitable engineering materials.
- Predict mechanical and electrical properties.
- Design new alloys and composites.
- Explain heat treatment behaviour.
- Understand crystal structures and defects.
- Develop advanced materials for aerospace, biomedical, and electronic applications.

### **Key Points to Remember**

- The atom is the basic unit of matter.
- Protons and neutrons are located in the nucleus; electrons occupy shells around it.

- Valence electrons control chemical bonding.
- Atoms form bonds to attain a stable, low-energy state.
- Attractive and repulsive forces determine the equilibrium bond distance.
- Bond energy influences strength, hardness, melting point, and stiffness.
- The nature of bonding determines the engineering properties of materials.

### **Viva Questions**

1. Define an atom.
2. Name the three subatomic particles.
3. What is the atomic number?
4. What is the mass number?
5. Define valence electrons.
6. Why do atoms form bonds?
7. What are attractive and repulsive forces?
8. Define equilibrium bond distance.
9. What is bond energy?
10. How does bond energy affect the properties of engineering materials?

### **Examination Questions**

#### **Short Questions (2 Marks)**

1. Define an atom.
2. What is the atomic number?
3. Define valence electrons.
4. What is bond energy?
5. State one effect of high bond energy.

#### **Long Questions (10 Marks)**

1. Explain the fundamental concepts of atoms with a neat labelled diagram.
2. Describe the structure of an atom, atomic number, mass number, and electronic configuration.
3. Explain bonding forces and bond energy with a potential energy curve. Discuss their significance in Materials Engineering.

### **Summary**

Atomic structure explains **what materials are made of**, while bonding forces explain **why atoms stay together**. The strength and type of bonding determine the crystal structure, mechanical properties, electrical conductivity, thermal stability, and overall performance of engineering materials. These concepts provide the essential foundation for studying **interatomic bonds, crystal structures, crystal defects, and engineering materials** in the subsequent chapters.

## Lecture-10

### UNIT–1: INTRODUCTION TO MATERIALS ENGINEERING

#### Chapter–4: Interatomic Bonds

#### (Covalent Bond, Metallic Bond, Ionic Bond, Hydrogen Bond and Van der Waals Bond)

**Course:** MTPC201 – Introduction to Materials Engineering

**Semester:** 3rd Semester Diploma in Metallurgical Engineering

**Syllabus Covered:** Interatomic Bonds (Covalent bond, Metallic bond, Ionic bond, Hydrogen bond and Van der Waals bond). The chapter follows your uploaded syllabus and is expanded using standard references including William D. Callister, V. Raghavan, Van Vlack, W.F. Smith, Sidney H. Avner, and E.C. Rollason.

#### Learning Outcomes

After studying this chapter, students will be able to:

- Define interatomic bonding.
- Explain why atoms form chemical bonds.
- Describe the formation of ionic, covalent, metallic, hydrogen, and van der Waals bonds.
- Compare different types of bonds.
- Relate bond type to engineering properties and applications.
- Select suitable materials based on their bonding characteristics.

#### 1. Introduction

An isolated atom is generally unstable because its outermost electron shell is incomplete. To become more stable, atoms interact with neighbouring atoms by transferring, sharing, or delocalizing electrons.

The force that holds atoms together is called an **interatomic bond**.

The type of bond present determines the material's:

- Strength
- Hardness
- Ductility
- Electrical conductivity

- Thermal conductivity
- Melting point
- Corrosion resistance

Hence, **bonding is the origin of material properties.**

## **2. What is an Interatomic Bond?**

### **Definition**

An **interatomic bond** is the attractive force that holds two or more atoms together in a solid, liquid, or molecule.

The bond is formed because the system becomes more stable by lowering its total energy.

## **3. Why Do Atoms Form Bonds?**

Atoms form bonds to:

- Achieve a stable electronic configuration.
- Complete their outermost shell (Octet Rule for most atoms).
- Reduce potential energy.
- Increase chemical stability.

Example:

- Sodium loses one electron.
- Chlorine gains one electron.
- Both become stable.

## **4. Classification of Interatomic Bonds**

Interatomic bonds are divided into two groups.

### **Primary Bonds (Strong Bonds)**

- Ionic Bond
- Covalent Bond
- Metallic Bond

These determine the basic structure and properties of engineering materials.

### **Secondary Bonds (Weak Bonds)**

- Hydrogen Bond
- Van der Waals Bond



These influence polymers, biological materials, molecular solids, and surface interactions.

## 5. Ionic Bond

### Definition

An **ionic bond** is formed by the complete transfer of one or more electrons from one atom to another. The resulting positively and negatively charged ions are held together by electrostatic attraction.

It usually forms between a **metal** and a **non-metal**.

### Formation of Sodium Chloride (NaCl)

#### Sodium

Electronic configuration:

2,8,1

Loses one electron

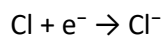


#### Chlorine

Electronic configuration:

2,8,7

Gains one electron



$\text{Na}^+$  and  $\text{Cl}^-$  attract each other to form NaCl.

### Characteristics of Ionic Bond

- Strong electrostatic attraction
- Non-directional
- High melting point
- High boiling point
- Hard
- Brittle
- Poor electrical conductor in solid state
- Good conductor when molten or dissolved in water

### Engineering Examples

- Sodium chloride (NaCl)
- Magnesium oxide (MgO)
- Calcium fluoride (CaF<sub>2</sub>)
- Aluminium oxide (Al<sub>2</sub>O<sub>3</sub>)

### **Applications**

- Ceramic insulators
- Refractory bricks
- Furnace linings
- Electrical insulation

## **6. Covalent Bond**

### **Definition**

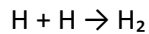
A **covalent bond** is formed when two atoms share one or more pairs of valence electrons.

It generally occurs between **non-metal atoms**.

### **Formation of Hydrogen Molecule**

Each hydrogen atom has one electron.

By sharing electrons:



Both atoms attain a stable configuration.

### **Characteristics**

- Very strong
- Directional
- High melting point
- High hardness
- Excellent chemical stability
- Poor electrical conductivity (except graphite)

### **Engineering Examples**

- Diamond
- Silicon
- Germanium

- Silicon carbide (SiC)

### **Applications**

- Cutting tools
- Semiconductor devices
- Solar cells
- Integrated circuits
- Abrasives

## **7. Metallic Bond**

### **Definition**

A **metallic bond** is formed when positively charged metal ions are surrounded by a "sea" of freely moving (delocalized) electrons.

These free electrons hold the metal ions together.

### **Electron Sea Model**

Metal atoms lose their valence electrons.

The released electrons move freely throughout the crystal.

This "electron sea" binds all metal ions together.

### **Characteristics**

- Excellent electrical conductivity
- Excellent thermal conductivity
- High ductility
- High malleability
- Metallic lustre
- Moderate to high melting point
- Non-directional bond

### **Engineering Examples**

- Iron
- Copper
- Aluminium
- Silver

- Gold
- Nickel

### **Applications**

- Electrical wires
- Heat exchangers
- Structural steel
- Automobile parts
- Aircraft components

## **8. Hydrogen Bond**

### **Definition**

A **hydrogen bond** is a weak secondary bond formed between a hydrogen atom already covalently bonded to a highly electronegative atom (such as oxygen, nitrogen, or fluorine) and another electronegative atom.

### **Formation**

Example:

Water ( $\text{H}_2\text{O}$ )

The hydrogen atom of one water molecule is attracted to the oxygen atom of another water molecule.

### **Characteristics**

- Stronger than van der Waals forces
- Weaker than primary bonds
- Directional
- Increases boiling point
- Improves molecular stability

### **Examples**

- Water
- Ice
- DNA
- Proteins
- Nylon

### **Applications**

- Polymer fibres
- Biomaterials
- Pharmaceuticals
- Biological systems

## **9. Van der Waals Bond**

### **Definition**

Van der Waals bonds are weak attractive forces between neutral atoms or molecules due to temporary or induced dipoles.

### **Characteristics**

- Weakest interatomic bond
- Acts over short distances
- Easily broken
- Responsible for intermolecular attraction

### **Examples**

- Paraffin wax
- Polyethylene
- Solid argon
- Solid nitrogen

### **Applications**

- Polymer flexibility
- Adhesives
- Molecular crystals
- Surface coatings

## **10. Comparison of Interatomic Bonds**

| <b>Property</b> | <b>Ionic</b>      | <b>Covalent</b>  | <b>Metallic</b> | <b>Hydrogen</b>     | <b>Van der Waals</b> |
|-----------------|-------------------|------------------|-----------------|---------------------|----------------------|
| Bond formation  | Electron transfer | Electron sharing | Delocalized     | Hydrogen attraction | Temporary            |

| Property                | Ionic           | Covalent    | Metallic        | Hydrogen    | Van der Waals   |
|-------------------------|-----------------|-------------|-----------------|-------------|-----------------|
|                         |                 |             | electrons       |             | dipoles         |
| Bond strength           | High            | Very High   | Moderate –High  | Moderate    | Low             |
| Directionality          | Non-directional | Directional | Non-directional | Directional | Non-directional |
| Electrical conductivity | Poor (solid)    | Poor        | Excellent       | Poor        | Poor            |
| Hardness                | High            | Very High   | Moderate        | Low         | Very Low        |
| Melting point           | High            | Very High   | Moderate –High  | Moderate    | Low             |
| Typical examples        | NaCl            | Diamond     | Copper          | Water       | Paraffin        |

## Types of Interatomic Bonds (3D Illustrations)

### 1. COVALENT BOND

Shared Electron Pair

Example:  $H_2$  Molecule

$H - H$

- Atoms share one or more pairs of electrons.
- Strong and directional bond.
- Usually between non-metal atoms.
- Example: Diamond (C), SiC, Si, Ge.

### 2. METALLIC BOND

Metal Cation

Sea of Delocalized Electrons

Example: Copper (Cu)

- Metal cations held together by delocalized electrons.
- Non-directional bond.
- Good electrical and thermal conductivity.
- Examples: Cu, Al, Fe, Ni, Ag.

### 3. IONIC BOND

$Cl^-$  (Anion)

$Na^+$  (Cation)

Example: Sodium Chloride (NaCl)

- Complete transfer of electrons from one atom to another.
- Electrostatic attraction holds ions together.
- High melting point, brittle.
- Examples: NaCl, MgO,  $CaF_2$ .

### 4. HYDROGEN BOND

Hydrogen Bond

Example: Between Water Molecules ( $H_2O$ )

- Attraction between H (covalently bonded to N, O, or F) and a lone pair of another N, O, or F atom.
- Stronger than van der Waals forces but weaker than covalent bonds.
- Responsible for high boiling point of water, DNA structure, protein stability.

### 5. VAN DER WAALS BOND

Instantaneous Dipole

Induced Dipole

Weak Attraction

Example: Between Two Non-polar Molecules

- Weakest type of bonding.
- Caused by temporary dipoles induced in atoms or molecules.
- Present in non-polar molecules.
- Examples: Noble gases (Ar, Ne), Paraffin wax, Polymers.

## 11. Effect of Bonding on Engineering Properties

| Bond Type     | Material Behaviour                                     |
|---------------|--------------------------------------------------------|
| Ionic         | Hard, brittle, high melting point                      |
| Covalent      | Extremely hard, chemically stable                      |
| Metallic      | Ductile, malleable, electrically conductive            |
| Hydrogen      | Improves strength of polymers and biological molecules |
| Van der Waals | Soft, flexible, low melting point                      |

## 12. Engineering Case Studies

### Diamond

- Bond: Covalent
- Property: Extremely hard
- Application: Cutting and grinding tools

### Copper

- Bond: Metallic
- Property: Excellent electrical conductivity
- Application: Electrical transmission cables

#### **Sodium Chloride**

- Bond: Ionic
- Property: Hard and brittle
- Application: Chemical and ceramic industries

#### **Nylon**

- Bond: Hydrogen bonding between polymer chains
- Property: High tensile strength
- Application: Textile fibres and machine components

#### **Polyethylene**

- Bond: Van der Waals forces between polymer chains
- Property: Flexible and lightweight
- Application: Packaging materials

### **13. Importance of Interatomic Bonds in Metallurgical Engineering**

Knowledge of interatomic bonding helps engineers to:

- Select suitable engineering materials.
- Predict mechanical and electrical properties.
- Understand heat treatment and phase transformations.
- Explain corrosion behaviour.
- Develop advanced alloys and composites.
- Design materials for aerospace, biomedical, and electronic applications.

#### **Key Points to Remember**

- Atoms form bonds to attain a stable, low-energy electronic configuration.
- Primary bonds (ionic, covalent, metallic) are much stronger than secondary bonds.
- Metallic bonding is responsible for the excellent electrical conductivity and ductility of metals.
- Covalent bonding provides very high hardness and chemical stability.
- Ionic bonding produces hard but brittle materials with high melting points.



- Hydrogen and van der Waals bonds, although weaker, significantly influence polymers, biological materials, and molecular solids.

### **Viva Questions**

1. Define an interatomic bond.
2. Why do atoms form bonds?
3. Explain the formation of an ionic bond with an example.
4. What is a covalent bond?
5. Describe the electron sea model of metallic bonding.
6. What is a hydrogen bond?
7. Define van der Waals forces.
8. Why are metals good electrical conductors?
9. Why are ionic solids brittle?
10. Compare primary and secondary bonds.

### **Examination Questions**

#### **Short Questions (2 Marks)**

1. Define an ionic bond.
2. Define a covalent bond.
3. What is metallic bonding?
4. What is a hydrogen bond?
5. State two characteristics of van der Waals forces.

#### **Long Questions (10 Marks)**

1. Explain the formation, characteristics, properties, and engineering applications of ionic, covalent, and metallic bonds.
2. Compare ionic, covalent, metallic, hydrogen, and van der Waals bonds using suitable examples and diagrams.
3. Discuss how different types of interatomic bonds influence the mechanical, electrical, thermal, and chemical properties of engineering materials.

### **Chapter Summary**

Interatomic bonding is the **fundamental reason why engineering materials exist and perform differently**. The way atoms transfer, share, or delocalize electrons determines whether a material behaves as a metal, ceramic, polymer, or semiconductor. Understanding these bonding

mechanisms enables engineers to predict material properties, select appropriate materials, and design new materials for advanced engineering applications.

## **Lecture-11**

### **UNIT-2: THE STRUCTURE OF CRYSTALLINE SOLIDS**

**Course:** MTPC201 (Th-1) – Introduction to Materials Engineering

**Semester:** 3rd Semester Diploma in Metallurgical Engineering

#### **Reference Books**

1. William D. Callister Jr. & David G. Rethwisch – *Materials Science and Engineering: An Introduction* (10th Edition)
2. V. Raghavan – *Materials Science and Engineering*
3. Donald R. Askeland – *The Science and Engineering of Materials*
4. Van Vlack – *Elements of Materials Science and Engineering*
5. W.F. Smith – *Foundations of Materials Science and Engineering*
6. E.C. Rollason – *Metallurgy for Engineers*

### **UNIT-2: THE STRUCTURE OF CRYSTALLINE SOLIDS**

#### **Introduction**

The performance of every engineering material depends not only on its chemical composition but also on the **arrangement of atoms** inside the material.

Two materials having identical chemical composition can exhibit completely different properties if their atoms are arranged differently.

#### **Example**

Diamond and Graphite

Both consist entirely of carbon atoms.

Yet,

- Diamond is one of the hardest known materials.
- Graphite is soft and slippery.

This difference arises because the arrangement of carbon atoms is different.

Hence,

**The structure of crystalline solids is one of the most fundamental topics in Materials Engineering.**

Understanding crystal structures enables engineers to explain:

- Strength
- Hardness
- Ductility
- Conductivity
- Density
- Corrosion resistance
- Heat treatment
- Phase transformation
- Material failure

### **Importance of Studying Crystal Structure**

Crystal structure helps engineers to

- ✓ Select suitable engineering materials
- ✓ Design stronger alloys
- ✓ Understand heat treatment
- ✓ Predict mechanical properties
- ✓ Explain deformation
- ✓ Develop advanced materials
- ✓ Design aerospace materials
- ✓ Develop biomedical implants
- ✓ Manufacture semiconductors

This unit forms the backbone of Materials Science.

### **1. Crystal and Crystallography**

- Crystal
- Crystal lattice
- Crystallography
- Crystal symmetry

### **2. Bravais Lattices**

- Seven crystal systems

- Fourteen Bravais lattices
- Primitive and centred lattices

### **3. Unit Cells**

- Building block of crystals
- Lattice parameters
- Primitive and non-primitive cells

### **4. Crystal Structures**

- Simple Cubic (SC)
- Body Centred Cubic (BCC)
- Face Centred Cubic (FCC)
- Hexagonal Close Packed (HCP)

including

- Number of atoms
- Atomic packing
- Coordination number
- Applications

### **5. Point Coordinates**

Location of atoms inside unit cells.

### **6. Crystallographic Directions**

Representation of atomic directions using

- Direction indices

Applications

- Slip
- Plastic deformation

### **7. Crystallographic Planes**

Identification of crystal planes using

- Miller Indices

Applications

- XRD

- Heat treatment
- Grain orientation

### **8. Linear Density**

Number of atoms along a crystallographic direction.

### **9. Planar Density**

Number of atoms present on a crystallographic plane.

### **10. Close Packed Structures**

Students will understand

- Atomic packing
- Packing efficiency

Comparison between

- FCC
- HCP

### **11. Coordination Number**

Number of nearest neighbouring atoms.

### **12. Atomic Packing Factor (APF)**

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

### **13. Density of Crystal**

calculate theoretical density using

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

where

$\rho$  = Density

$n$  = Number of atoms

$A$  = Atomic weight

$N_A$  = Avogadro number

$V_c$  = Unit cell volume

## 14. Crystal Defects

Real engineering materials are never perfect.

### Point Defects

- Vacancy
- Self-interstitial

### Line Defects

- Edge dislocation
- Screw dislocation

### Surface Defects

- Grain boundary
- Twin boundary

### Volume Defects

- Pores
- Cracks
- Inclusions

## Flow Chart of Unit–2

Atoms



Interatomic Bonding



Crystal



Crystal Lattice



Unit Cell



Crystal Structures

(SC, BCC, FCC, HCP)



Crystal Planes & Directions



Atomic Packing



Density & APF



Crystal Defects



Engineering Properties

**Engineering Field**

**Application**

Metallurgy

Steel design and heat treatment

Mechanical Engineering

Machine components

Aerospace

Titanium and nickel superalloys

Civil Engineering

Structural steel

Electronics

Silicon crystals

Biomedical

Titanium implants

| Engineering Field           | Application                    |
|-----------------------------|--------------------------------|
| Nanotechnology              | Carbon nanotubes and graphene  |
| Mining & Mineral Processing | Crystal identification of ores |

### Learning Outcomes

After completing Unit–2, students will be able to

- Explain crystal structures.
- Identify unit cells.
- Distinguish SC, BCC, FCC and HCP.
- Calculate APF.
- Calculate crystal density.
- Identify crystallographic planes and directions.
- Explain crystal defects.
- Relate crystal structure to engineering properties.

### Key Points to Remember

- All engineering materials are composed of atoms arranged in a definite pattern.
- Crystal structure determines the physical and mechanical properties of materials.
- SC, BCC, FCC, and HCP are the most important crystal structures.
- FCC and HCP have the highest packing efficiency (74%).
- Crystal defects significantly influence strength, ductility, and conductivity.
- Knowledge of crystal structures is essential for metallurgy, mechanical engineering, aerospace, electronics, and biomedical engineering.

## Chapter–1: Crystal and Crystallography

### Introduction

Every engineering material, such as steel, aluminium, copper, ceramics, and semiconductors, is composed of atoms arranged in a specific manner. The study of these arrangements is known as **crystallography**.

Crystallography is one of the most important branches of Materials Science because it explains why materials exhibit different mechanical, electrical, thermal, and optical properties.

For example:

- Copper is highly ductile because it has an **FCC** crystal structure.



- Ferrite ( $\alpha$ -iron) is stronger because it has a **BCC** structure.
- Diamond is extremely hard due to its covalent crystal network.

Thus, the arrangement of atoms directly determines material behavior.

### **What is a Crystal?**

#### **Definition**

A **crystal** is a solid in which atoms, ions, or molecules are arranged in a **regular, repeating three-dimensional pattern** extending throughout the material.

#### **Simple Definition (Exam)**

A crystal is a solid having a regular and periodic arrangement of atoms in three dimensions.

#### **Characteristics of a Crystal**

- Regular atomic arrangement.
- Long-range order.
- Definite geometric shape.
- Sharp melting point.
- Anisotropic properties (in single crystals).
- High structural stability.

#### **Examples**

- Iron (Fe)
- Copper (Cu)
- Aluminium (Al)
- Diamond
- Silicon
- Sodium chloride (NaCl)

### **What is Crystallography?**

#### **Definition**

**Crystallography** is the branch of science that studies:

- Crystal structures
- Atomic arrangements
- Crystal symmetry

- Crystal systems
- Crystal planes
- Crystal directions

### **Importance**

Crystallography enables engineers to understand:

- Why materials are strong or weak.
- Why some metals are ductile while others are brittle.
- How crystal orientation affects deformation.
- How X-ray diffraction identifies crystal structures.

### **Crystal Lattice**

A **crystal lattice** is an imaginary three-dimensional array of lattice points representing the periodic positions of atoms.

### **Important Relation**

Crystal Structure=Lattice+Basis

where:

- **Lattice** = Geometrical arrangement of points.
- **Basis** = Atom or group of atoms attached to each lattice point.

### **Types of Solids**

#### **Crystalline Solids**

- Regular arrangement of atoms.
- Long-range order.
- Sharp melting point.

Examples:

- Iron
- Copper
- Aluminium

#### **Amorphous Solids**

- Random arrangement of atoms.
- Only short-range order.

- No definite melting point.

Examples:

- Glass
- Rubber
- Plastics

**Comparison**

| Property           | Crystalline  | Amorphous         |
|--------------------|--------------|-------------------|
| Atomic arrangement | Regular      | Random            |
| Long-range order   | Present      | Absent            |
| Melting point      | Sharp        | Gradual softening |
| Examples           | Iron, Copper | Glass, Rubber     |

**Importance of Crystallography**

Crystallography helps engineers to:

- Determine crystal structures.
- Predict material properties.
- Design high-strength alloys.
- Analyze crystal defects.
- Interpret X-ray diffraction (XRD) patterns.
- Improve manufacturing processes.

**Real-Life Examples**

| Material             | Crystal Structure | Engineering Application      |
|----------------------|-------------------|------------------------------|
| Iron ( $\alpha$ -Fe) | BCC               | Structural steel             |
| Copper               | FCC               | Electrical wiring            |
| Aluminium            | FCC               | Aircraft structures          |
| Magnesium            | HCP               | Lightweight automotive parts |
| Silicon              | Diamond cubic     | Microchips and solar cells   |

# CRYSTAL AND CRYSTALLOGRAPHY

## 1. CRYSTAL

A crystal is a solid in which the atoms, ions or molecules are arranged in a regular, repeating three-dimensional pattern.

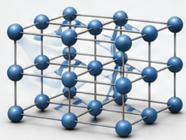


### Characteristics

- Definite geometric shape
- Flat faces and sharp edges
- Anisotropic properties
- Definite melting point
- Orderly internal arrangement

## 2. CRYSTAL vs AMORPHOUS

### Crystalline



- Long range order
- Regular arrangement
- Definite shape
- Sharp melting point
- Example: Salt, Quartz, Metal

### Amorphous

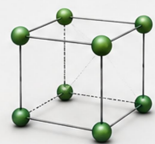


- Short range order only
- Irregular arrangement
- No definite shape
- No sharp melting point
- Example: Glass, Plastic, Rubber

## 3. BASIC CRYSTALLOGRAPHIC CONCEPTS

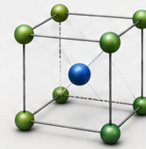
### 3.1 LATTICE

An array of points in space that show the periodicity of a crystal.



### 3.2 UNIT CELL

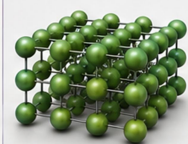
The smallest repeating unit of a crystal lattice.



Example: Simple Cubic (SC) Unit Cell

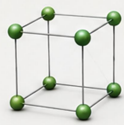
### 3.3 SPACE LATTICE

The three dimensional arrangement of lattice points in space.



## 4. COMMON CRYSTAL STRUCTURES

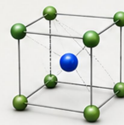
### 4.1 SIMPLE CUBIC (SC)



- Atoms at 8 corners
- Coordination No. = 6
- Atomic Packing Factor (APF) = 0.52



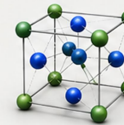
### 4.2 BODY CENTERED CUBIC (BCC)



- Atoms at 8 corners and 1 at body center
- Coordination No. = 8
- APF = 0.68



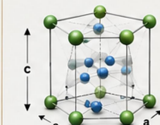
### 4.3 FACE CENTERED CUBIC (FCC)



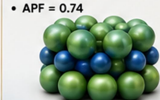
- Atoms at 8 corners and 6 at face centers
- Coordination No. = 12
- APF = 0.74



### 4.4 HEXAGONAL CLOSE PACKED (HCP)



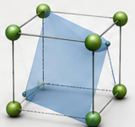
- Atoms at 12 corners, 2 at center of top & bottom faces and 3 inside
- Coordination No. = 12
- APF = 0.74



## 5. CRYSTALLOGRAPHIC ELEMENTS

### 5.1 CRYSTAL PLANES

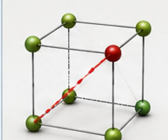
Imaginary flat surface passing through lattice points.



Example: (100) Plane (110) Plane (111) Plane

### 5.2 CRYSTAL DIRECTIONS

Straight lines along which atoms are closely packed.

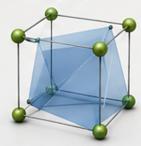


Example: [100], [110], [111]

### 5.3 MILLER INDICES

A set of three smallest integers (h k l) used to represent a plane.

- Steps:
1. Find intercepts
  2. Take reciprocals
  3. Clear fractions
  4. Write (h k l)



## 6. IMPORTANCE OF CRYSTALS & CRYSTALLOGRAPHY

- Helps in understanding the internal structure of materials.
- Basis for study of mechanical, electrical, optical properties.
- Important in metallurgy, ceramics, semiconductors and polymers.
- Essential for analysis of crystal defects and phase transformations.



## 7. APPLICATIONS



Aerospace Alloys



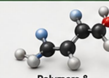
Semiconductors



Cutting Tools (Diamond)



Ceramics



Polymers & Biomaterials

## Key Points to Remember

- A crystal has a periodic arrangement of atoms.
- Crystallography is the science of crystal structures and symmetry.
- Crystal structure = Lattice + Basis.
- Crystalline materials exhibit long-range order, whereas amorphous materials do not.
- Understanding crystallography is essential for materials selection, heat treatment, alloy development, and failure analysis.

## Viva Questions

1. Define a crystal.
2. What is crystallography?
3. Differentiate between crystalline and amorphous solids.
4. What is a crystal lattice?
5. State the relation between lattice and crystal structure.
6. Why is crystallography important in metallurgy?

7. Give four examples of crystalline materials.
8. Name two amorphous materials.

### **Examination Questions**

#### **Chapter–1: Crystal and Crystallography**

##### **Part-A: Very Short Questions (2 Marks)**

1. Define a crystal.
2. What is crystallography?
3. Define a crystal lattice.
4. Define a lattice point.
5. What is meant by long-range order?
6. What is an amorphous solid?
7. State any two characteristics of crystalline solids.
8. State any two characteristics of amorphous solids.
9. Give two examples of crystalline materials.
10. Give two examples of amorphous materials.
11. Write the relation between crystal structure, lattice and basis.
12. What is the difference between crystal and crystal lattice?
13. Why is diamond harder than graphite?
14. State two engineering applications of crystallography.
15. Why is crystal structure important in materials engineering?

##### **Part-B: Short Answer Questions (5 Marks)**

###### **Question 1**

Define a crystal. Explain the characteristics of crystalline solids with suitable examples.

###### **Question 2**

Explain the difference between crystalline and amorphous solids.

###### **Question 3**

What is crystallography? Explain its importance in Materials Engineering.

###### **Question 4**

Explain the concept of crystal lattice and lattice points with neat diagrams.

**Question 5**

Differentiate between crystalline and amorphous solids.

**Question 6**

Write short notes on:

- Crystal
- Crystal lattice
- Basis
- Crystal structure

**Question 7**

Explain the significance of crystallography in metallurgy.

**Question 8**

Explain the concept of long-range order and short-range order.

**Question 9**

Discuss the engineering applications of crystal structures.

**Question 10**

Explain the relationship between crystal structure and engineering properties.

**Part-C: Long Answer Questions (10 Marks)****Question 1**

Define crystal and crystallography.

Explain:

- Crystal
- Crystal lattice
- Basis
- Crystal structure

with suitable diagrams and engineering examples.

**Question 2**

What is crystallography?

Explain its role in understanding

- crystal structures

- material properties
- heat treatment
- alloy design
- X-ray diffraction
- engineering applications

### **Question 3**

Differentiate between crystalline and amorphous solids.

Compare them with respect to:

- Atomic arrangement
- Melting point
- Mechanical properties
- Electrical properties
- Examples
- Applications

### **Question 4**

Explain the concept of crystal lattice and basis.

Derive the relationship

**Crystal Structure = Lattice + Basis**

with suitable illustrations.

### **Question 5**

Discuss the importance of crystallography in Materials Engineering.

Explain how crystal structures influence

- Strength
- Hardness
- Ductility
- Conductivity
- Density
- Corrosion resistance

### **Question 6**

Write detailed notes on:

- Crystal
- Crystallography
- Crystal lattice
- Lattice point
- Basis
- Engineering applications

**Numerical/Concept-Based Questions (5–10 Marks)**

1. Explain why diamond and graphite have different properties although both are made of carbon.
2. Why are most metals crystalline while glass is amorphous?
3. Explain why knowledge of crystallography is essential for heat treatment of steels.
4. Describe how atomic arrangement affects the engineering properties of materials.

**Viva-Voce Questions**

1. What is a crystal?
2. What is the difference between crystal and crystallography?
3. Why do metals generally have crystalline structures?
4. Why is glass considered amorphous?
5. What is meant by long-range order?
6. What is a lattice point?
7. What is basis?
8. Define crystal structure.
9. Give two examples of crystalline solids.
10. Give two examples of amorphous solids.
11. What is the importance of crystallography in metallurgy?
12. Why is diamond harder than graphite?
13. Why is copper more ductile than iron?
14. Name one application of crystallography in engineering.
15. What is the relationship between lattice and crystal structure?



## Lecture-12

### UNIT–2: THE STRUCTURE OF CRYSTALLINE SOLIDS

#### Chapter–2: Bravais Lattices

**Course:** MTPC201 – Introduction to Materials Engineering

**Semester:** 3rd Semester Diploma in Metallurgical Engineering

**Syllabus Covered:** Bravais Lattices. This note expands the syllabus using standard references such as William D. Callister, V. Raghavan, Van Vlack, W.F. Smith, Sidney H. Avner, and E.C. Rollason.

#### Learning Outcomes

After studying this chapter, students will be able to:

- Define a Bravais lattice.
- Explain the concept of lattice points.
- Describe the seven crystal systems.
- Classify the fourteen Bravais lattices.
- Differentiate between primitive and centered lattices.
- Explain the importance of Bravais lattices in Materials Engineering.

#### 1. Introduction

Every crystalline material is formed by the regular repetition of atoms in three-dimensional space. Although there are millions of ways atoms can appear to be arranged, **French crystallographer Auguste Bravais** proved in **1848** that there are only **14 unique repeating lattice arrangements** possible.

These are called the **Bravais Lattices**.

They form the mathematical foundation of crystallography.

#### 2. What is a Bravais Lattice?

##### Definition

A **Bravais lattice** is an infinite three-dimensional arrangement of lattice points in which every lattice point has an identical environment.

##### Simple Definition (Exam)

A Bravais lattice is a regular three-dimensional arrangement of lattice points that repeats throughout a crystal.

#### 3. What is a Lattice Point?

A **lattice point** is an imaginary point representing the position where one atom or a group of atoms (basis) may be placed.

**Important Note:**

- A lattice point is **not an atom**.
- When a basis is attached to every lattice point, a crystal structure is obtained.

Therefore,

**Crystal Structure = Bravais Lattice + Basis**

This is one of the most important concepts in crystallography.

**4. History of Bravais Lattices**

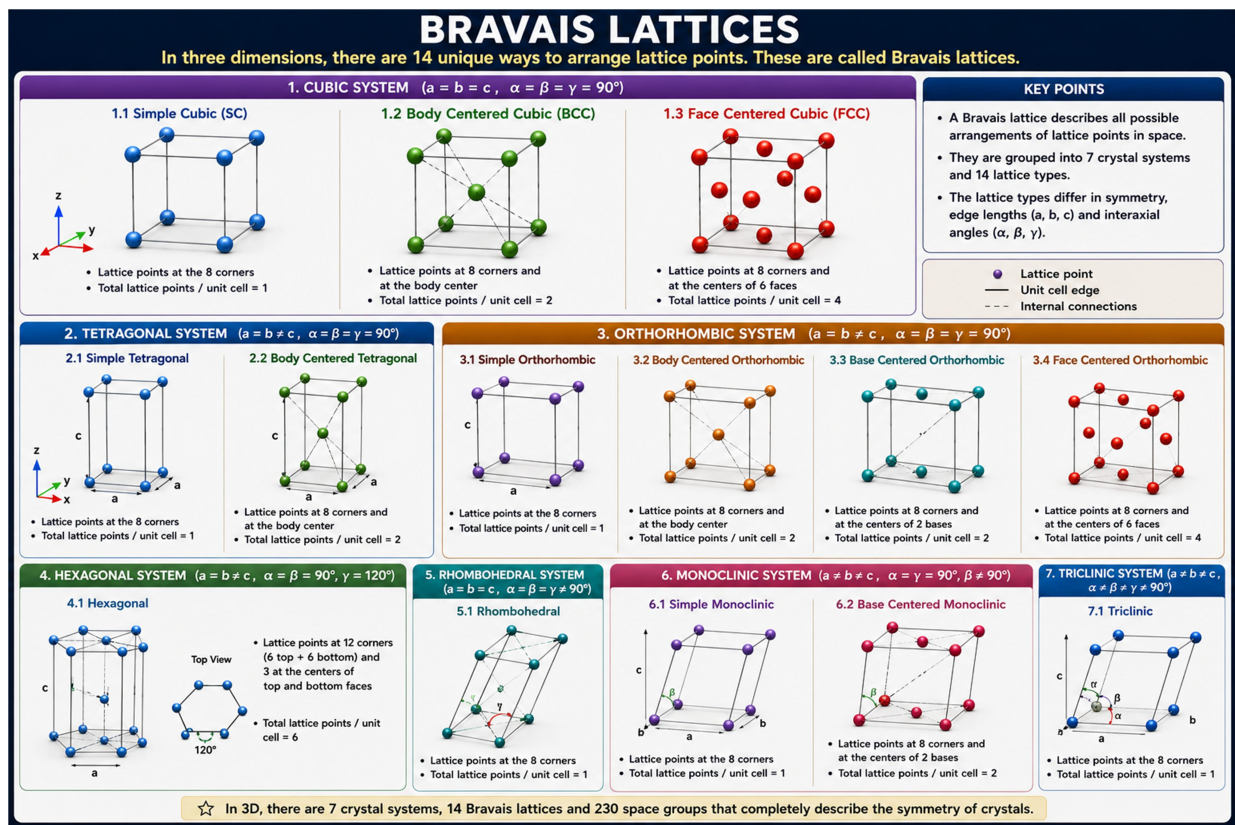
In 1848, **Auguste Bravais** demonstrated mathematically that all crystal structures can be described using only **14 distinct lattice types**.

These lattices explain the arrangement of atoms in almost all crystalline engineering materials.

**5. Crystal Systems**

The 14 Bravais lattices are grouped into **7 crystal systems** based on unit-cell geometry.

| Crystal System          | Edge Lengths      | Interaxial Angles                                 |
|-------------------------|-------------------|---------------------------------------------------|
| Cubic                   | $a = b = c$       | $\alpha = \beta = \gamma = 90^\circ$              |
| Tetragonal              | $a = b \neq c$    | $\alpha = \beta = \gamma = 90^\circ$              |
| Orthorhombic            | $a \neq b \neq c$ | $\alpha = \beta = \gamma = 90^\circ$              |
| Hexagonal               | $a = b \neq c$    | $\alpha = \beta = 90^\circ, \gamma = 120^\circ$   |
| Trigonal (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               | $a \neq b \neq c$ | $\alpha \neq \beta \neq \gamma \neq 90^\circ$     |



## 6. Types of Centering

A Bravais lattice may contain lattice points at different positions.

### (A) Primitive (P)

Lattice points only at the corners.

Also called **Simple** lattice.

### (B) Body-Centered (I)

Lattice points at:

- Eight corners
- One body center

Example:

- Body-Centered Cubic (BCC)

### (C) Face-Centered (F)

Lattice points at:

- Eight corners
- Centers of all six faces

Example:

- Face-Centered Cubic (FCC)

#### **(D) Base-Centered (C)**

Lattice points at:

- Eight corners
- Centers of one pair of opposite faces

Common in some orthorhombic and monoclinic systems.

### **7. The Fourteen Bravais Lattices**

| <b>Crystal System</b>      | <b>Bravais Lattices</b>                                                |
|----------------------------|------------------------------------------------------------------------|
| Cubic                      | Primitive Cubic (P), Body-Centered Cubic (I), Face-Centered Cubic (F)  |
| Tetragonal                 | Primitive (P), Body-Centered (I)                                       |
| Orthorhombic               | Primitive (P), Base-Centered (C), Body-Centered (I), Face-Centered (F) |
| Monoclinic                 | Primitive (P), Base-Centered (C)                                       |
| Triclinic                  | Primitive (P)                                                          |
| Hexagonal                  | Primitive (P)                                                          |
| Trigonal<br>(Rhombohedral) | Rhombohedral (R)                                                       |

**Total = 14 Bravais Lattices**

### **8. Distribution of Bravais Lattices**

| <b>Crystal System</b> | <b>Number of Bravais Lattices</b> |
|-----------------------|-----------------------------------|
| Cubic                 | 3                                 |
| Tetragonal            | 2                                 |
| Orthorhombic          | 4                                 |
| Monoclinic            | 2                                 |
| Triclinic             | 1                                 |
| Hexagonal             | 1                                 |

| Crystal System | Number of Bravais Lattices |
|----------------|----------------------------|
|----------------|----------------------------|

|          |   |
|----------|---|
| Trigonal | 1 |
|----------|---|

|              |           |
|--------------|-----------|
| <b>Total</b> | <b>14</b> |
|--------------|-----------|

## 9. Primitive vs Centered Lattices

| Primitive Lattice | Centered Lattice |
|-------------------|------------------|
|-------------------|------------------|

|                                |                                                          |
|--------------------------------|----------------------------------------------------------|
| Lattice points only at corners | Additional lattice points at body, face, or base centers |
|--------------------------------|----------------------------------------------------------|

|                     |                          |
|---------------------|--------------------------|
| Simpler arrangement | More complex arrangement |
|---------------------|--------------------------|

|                          |                           |
|--------------------------|---------------------------|
| Lower packing efficiency | Higher packing efficiency |
|--------------------------|---------------------------|

|                       |                    |
|-----------------------|--------------------|
| Example: Simple Cubic | Examples: BCC, FCC |
|-----------------------|--------------------|

## 10. Importance of Bravais Lattices

Bravais lattices help engineers to:

- Understand crystal symmetry.
- Describe atomic arrangements.
- Identify crystal structures.
- Calculate crystal density.
- Determine atomic packing factor (APF).
- Analyze crystal defects.
- Explain deformation mechanisms.
- Predict material properties.

## 11. Engineering Applications

### Steel Industry

Ferrite has a **Body-Centered Cubic (BCC)** structure.

This influences:

- Strength
- Ductility
- Heat-treatment behavior

### Aluminium Industry

Aluminium has a **Face-Centered Cubic (FCC)** structure.

Therefore it has:

- Excellent ductility
- High formability
- Good corrosion resistance

### **Titanium Industry**

Titanium changes its crystal structure with temperature:

- **HCP** at room temperature
- **BCC** at higher temperatures

This affects its mechanical properties and processing.

### **12. Advantages of Studying Bravais Lattices**

Understanding Bravais lattices enables engineers to:

- Design advanced alloys.
- Select suitable engineering materials.
- Understand phase transformations.
- Interpret X-ray diffraction patterns.
- Predict mechanical behavior.
- Develop new materials for aerospace, biomedical, and electronic applications.

### **13. Key Formula**

$$\{\text{Crystal Structure}\} = \{\text{Bravais Lattice}\} + \{\text{Basis}\}$$

This is one of the most frequently asked concepts in crystallography.

### **Key Points to Remember**

- A Bravais lattice is a periodic arrangement of lattice points.
- Auguste Bravais proposed the concept in **1848**.
- There are **14 Bravais lattices** grouped into **7 crystal systems**.
- Primitive lattices have lattice points only at the corners, whereas centered lattices have additional lattice points.
- Bravais lattices are fundamental to understanding crystal structures and material properties.

### **Frequently Asked Viva Questions**

1. What is a Bravais lattice?
2. Who proposed the Bravais lattice concept?
3. How many Bravais lattices are there?
4. How many crystal systems exist?
5. What is a lattice point?
6. Differentiate between primitive and body-centered lattices.
7. State the relationship between crystal structure, lattice, and basis.
8. Which Bravais lattice is adopted by aluminium?
9. Which crystal system contains the largest number of Bravais lattices?
10. Why are Bravais lattices important in Materials Engineering?

### **Examination Questions**

#### **Short Questions (2 Marks)**

1. Define a Bravais lattice.
2. What is a lattice point?
3. How many Bravais lattices are there?
4. Name the seven crystal systems.
5. State the difference between primitive and centered lattices.

#### **Long Questions (10 Marks)**

1. Explain the concept of Bravais lattices. Discuss the seven crystal systems and the fourteen Bravais lattices with suitable diagrams.
2. Define a Bravais lattice and explain its importance in crystallography and Materials Engineering.
3. Differentiate between primitive, body-centered, face-centered, and base-centered lattices with suitable examples.

### **Lecture-13**

#### **UNIT-2: THE STRUCTURE OF CRYSTALLINE SOLIDS**

##### **Detailed Lecture Notes: Unit Cells**

**Course:** MTPC201 – Introduction to Materials Engineering

**Semester:** 3rd Semester Diploma in Metallurgical Engineering

**Subject Area:** Unit-2 — The Structure of Crystalline Solids

**Reference base:** William D. Callister, V. Raghavan, Sidney H. Avner, Van Vlack and W.F. Smith.

## 1. INTRODUCTION TO UNIT CELLS

A crystalline material consists of atoms arranged in a **regular and repeating three-dimensional pattern**.

It is not necessary to draw the entire crystal to describe this arrangement. Instead, we identify the smallest geometrical portion whose repetition can generate the complete crystal.

This fundamental repeating unit is called the:

**Unit Cell**

**Simple idea**

Think of a tiled floor.

One tile represents the basic repeating pattern. By repeating the tile, the entire floor can be constructed.

Similarly:

**Unit Cell → Repeated in 3D → Crystal**

## 2. DEFINITION OF UNIT CELL

### Definition

A **unit cell** is the smallest repeating three-dimensional volume of a crystal lattice which, when translated repeatedly along its three principal directions, reproduces the complete crystal structure.

### Important points

A unit cell:

- has a definite geometry;
- contains one or more lattice points/atoms depending on the chosen cell;
- possesses definite dimensions;
- repeats periodically in three dimensions;
- represents the symmetry of the crystal.

## 3. CRYSTAL LATTICE AND UNIT CELL

Before understanding the unit cell, distinguish between **lattice** and **unit cell**.

### Crystal lattice

A lattice is an imaginary three-dimensional arrangement of points having identical surroundings.

### Unit cell



A unit cell is the smallest repeating geometrical region used to represent that lattice.

Thus:

Crystal lattice = periodic arrangement of lattice points

And Unit cell = repeating building block of that lattice

#### 4. UNIT CELL AND CRYSTAL STRUCTURE

A very important relationship is:

Crystal Structure=Lattice+Basis

Where:

##### **Lattice**

Defines the geometrical arrangement of points.

##### **Basis**

An atom or group of atoms attached to each lattice point.

Therefore, the lattice tells us **where** the repeating points are located, while the basis tells us **what is placed at those points**.

#### 5. LATTICE PARAMETERS

A unit cell is mathematically described by six parameters.

These are:

##### **Three axial lengths**

$a, b, c$

##### **Three interaxial angles**

$\alpha, \beta, \gamma$

Therefore:

$a, b, c, \alpha, \beta, \gamma$

are called the **lattice parameters**.

#### 6. MEANING OF THE LATTICE PARAMETERS

Consider a general unit cell.

- $a$  = length along x-axis
- $b$  = length along y-axis
- $c$  = length along z-axis

The angles are:

- $\alpha$  = angle between  $b$  and  $c$
- $\beta$  = angle between  $a$  and  $c$
- $\gamma$  = angle between  $a$  and  $b$

Thus a crystal system can be identified from the relationships among  $a, b, c$  and  $\alpha, \beta, \gamma$ .

## 7. UNIT CELL OF THE CUBIC SYSTEM

The cubic system is particularly important in Metallurgy because many metals crystallize in cubic structures.

For a cubic unit cell:

$$a = b = c$$

and

$$\alpha = \beta = \gamma = 90^\circ$$

Therefore, only one lattice parameter is required:

$$a$$

## 8. TYPES OF UNIT CELLS

Unit cells can be classified according to the location of their lattice points.

The major types are:

1. Primitive or Simple unit cell
2. Body-centred unit cell
3. Face-centred unit cell
4. Base-centred unit cell

For the structures emphasized in this course:

- SC  $\rightarrow$  Simple/primitive
- BCC  $\rightarrow$  Body-centred
- FCC  $\rightarrow$  Face-centred
- HCP  $\rightarrow$  Hexagonal close-packed

# UNIT CELLS

The smallest repeating unit which, when stacked in three dimensions, builds the entire crystal.

## 1. WHAT IS A UNIT CELL?

A unit cell is the smallest volume that represents the geometry of a crystal lattice. Repetition of this cell in space produces the entire crystal.

**Key Point**  
All lattice points of a crystal can be generated by translating the unit cell along three axes.

## 2. ELEMENTS OF A UNIT CELL

$a, b, c$  : Edge lengths (Unit cell parameters)  
 $\alpha$  : Angle between  $b$  and  $c$   
 $\beta$  : Angle between  $a$  and  $c$   
 $\gamma$  : Angle between  $a$  and  $b$   
 Interaxial angles :  $0^\circ < \alpha, \beta, \gamma \leq 180^\circ$

### Types of Lattice Points

Corner (1/8)

Face Center (1/2)

Body Center (1)

Edge Center (1/4)

Number in bracket = Contribution to one unit cell

## 3. TYPES OF UNIT CELLS (BY SHAPE)

### 1. Cubic

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

### 2. Tetragonal

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

### 3. Orthorhombic

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

### 4. Hexagonal

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

### 5. Monoclinic

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

### 6. Triclinic

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

## 4. BRAVAIS LATTICES & UNIT CELLS

| Crystal System          | Bravais Lattices | Unit Cell Characteristics                                             | No. of Lattices |
|-------------------------|------------------|-----------------------------------------------------------------------|-----------------|
| Cubic                   | P, I, F          | $a = b = c$ ; $\alpha = \beta = \gamma = 90^\circ$                    | 3               |
| Tetragonal              | P, I             | $a = b \neq c$ ; $\alpha = \beta = \gamma = 90^\circ$                 | 2               |
| Orthorhombic            | P, C, I, F       | $a \neq b \neq c$ ; $\alpha = \beta = \gamma = 90^\circ$              | 4               |
| Hexagonal               | P                | $a = b \neq c$ ; $\alpha = \beta = 90^\circ, \gamma = 120^\circ$      | 1               |
| Rhombohedral (Trigonal) | R                | $a = b = c$ ; $\alpha = \beta = \gamma \neq 90^\circ$                 | 1               |
| Monoclinic              | P, C             | $a \neq b \neq c$ ; $\alpha = \gamma = 90^\circ, \beta \neq 90^\circ$ | 2               |
| Triclinic               | P                | $a \neq b \neq c$ ; $\alpha \neq \beta \neq \gamma \neq 90^\circ$     | 1               |

Total Bravais lattices = 14

P = Primitive (simple)    I = Body centered    F = Face centered    C = Base centered    R = Rhombohedral

## 5. COMMON EXAMPLES

|                                                                               |                                                                                 |                                                                                          |
|-------------------------------------------------------------------------------|---------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| <b>Simple Cubic (SC)</b><br><br>Example: Polonium                             | <b>Body Centered Cubic (BCC)</b><br><br>Example: Iron ( $\alpha$ -Fe), Chromium | <b>Face Centered Cubic (FCC)</b><br><br>Example: Copper, Aluminium, Nickel, Silver, Gold |
| <b>Hexagonal Close Packed (HCP)</b><br><br>Example: Magnesium, Zinc, Titanium | <b>Rhombohedral</b><br><br>Example: Bismuth                                     | <b>Diamond Cubic</b><br><br>Example: Diamond, Silicon, Germanium                         |

## 6. IMPORTANCE

- Helps in understanding the internal arrangement of atoms.
- Basis for calculation of density, atomic packing factor (APF) and coordination number.
- Important in determining physical properties like strength, hardness, conductivity, etc.
- Essential for studying crystal planes, directions and Miller indices.
- Foundation for phase transformations, slip systems and material behavior.

Unit cell is the building block of all crystals.

## 9. PRIMITIVE OR SIMPLE UNIT CELL

A **primitive unit cell** contains lattice points only at its corners.

For a cubic primitive cell:

Simple Cubic (SC)

There are eight corner positions.

However, a corner atom is shared among eight neighbouring unit cells.

Therefore, the contribution of each corner atom is:

$$\frac{1}{8}$$

Hence:

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

Therefore, a simple cubic unit cell contains:

1 atom per unit cell

## 10. ATOMIC CONTRIBUTION IN A UNIT CELL

This is one of the **most important concepts for examination and numerical problems**.

Atoms may occupy:

- corners;
- edges;
- faces;
- body centre.

Their contribution to one unit cell is different.

### **10.1 Corner Atom**

A corner atom is shared by:  
8 unit cells.

Therefore:

Contribution= $\frac{1}{8}$

### **10.2 Edge Atom**

An atom situated exactly at the middle of an edge is shared by:  
4 unit cells.

Therefore:

Contribution= $\frac{1}{4}$

### **10.3 Face-Centred Atom**

An atom at the centre of a face is shared by:  
2 unit cells.

Therefore:

Contribution= $\frac{1}{2}$

### **10.4 Body-Centred Atom**

An atom completely inside the unit cell belongs entirely to that unit cell.

Therefore:

Contribution=1

## **11. MASTER TABLE: ATOMIC CONTRIBUTION**

| <b>Position</b> | <b>Number of unit cells sharing atom</b> | <b>Contribution to one unit cell</b> |
|-----------------|------------------------------------------|--------------------------------------|
| Corner          | 8                                        | $\left(\frac{1}{8}\right)$           |

| Position    | Number of unit cells sharing atom | Contribution to one unit cell |
|-------------|-----------------------------------|-------------------------------|
| Edge        | 4                                 | (1/4)                         |
| Face centre | 2                                 | (1/2)                         |
| Body centre | 1                                 | (1)                           |

**Easy memory trick**

**Corner  $\rightarrow 8 \rightarrow 1/8$**

**Edge  $\rightarrow 4 \rightarrow 1/4$**

**Face  $\rightarrow 2 \rightarrow 1/2$**

**Body  $\rightarrow 1 \rightarrow 1$**

## 12. NUMBER OF ATOMS IN SIMPLE CUBIC UNIT CELL

There are:

8

corner atoms.

Contribution of each:

$\frac{1}{8}$

Therefore:

$$N = 8 \times \frac{1}{8}$$

$$\boxed{N = 1}$$

**A Simple Cubic unit cell contains one effective atom.**

## 13. BODY-CENTRED CUBIC UNIT CELL

In a BCC structure:

- 8 atoms are present at the corners.
- 1 atom is present at the body centre.

Corner contribution:

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

Body-centre contribution:

$$1 \times 1 = 1$$

Therefore:

$$N = 1 + 1$$

$$\boxed{N = 2}$$

Thus:

**BCC contains two effective atoms per unit cell.**

#### 14. FACE-CENTRED CUBIC UNIT CELL

FCC contains:

- 8 corner atoms
- 6 face-centred atoms

Corner contribution:

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

Face contribution:

$$6 \times \frac{1}{2} = 3$$

Therefore:

$$N = 1 + 3$$

$$\boxed{N = 4}$$

**FCC contains four effective atoms per unit cell.**

## 15. COMPARISON OF SC, BCC AND FCC

| Feature                   | SC   | BCC  | FCC  |
|---------------------------|------|------|------|
| Corner atoms              | 8    | 8    | 8    |
| Face atoms                | 0    | 0    | 6    |
| Body atoms                | 0    | 1    | 0    |
| Effective atoms/unit cell | 1    | 2    | 4    |
| Coordination number       | 6    | 8    | 12   |
| APF                       | 0.52 | 0.68 | 0.74 |
| Packing efficiency        | 52%  | 68%  | 74%  |

## 16. CONVENTIONAL VS PRIMITIVE UNIT CELL

This distinction is important at higher levels of crystallography.

### Primitive unit cell

Contains exactly **one lattice point**.

### Conventional unit cell

Chosen to display the symmetry of the crystal conveniently and may contain more than one lattice point.

For example, the conventional FCC cubic cell contains four lattice points effectively.

## 17. WHY DO WE USE UNIT CELLS?

Unit cells allow engineers and scientists to describe complicated crystal structures using a simple geometrical model.

They help determine:

### 1. Number of atoms

N

### 2. Atomic packing factor

APF

### Theoretical density

$$\rho$$

### 4. Atomic radius

r

### 5. Coordination number

CN

## 6. Crystallographic directions

[uvw]

## 7. Crystal planes

(hkl)

## 18. UNIT CELL AND ATOMIC RADIUS

In many crystal structures, atoms are considered as hard spheres.

The relationship between atomic radius ( $r$ ) and lattice parameter ( $a$ ) depends on the direction in which atoms touch.

This is extremely important for numerical problems.

## 19. SIMPLE CUBIC: RELATION BETWEEN ( $a$ ) AND ( $r$ )

In SC, atoms touch along the cube edge.

Therefore:

$$a = 2r$$

Hence:

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

## 20. BCC: RELATION BETWEEN ( $a$ ) AND ( $r$ )

In BCC, atoms touch along the **body diagonal**.



For a cube:

$$\text{Body diagonal} = \sqrt{3}a$$

Along the body diagonal there are effectively four atomic radii:

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

Therefore:

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

or

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

## 21. FCC: RELATION BETWEEN (a) AND (r)

In FCC, atoms touch along the **face diagonal**.

Face diagonal:

$$\sqrt{2}a$$

There are four atomic radii along the face diagonal:

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

Therefore:

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

or:

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

## 22. IMPORTANT RELATIONSHIPS

| Structure | Contact direction | Relationship |
|-----------|-------------------|--------------|
| SC        | Cube edge         | (a=2r)       |

| Structure | Contact direction | Relationship     |
|-----------|-------------------|------------------|
| BCC       | Body diagonal     | $(\sqrt{3}a=4r)$ |
| FCC       | Face diagonal     | $(\sqrt{2}a=4r)$ |

**Examination memory:**

SC → Edge

BCC → Body diagonal

FCC → Face diagonal

### 23. UNIT CELL VOLUME

For a cubic unit cell:

For a cubic unit cell:

$$V_c = a^3$$

If  $a$  is expressed in cm, volume is obtained in:

$$cm^3$$

If  $a$  is expressed in nm:

$$V_c = nm^3$$

### 24. UNIT CONVERSION — VERY IMPORTANT

Students frequently make mistakes in density calculations because of unit conversion.

Remember:

$$1\text{ nm} = 10^{-7}\text{ cm}$$

Therefore:

$$1\text{ nm}^3 = 10^{-21}\text{ cm}^3$$

Also:

$$1\text{ Å} = 10^{-8}\text{ cm}$$

and:

$$1\text{ nm} = 10\text{ Å}$$

## 25. THEORETICAL DENSITY FROM UNIT CELL

The mass contained in one unit cell can be calculated from the number of atoms present.

If:

- (n) = number of atoms per unit cell
- (A) = atomic weight
- ( $N_A$ ) = Avogadro's number

then mass of one atom is:

$$\frac{A}{N_A}$$

Therefore mass of unit cell:

$$m_c = \frac{nA}{N_A}$$

Since:

$$\rho = \frac{m}{V}$$

we obtain:

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

For cubic crystals:

$$\rho = \frac{nA}{N_A a^3}$$

This is one of the most important equations in crystal structure calculations.

## 26. EXAMPLE: NUMBER OF ATOMS IN FCC

### Problem

Calculate the effective number of atoms in an FCC unit cell.

### Solution

Corner contribution:

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

Face contribution:

$$6 \times \frac{1}{2} = 3$$

Therefore:

$$N = 1 + 3$$

$$\boxed{N = 4}$$

### 27. EXAMPLE: FIND ATOMIC RADIUS OF BCC METAL

Suppose a BCC metal has:

$$a = 0.2866 \text{ nm}$$

For BCC:

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

Therefore:

$$r = \frac{1.732(0.2866)}{4}$$

$$\boxed{r \approx 0.124 \text{ nm}}$$

### 28. EXAMPLE: FIND LATTICE PARAMETER OF FCC

Suppose:

$$r = 0.128 \text{ nm}$$

For FCC:

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

Therefore:

$$a = 2(1.414)(0.128)$$

$$a \approx 0.362 \text{ nm}$$

## 29. UNIT CELL AND COORDINATION NUMBER

The **coordination number (CN)** is the number of nearest-neighbour atoms surrounding a selected atom.

For the major cubic structures:

| Structure | Coordination Number |
|-----------|---------------------|
| SC        | 6                   |
| BCC       | 8                   |
| FCC       | 12                  |

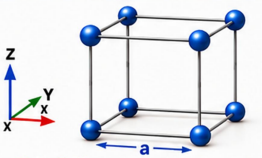
The HCP structure also has:

{CN=12}

# CRYSTAL STRUCTURES

Most Common Crystal Structures in Materials Science

### 1. SIMPLE CUBIC (SC)



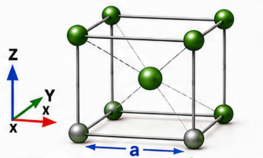
**Unit Cell**  
Atoms are located only at the eight corners of the cube.

|                             |                                                     |
|-----------------------------|-----------------------------------------------------|
| Unit Cell Parameter         | $a = b = c$<br>$\alpha = \beta = \gamma = 90^\circ$ |
| Atoms per Unit Cell         | 1                                                   |
| Atomic Packing Factor (APF) | 0.52                                                |
| Coordination Number         | 6                                                   |
| Examples                    | Polonium ( $\alpha$ -Po)                            |

Atomic Packing



### 2. BODY CENTERED CUBIC (BCC)



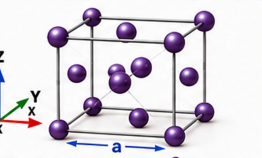
**Unit Cell**  
Atoms are located at the eight corners and one at the body center.

|                             |                                                     |
|-----------------------------|-----------------------------------------------------|
| Unit Cell Parameter         | $a = b = c$<br>$\alpha = \beta = \gamma = 90^\circ$ |
| Atoms per Unit Cell         | 2                                                   |
| Atomic Packing Factor (APF) | 0.68                                                |
| Coordination Number         | 8                                                   |
| Examples                    | Iron ( $\alpha$ -Fe), Chromium, Vanadium            |

Atomic Packing



### 3. FACE CENTERED CUBIC (FCC)



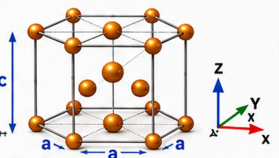
**Unit Cell**  
Atoms are located at the eight corners and at the centers of all six faces.

|                             |                                                     |
|-----------------------------|-----------------------------------------------------|
| Unit Cell Parameter         | $a = b = c$<br>$\alpha = \beta = \gamma = 90^\circ$ |
| Atoms per Unit Cell         | 4                                                   |
| Atomic Packing Factor (APF) | 0.74                                                |
| Coordination Number         | 12                                                  |
| Examples                    | Copper, Aluminium, Nickel, Silver, Gold             |

Atomic Packing



### 4. HEXAGONAL CLOSE PACKED (HCP)



**Unit Cell**  
Atoms are located at the corners of hexagonal faces and three atoms inside the cell.

|                             |                                                                   |
|-----------------------------|-------------------------------------------------------------------|
| Unit Cell Parameter         | $a = b \neq c$<br>$\alpha = \beta = 90^\circ, \gamma = 120^\circ$ |
| Atoms per Unit Cell         | 6                                                                 |
| Atomic Packing Factor (APF) | 0.74                                                              |
| Coordination Number         | 12                                                                |
| Examples                    | Magnesium, Zinc, Titanium, Cobalt                                 |

Atomic Packing



#### COMPARISON OF CRYSTAL STRUCTURES

| Property                    | SC                                                  | BCC                                                 | FCC                                                 | HCP                                                               |
|-----------------------------|-----------------------------------------------------|-----------------------------------------------------|-----------------------------------------------------|-------------------------------------------------------------------|
| Unit Cell Shape             | Cube                                                | Cube                                                | Cube                                                | Hexagonal Prism                                                   |
| Atoms per Unit Cell         | 1                                                   | 2                                                   | 4                                                   | 6                                                                 |
| Atomic Packing Factor (APF) | 0.52                                                | 0.68                                                | 0.74                                                | 0.74                                                              |
| Coordination Number         | 6                                                   | 8                                                   | 12                                                  | 12                                                                |
| Unit Cell Parameter         | $a = b = c$<br>$\alpha = \beta = \gamma = 90^\circ$ | $a = b = c$<br>$\alpha = \beta = \gamma = 90^\circ$ | $a = b = c$<br>$\alpha = \beta = \gamma = 90^\circ$ | $a = b \neq c$<br>$\alpha = \beta = 90^\circ, \gamma = 120^\circ$ |

#### LEGEND

- Corner atom (shared by 8 unit cells)
- Face centered atom (shared by 2 unit cells)
- Body centered atom (fully inside unit cell)
- Atoms in HCP structure (shared in the cell)

#### KEY POINTS

- ◆ Crystal structures determine the properties of materials.
- ◆ Higher APF means more efficient packing.
- ◆ FCC and HCP have the highest packing (74%).
- ◆ BCC has higher strength and hardness.
- ◆ SC is least densely packed.

## 30. UNIT CELL AND ATOMIC PACKING FACTOR

The **Atomic Packing Factor (APF)** is the fraction of unit-cell volume occupied by atoms, treating atoms as hard spheres.

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

Values

$$SC = 0.52$$

$$BCC = 0.68$$

$$FCC = 0.74$$

The close-packed FCC and HCP structures both have approximately:

$$APF = 0.74$$

## 31. WHY FCC HAS HIGHER PACKING THAN BCC

Compare:

$$SC = 52\%$$

$$BCC = 68\%$$

$$FCC = 74\%$$

Therefore FCC uses the available space more efficiently.

The idealized packing efficiency increases in the sequence:

$$SC < BCC < FCC$$

## Lecture-14

### 32. UNIT CELL OF HCP

HCP is different from the cubic structures because its geometry is hexagonal.

The conventional HCP cell contains:

6 atoms

The atoms are arranged in close-packed layers.

The stacking sequence is:

ABABAB...

HCP has:

CN=12

and:

APF=0.74

### 33. FCC VS HCP

Both are close-packed structures.

#### FCC

ABCABCABC...

#### HCP

ABABABAB...

Both:

CN=12

and:

APF=0.74

This is an important conceptual question.

### 34. UNIT CELL AND CRYSTAL PROPERTIES

The atomic arrangement represented by the unit cell influences:

- Density
- Plastic deformation
- Slip
- Electrical conductivity
- Thermal behaviour
- Diffusion
- Elastic properties
- Fracture behaviour

Thus:

Unit Cell → Crystal Structure → Material Properties

### 35. COMMON MISTAKES BY STUDENTS

#### Mistake 1

Writing:

BCC has 8 atoms because it has 8 corner atoms.

**Incorrect.**

The effective number is:

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

#### Mistake 2

Writing FCC has six atoms.



The six face-centred atoms contribute:

$$6 \times \frac{1}{2} = 3$$

plus one effective atom from corners.

Therefore:

$$\boxed{4}$$

### Mistake 3

Using the wrong radius relationship.

Remember:

$$SC : a = 2r$$

$$BCC : \sqrt{3}a = 4r$$

$$FCC : \sqrt{2}a = 4r$$

### Mistake 4

Confusing APF with number of atoms.

For example:

FCC has:

4atoms/unit cell

APF=0.74

These are completely different quantities.

### 36. QUICK REVISION TABLE

| Quantity                  | SC   | BCC           | FCC           |
|---------------------------|------|---------------|---------------|
| Effective atoms/unit cell | 1    | 2             | 4             |
| CN                        | 6    | 8             | 12            |
| APF                       | 0.52 | 0.68          | 0.74          |
| Atomic contact            | Edge | Body diagonal | Face diagonal |

| Quantity             | SC       | BCC              | FCC              |
|----------------------|----------|------------------|------------------|
| Packing efficiency   | 52%      | 68%              | 74%              |
| $a - r$ relationship | $a = 2r$ | $\sqrt{3}a = 4r$ | $\sqrt{2}a = 4r$ |

### 37. DEFINITIONS

#### Unit Cell

The unit cell is the smallest repeating three-dimensional portion of a crystal lattice which generates the entire crystal through translational repetition.

#### Lattice Parameter

Lattice parameters are the three axial dimensions ( $a, b, c$ ) and three interaxial angles ( $\alpha, \beta, \gamma$ ) that define the geometry of a unit cell.

#### Primitive Unit Cell

A primitive unit cell contains one effective lattice point.

#### Body-Centred Unit Cell

A body-centred unit cell contains lattice points at the corners and one additional lattice point at the body centre.

#### Face-Centred Unit Cell

A face-centred unit cell contains lattice points at the corners and at the centres of all faces.

#### Coordination Number

Coordination number is the number of nearest-neighbour atoms surrounding a particular atom in a crystal.

#### Atomic Packing Factor

Atomic packing factor is the ratio of the volume occupied by atoms to the total volume of the unit cell.

## 38. KEY FORMULAS TO MEMORIZE

### Effective atoms

$$N = N_c \frac{1}{8} + N_e \frac{1}{4} + N_f \frac{1}{2} + N_b$$

where:

- $N_c$  = corner atoms
- $N_e$  = edge atoms
- $N_f$  = face atoms
- $N_b$  = body-centre atoms

### Cubic unit-cell volume

$$V_c = a^3$$

### Theoretical density

$$\rho = \frac{nA}{N_A a^3}$$

### SC

$$a = 2r$$

### BCC

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

### FCC

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

### APF

$$APF = \frac{n(4/3)\pi r^3}{a^3}$$

## 39. 2-MARK EXAMINATION QUESTIONS

1. Define a unit cell.
2. What is meant by a crystal lattice?
3. What are lattice parameters?
4. Name the six lattice parameters of a general unit cell.
5. What is a primitive unit cell?
6. What is a body-centred unit cell?
7. What is a face-centred unit cell?

8. What fraction of a corner atom belongs to a unit cell?
9. What fraction of a face-centred atom belongs to a unit cell?
10. What fraction of a body-centred atom belongs to a unit cell?
11. How many effective atoms are present in an SC unit cell?
12. How many effective atoms are present in a BCC unit cell?
13. How many effective atoms are present in an FCC unit cell?
14. State the coordination number of SC.
15. State the coordination number of BCC.
16. State the coordination number of FCC.
17. Define atomic packing factor.
18. State the APF of SC, BCC and FCC.
19. State the relationship between (a) and (r) for BCC.
20. State the relationship between (a) and (r) for FCC.
21. What is meant by a conventional unit cell?
22. What is the difference between a primitive and conventional unit cell?
23. What is the volume of a cubic unit cell?
24. State the theoretical density equation for a cubic crystal.
25. What is the stacking sequence of HCP?

#### **40. 5-MARK EXAMINATION QUESTIONS**

1. Define a unit cell and explain its significance in crystallography.
2. Explain the six lattice parameters of a general unit cell.
3. Explain the contribution of corner, edge, face and body-centred atoms to a unit cell.
4. Calculate the number of effective atoms in SC, BCC and FCC unit cells.
5. Explain the structure of a simple cubic unit cell.
6. Explain the structure of a BCC unit cell.
7. Explain the structure of an FCC unit cell.
8. Differentiate between primitive and conventional unit cells.
9. Explain the relationship between atomic radius and lattice parameter in SC, BCC and FCC.

10. Compare SC, BCC and FCC structures with respect to number of atoms, coordination number and APF.
11. Define APF and explain its significance.
12. Explain how the theoretical density of a crystal can be determined from its unit-cell parameters.
13. Explain the HCP unit cell and its atomic arrangement.
14. Compare FCC and HCP close-packed structures.
15. Explain why atoms at corners, faces and body centres have different contributions to a unit cell.

#### **41. 10-MARK EXAMINATION QUESTIONS**

**Q1.**

**Define a unit cell. Explain the concept of lattice parameters and discuss the contribution of corner, edge, face and body-centred atoms to a unit cell with suitable diagrams.**

**Q2.**

**Explain Simple Cubic, Body-Centred Cubic and Face-Centred Cubic unit cells. Calculate the effective number of atoms in each structure.**

**Q3.**

**Derive the relationship between atomic radius ( $r$ ) and lattice parameter ( $a$ ) for SC, BCC and FCC crystal structures.**

**Q4.**

**Compare SC, BCC, FCC and HCP structures with respect to:**

- number of atoms/unit cell,
- coordination number,
- atomic packing factor,
- atomic contact direction,
- packing efficiency,
- examples of metals.

**Q5.**

**Define Atomic Packing Factor. Derive the APF for the SC, BCC and FCC structures.**

**Q6.**

**Derive the expression for theoretical density of a crystalline material using unit-cell parameters. Explain the significance of each term in the equation.**

**Q7.**

**Explain primitive and conventional unit cells. Discuss different types of unit-cell centering with neat diagrams.**

**Q8.**

**Explain HCP structure in detail. Discuss its atomic arrangement, coordination number, packing efficiency and stacking sequence. Compare HCP with FCC.**

**Q9. Numerical**

A metal has a BCC crystal structure, atomic weight of 55.85 g/mol and lattice parameter of 0.2866 nm.

Calculate:

1. Number of atoms per unit cell.
2. Atomic radius.
3. Unit-cell volume.
4. Theoretical density.

**Q10. Numerical**

An FCC metal has an atomic radius of 0.128 nm and atomic weight of 63.5 g/mol.

Determine:

1. Lattice parameter.
2. Number of atoms per unit cell.
3. Unit-cell volume.
4. Theoretical density.

## 42. FINAL REVISION — "UNIT CELL IN ONE MINUTE"

Students should be able to recall this sequence:

Unit Cell → Lattice Parameters → Atomic Contribution → Atoms/Cell →  $CN$  →  $APF$  →

And remember:

$$SC = 1, \quad BCC = 2, \quad FCC = 4$$

$$CN : 6, 8, 12$$

$$APF : 0.52, 0.68, 0.74$$

$$SC : a = 2r$$

$$BCC : \sqrt{3}a = 4r$$

$$FCC : \sqrt{2}a = 4r$$

### Lecture-15

#### UNIT-II: THE STRUCTURE OF CRYSTALLINE SOLIDS

##### Lecture Notes: Point Coordinates, Crystallographic Directions & Crystallographic Planes

**Course:** MTPC201 – Introduction to Materials Engineering

**Semester:** 3rd Semester Diploma in Metallurgical Engineering

**Branch:** Metallurgical Engineering

The prescribed syllabus specifically includes **Point Coordinates, Crystallographic Directions and Crystallographic Planes**, followed by linear/planar densities, close-packed structures, crystal planes/directions, coordination number, APF and density.

**Note:** The uploaded syllabus specifies the topics but does not provide detailed teaching content for these three topics. The detailed explanations, derivations and examples below therefore expand the syllabus using standard crystallography conventions appropriate for Diploma Metallurgical Engineering.

#### 1. LEARNING OBJECTIVES

After completing this lecture, students should be able to:

1. Define point coordinates in a crystal.
2. Locate a point within a unit cell using fractional coordinates.
3. Understand the crystallographic coordinate system.
4. Define crystallographic directions.
5. Determine direction indices  $[uvw]$ .
6. Understand the significance of negative indices.

7. Differentiate between a direction and a family of directions.
8. Define crystallographic planes.
9. Determine Miller indices (hkl).
10. Understand the significance of negative Miller indices.
11. Determine Miller indices from plane intercepts.
12. Draw simple crystallographic planes and directions.
13. Distinguish between [uvw],  $\langle uvw \rangle$ , (hkl) and {hkl}.
14. Relate crystallographic directions and planes to slip, deformation and anisotropy.

## **PART-A: POINT COORDINATES**

### **2. INTRODUCTION**

A crystal contains an enormous number of atoms arranged periodically.

For example, even a very small piece of metal may contain billions of atoms. It is impossible and unnecessary to individually describe every atom.

Instead, crystallographers establish a coordinate system associated with the unit cell.

This allows us to specify the exact position of any point in the crystal.

The basic idea is:

Coordinate system  $\rightarrow$  Position of point

### **3. CRYSTALLOGRAPHIC COORDINATE SYSTEM**

Consider a cubic unit cell.

Three mutually perpendicular axes are normally selected:

- x-axis
- y-axis
- z-axis

For a cubic crystal:

$$a=b=c$$

and:

$$\alpha=\beta=\gamma=90^\circ$$

The origin is generally taken at one corner of the unit cell.

For teaching purposes, students should visualize the origin as:



(0,0,0)

#### 4. WHAT ARE POINT COORDINATES?

The position of a point inside a unit cell is expressed by three numbers:

(x,y,z)

These are called the **point coordinates**.

Usually, the coordinates are expressed as fractions of the unit-cell dimensions.

Therefore:

x=distance along x-axis y=distance along y-axis z=distance along z-axis

Thus:

(x,y,z)

describes the position of a point relative to the crystallographic axes.

#### 5. EXAMPLES OF POINT COORDINATES

For a cubic unit cell:

**Origin**

(0,0,0)

**One corner**

(1,0,0)

**Opposite corner**

(1,1,1)

**Centre of the cube**

( $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ )

**Centre of one face**

For example:

( $\frac{1}{2}, \frac{1}{2}, 0$ )

#### 6. IMPORTANT RULE ABOUT POINT COORDINATES

Point coordinates are **not the same as Miller indices**.

This distinction is extremely important.

**Point coordinate:**

(x,y,z)

describes a **location**.

**Direction:**

$[uvw]$

describes a **direction**.

**Plane:**

$(hkl)$

describes a **crystallographic plane**.

## 7. POINT COORDINATE EXAMPLE

Suppose a point is located:

- $1/2$  of the unit-cell length along x,
- $1/4$  along y,
- $3/4$  along z.

Then:

$P=(21,41,43)$

This tells us exactly where the point is located.

## 8. WHY POINT COORDINATES ARE IMPORTANT

Point coordinates are useful for:

- locating atoms;
- describing positions of defects;
- identifying interstitial sites;
- describing basis atoms;
- constructing crystal structures;
- identifying atomic arrangements;
- computer modelling of crystals.

In materials engineering, point coordinates become particularly useful when studying:

- vacancies;
- interstitial atoms;
- substitutional atoms;
- crystal defects;

- diffusion;
- crystallographic directions and planes.

## **PART–B: CRYSTALLOGRAPHIC DIRECTIONS**

### **9. WHAT IS A CRYSTALLOGRAPHIC DIRECTION?**

A crystallographic direction represents a specific direction or line within a crystal lattice.

It is represented by three integers enclosed in **square brackets**:

$[uvw]$

where:

- $u$  = direction component along  $x$
- $v$  = direction component along  $y$
- $w$  = direction component along  $z$

### **10. DIRECTION NOTATION**

#### **Single direction**

$[uvw]$

Example:

$[100]$

represents the  $x$ -axis direction.

$[010]$

represents the  $y$ -axis direction.

$[001]$

represents the  $z$ -axis direction.

### **11. BASIC CRYSTALLOGRAPHIC DIRECTIONS**

For a cubic unit cell:

**$[100]$**

Direction along  $x$ -axis.

**$[010]$**

Direction along  $y$ -axis.

**$[001]$**

Direction along  $z$ -axis.

**[110]**

Direction lying in the xy-plane with equal x and y components.

**[111]**

Direction along the body diagonal.

A useful visualization:

[100] → Along x-axis

[010] → Along y-axis

[001] → Along z-axis

[110] → Face diagonal

[111] → Body diagonal

**12. PROCEDURE FOR DETERMINING DIRECTION INDICES**

This is an important examination procedure.

Suppose a direction begins at point:

$$P1=(x1,y1,z1)$$

and ends at:

$$P2=(x2,y2,z2)$$

**Step 1: Determine the vector components**

$$\Delta x=x2-x1 \quad \Delta y=y2-y1 \quad \Delta z=z2-z1$$

Therefore:

$$(\Delta x, \Delta y, \Delta z)$$

**Step 2: Convert to the smallest integers**

Remove fractions by multiplying by the appropriate common factor.

**Step 3: Write the result in square brackets**

$$[uvw]$$

**13. EXAMPLE: DETERMINATION OF DIRECTION**

Suppose:

$$P1=(0,0,0)$$

and:

$$P2=(1,1,0)$$

Then:

$$\Delta x=1-0=1 \quad \Delta y=1-0=1 \quad \Delta z=0-0=0$$

Therefore:

$$[110]$$

#### 14. EXAMPLE WITH FRACTIONS

Suppose:

$$P1=(0,0,0)$$

and:

$$P2=(21,21,0)$$

The vector is:

$$(21,21,0)$$

Multiply by 2:

$$(1,1,0)$$

Therefore:

$$[110]$$

#### 15. NEGATIVE DIRECTIONS

A negative component is represented by placing a **bar over the number**.

For example:

$$[1\bar{1}0]$$

means:

- negative x-direction,
- positive y-direction,
- zero z-direction.

Similarly:

$$[11\bar{0}]$$

represents positive x, negative y and zero z.

**Important**

Do not write:

$[-110]$

in formal crystallographic notation.

Prefer:

$[1\bar{1}0]$

#### **16. DIRECTION $[111]$**

The direction:

$[111]$

has equal positive components along all three axes.

In a cubic unit cell, it corresponds to the **body diagonal**.

Thus:

$[111] \rightarrow$  body diagonal

This is a very important visual relationship.

#### **17. DIRECTION $[110]$**

The direction:

$[110]$

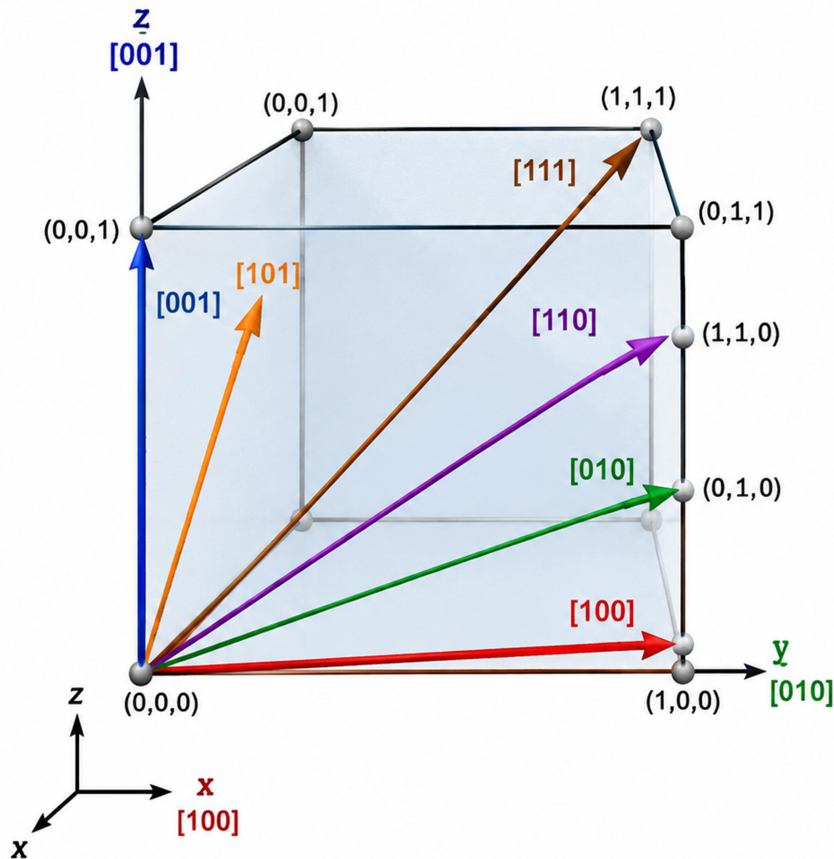
has:

$u=1, v=1, w=0$

Therefore it lies in the xy-plane.

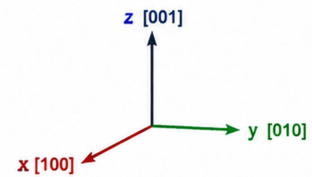
In a cubic crystal, it corresponds to a face-diagonal type direction.

# CRYSTALLOGRAPHIC DIRECTIONS



| Common Crystallographic Directions in a Cubic Crystal |                            |
|-------------------------------------------------------|----------------------------|
| Direction                                             | Miller Direction [ u v w ] |
| Along +x axis                                         | [100]                      |
| Along +y axis                                         | [010]                      |
| Along +z axis                                         | [001]                      |
| Along face diagonal (xy plane)                        | [110]                      |
| Along face diagonal (xz plane)                        | [101]                      |
| Along body diagonal (xyz)                             | [111]                      |

- Crystallographic directions are specified by Miller direction indices [u v w].
- They represent the direction of a vector parallel to the line joining lattice points.
- The smallest set of three integers (without common factor) is used.



## 18. EQUIVALENT CRYSTALLOGRAPHIC DIRECTIONS

In cubic crystals, several directions are geometrically equivalent because of the symmetry of the crystal.

For example:

[100], [010], [001]

belong to the same family of equivalent directions.

A family of directions is represented using:

$\langle uvw \rangle$

Thus:

$\langle 100 \rangle$

represents the family of equivalent [100]-type directions.

## 19. DIFFERENCE BETWEEN [UVW] AND $\langle UVW \rangle$

This is a frequent examination question.

| Notation              | Meaning                         |
|-----------------------|---------------------------------|
| $[uvw]$               | One specific direction          |
| $\langle uvw \rangle$ | Family of equivalent directions |

Example:

$[100]$

is one particular direction.

Whereas:

$\langle 100 \rangle$

represents all crystallographically equivalent directions of that type.

## **PART–C: CRYSTALLOGRAPHIC PLANES**

### **20. WHAT IS A CRYSTALLOGRAPHIC PLANE?**

A crystallographic plane is an imaginary plane passing through atoms or lattice points in a crystal.

Planes are extremely important because many important physical and mechanical phenomena occur preferentially on particular crystal planes.

Examples include:

- slip;
- cleavage;
- diffusion;
- surface reactions;
- crystal growth;
- X-ray diffraction.

### **21. MILLER INDICES**

Crystallographic planes are represented by **Miller indices**.

They are written in:

$(hkl)$

where:

- $h$  represents the reciprocal of the  $x$ -intercept;
- $k$  represents the reciprocal of the  $y$ -intercept;
- $l$  represents the reciprocal of the  $z$ -intercept.



## 22. WHY ARE MILLER INDICES USED?

Instead of describing a plane using complicated distances, Miller indices provide a simple set of integers.

For example:

(100) (110) (111)

represent important crystal planes in cubic structures.

## 23. PROCEDURE FOR FINDING MILLER INDICES

This is one of the **most important procedures in crystallography**.

To determine the Miller indices of a plane:

### Step 1

Determine the intercepts of the plane along:

x,y,z

in terms of:

a,b,c

### Step 2

Express the intercepts as numerical values.

### Step 3

Take the reciprocals.

### Step 4

Clear fractions to obtain the smallest integers.

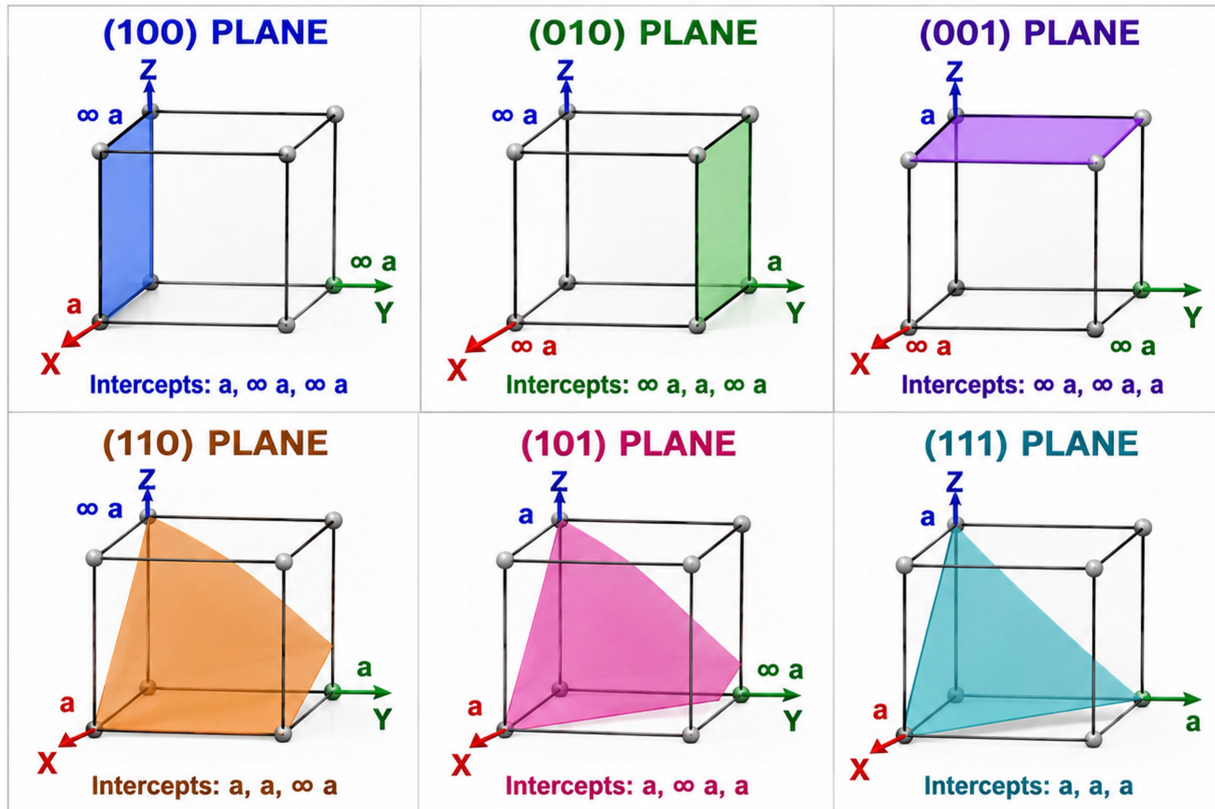
### Step 5

Write the integers inside parentheses:

(hkl)

# CRYSTALLOGRAPHIC PLANES

## PLANES IN A CUBIC CRYSTAL SYSTEM



### IMPORTANT POINTS

- A crystallographic plane is represented by **Miller indices** ( $h\ k\ l$ ) written in parentheses ( $hkl$ ).
- The indices are the reciprocals of the intercepts of the plane with the crystallographic axes (in units of  $a$ ).
- If a plane is parallel to an axis, its intercept is  $\infty$  (infinity) and the corresponding Miller index is 0.
- Clearer high-contrast colors are used to easily visualize each plane.

### 24. MILLER INDEX EXAMPLE — PLANE (111)

Suppose a plane intercepts all three axes at:

$a, b, c$

In fractional units:

$(1, 1, 1)$

Take reciprocals:

$(1/1, 1/1, 1/1)$

Therefore:

$(1, 1, 1)$

Hence:

$(111)$

### 25. MILLER INDEX EXAMPLE — PLANE (100)

Suppose a plane:

- intersects x-axis at a;
- is parallel to y-axis;
- is parallel to z-axis.

The intercepts are:

$(1, \infty, \infty)$

Take reciprocals:

$(1, \infty^{-1}, \infty^{-1})$

Since:

$$\infty^{-1} = 0$$

we obtain:

$(100)$

### **Important rule**

A plane parallel to an axis has an infinite intercept along that axis, and its corresponding Miller index is zero.

### **26. MILLER INDEX EXAMPLE — PLANE (110)**

Suppose the plane intercepts:

$$x=a \ y=b$$

and is parallel to z.

Therefore:

Intercepts= $(1, 1, \infty)$

Reciprocals:

$(1, 1, 0)$

Therefore:

$(110)$

### **27. NEGATIVE MILLER INDICES**

If a plane intercepts an axis on the negative side, the corresponding Miller index is negative.

A negative Miller index is represented using a bar.

For example:

$(1^{-1}0)$

means:

$h=-1, k=1, l=0$

## 28. IMPORTANT RULES FOR MILLER INDICES

Remember these rules:

### Rule 1

Miller indices are written in:

$(hkl)$

### Rule 2

They are obtained from the **reciprocals of intercepts**.

### Rule 3

Fractions are converted to the smallest whole numbers.

### Rule 4

An infinite intercept gives:

0

### Rule 5

Negative intercept  $\rightarrow$  negative Miller index shown by a bar.

## 29. PLANE (100)

The (100) plane:

- cuts the x-axis;
- is parallel to y;
- is parallel to z.

Therefore it is perpendicular to the x-axis.

## 30. PLANE (110)

The (110) plane:

- cuts x-axis;
- cuts y-axis;
- is parallel to z-axis.

Therefore it appears as a vertical diagonal plane in a cubic cell.

### 31. PLANE (111)

The (111) plane cuts all three axes at equal distances.

Therefore:

$$x=a, y=b, z=c$$

for a cubic cell.

It is an inclined triangular plane within the cube.

### Lecture-16

### 32. VERY IMPORTANT: (hkl) IS NOT [uvw]

Students frequently confuse these two notations.

| Symbol | Meaning                         |
|--------|---------------------------------|
| (hkl)  | One crystallographic plane      |
| {hkl}  | Family of equivalent planes     |
| [uvw]  | One crystallographic direction  |
| ⟨uvw⟩  | Family of equivalent directions |

#### Easy memory trick

**Square brackets → Direction**

[uvw]

**Round brackets → Plane**

(hkl)

**Angle brackets → Direction family**

⟨uvw⟩

**Curly brackets → Plane family**

{hkl}

### 33. FAMILY OF PLANES

Equivalent crystallographic planes are represented using:

{hkl}

For example:

{100}

represents the family of equivalent (100)-type planes.

In cubic crystals:

(100), (010), (001)

are equivalent members of the {100} family.

#### 34. IMPORTANT NOTATION TABLE

| Notation              | Meaning                         | Example                                     |
|-----------------------|---------------------------------|---------------------------------------------|
| (hkl)                 | Specific plane                  | (111)                                       |
| {hkl}                 | Family of equivalent planes     | {111}                                       |
| [uvw]                 | Specific direction              | [110]                                       |
| $\langle uvw \rangle$ | Family of equivalent directions | $\langle 110 \rangle$                       |
| (x,y,z)               | Point coordinate                | ( $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ ) |

#### 35. RELATIONSHIP BETWEEN PLANES AND DIRECTIONS

In a **cubic crystal**, an important relationship exists:

$[hkl] \perp (hkl)$

That is, the direction [hkl] is normal to the plane (hkl).

##### Example

For plane:

(111)

the normal direction is:

[111]

Similarly:

$(100) \perp [100]$

and:

$(110) \perp [110]$

##### Important qualification

This direct numerical relationship between plane indices and a normal direction is particularly straightforward for **cubic crystals**. It should not be blindly applied to all crystal systems.

#### 36. ANGLE BETWEEN CRYSTALLOGRAPHIC DIRECTIONS

For cubic crystals, the angle between two directions:

$$[u_1 v_1 w_1]$$

and

$$[u_2 v_2 w_2]$$

can be calculated using:

$$\cos \theta = \frac{u_1 u_2 + v_1 v_2 + w_1 w_2}{\sqrt{u_1^2 + v_1^2 + w_1^2} \sqrt{u_2^2 + v_2^2 + w_2^2}}$$

This is useful for advanced numerical problems.

### 37. EXAMPLE: ANGLE BETWEEN [100] AND [110]

For:

$$[100]$$

and:

$$[110]$$

we have:

$$u_1 = 1, \quad v_1 = 0, \quad w_1 = 0$$

and:

$$u_2 = 1, \quad v_2 = 1, \quad w_2 = 0$$

Therefore:

$$\cos \theta = \frac{1}{\sqrt{1} \sqrt{2}}$$

$$\cos \theta = \frac{1}{\sqrt{2}}$$

Hence:

$$\theta = 45^\circ$$

### 38. ANGLE BETWEEN [100] AND [111]

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

Therefore:

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

Hence:

$$\theta \approx 54.74^\circ$$

### 39. WHY CRYSTALLOGRAPHIC DIRECTIONS AND PLANES MATTER IN METALLURGY

These concepts are not merely mathematical notation.

They are fundamental to understanding:

#### **Plastic deformation**

Slip occurs on specific:

slip planes + slip directions

#### **Cleavage**

Some crystals fracture preferentially along particular planes.

#### **Diffusion**

Atomic diffusion can be faster along certain crystallographic paths.

#### **Crystal growth**

Growth rates may vary with crystallographic orientation.

#### **Anisotropy**

Properties can vary with crystallographic direction.

#### **X-ray diffraction**

Crystal planes are fundamental to diffraction analysis.

### 40. CRYSTALLOGRAPHY AND SLIP

Plastic deformation in crystalline metals commonly occurs through the movement of dislocations along favourable crystallographic systems.

A **slip system** consists of:

Slip plane+Slip direction

For FCC metals, the close-packed planes and directions are especially important.

The standard FCC close-packed plane family is:



$\{111\}$

and close-packed direction family:

$\langle 110 \rangle$

Thus the principal FCC slip systems are:

$\{111\}\langle 110 \rangle$

This is one reason crystallographic planes and directions are essential in Metallurgy.

#### **41. COMMON CONFUSIONS**

##### **Confusion 1: Point coordinate vs direction**

$(1/2, 1/2, 1/2)$

is a **point coordinate**.

$[111]$

is a **direction**.

##### **Confusion 2: Direction vs plane**

$[110]$

is a direction.

$(110)$

is a plane.

##### **Confusion 3: Direction family vs plane family**

$\langle 110 \rangle$

is a family of directions.

$\{110\}$

is a family of planes.

##### **Confusion 4: Coordinates vs Miller indices**

Point coordinates:

$(x, y, z)$

Miller indices:

$(hkl)$

They are obtained using completely different procedures.

#### **42. MASTER PROCEDURE — POINT COORDINATES**

To specify a point:

**Step 1**

Choose the origin.

**Step 2**

Measure the fractional distance along x.

**Step 3**

Measure the fractional distance along y.

**Step 4**

Measure the fractional distance along z.

**Step 5**

Write:

$(x,y,z)$

**43. MASTER PROCEDURE — CRYSTALLOGRAPHIC DIRECTION**

To determine  $[uvw]$ :

**Step 1**

Identify initial point.

**Step 2**

Identify final point.

**Step 3**

Subtract:

Final–Initial

**Step 4**

Reduce to smallest integers.

**Step 5**

Use square brackets:

$[uvw]$

**44. MASTER PROCEDURE — MILLER INDICES**

To determine  $(hkl)$ :

**Step 1**

Find x, y and z intercepts.

**Step 2**

Express them in terms of a,b,c.

**Step 3**

Take reciprocals.

**Step 4**

Clear fractions.

**Step 5**

Reduce to smallest integers.

**Step 6**

Write in parentheses:

(hkl)

**45. ONE COMPLETE EXAMPLE**

Suppose a plane intersects the crystallographic axes at:

$$x=2a \ y=3b$$

and is parallel to the z-axis.

**Step 1: Intercepts**

(2,3,∞)

**Step 2: Reciprocals**

(1/2,1/3,0)

**Step 3: Clear fractions**

LCM of 2 and 3 is 6.

Therefore:

$$(1/2,1/3,0) \times 6$$

gives:

(3,2,0)

Therefore the Miller indices are:

(320)

---

#### 46. ANOTHER EXAMPLE: NEGATIVE INTERCEPT

Suppose a plane has intercepts:

$$(-a, b, c)$$

Then:

$$(-1, 1, 1)$$

Reciprocals:

$$(-1, 1, 1)$$

Therefore:

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

The bar over 1 indicates a negative index.

#### 47. IMPORTANT EXAMINATION POINTS

Students should remember:

##### Point coordinates

$$(x, y, z)$$

##### Direction

$$[uvw]$$

##### Direction family

$$\langle uvw \rangle$$

##### Plane

$$(hkl)$$

##### Plane family

$$\{hkl\}$$

##### Miller indices

Reciprocals of intercepts

##### Parallel axis

$$\infty \rightarrow 0$$

##### Negative intercept

bar over index

#### 48. QUICK COMPARISON TABLE

| Feature       | Point Coordinates   | Direction                 | Plane                    |
|---------------|---------------------|---------------------------|--------------------------|
| Purpose       | Locate a point      | Specify orientation       | Specify plane            |
| Notation      | $(x,y,z)$           | $[uvw]$                   | $(hkl)$                  |
| Determination | Fractional position | Difference of coordinates | Reciprocal of intercepts |
| Brackets      | Parentheses         | Square brackets           | Round brackets           |
| Example       | $(1/2, 1/2, 1/2)$   | $[111]$                   | $(111)$                  |

#### 49. HIGH-YIELD REVISION TABLE

| Concept               | Must Remember                                               |
|-----------------------|-------------------------------------------------------------|
| Point coordinate      | $(x,y,z)$                                                   |
| One direction         | $[uvw]$                                                     |
| Direction family      | $\langle uvw \rangle$                                       |
| One plane             | $(hkl)$                                                     |
| Plane family          | $\{hkl\}$                                                   |
| Direction calculation | Final – Initial                                             |
| Plane calculation     | Intercepts $\rightarrow$ Reciprocals $\rightarrow$ Integers |
| Infinite intercept    | Index = 0                                                   |
| Negative value        | Use overbar                                                 |
| Cubic plane normal    | $[hkl] \perp (hkl)$                                         |
| FCC slip plane        | $\{111\}$                                                   |
| FCC slip direction    | $\langle 110 \rangle$                                       |

## 50. SHORT VIVA QUESTIONS

1. What is a crystallographic coordinate system?
2. Define point coordinates.
3. What does  $(x,y,z)$  represent?
4. What is a crystallographic direction?
5. What notation is used for a crystallographic direction?
6. What is the meaning of  $[100]$ ?
7. What is the meaning of  $[111]$ ?
8. What are direction indices?
9. What is a Miller index?
10. What notation is used for a crystal plane?
11. What is the procedure for finding Miller indices?
12. Why is the reciprocal taken while determining Miller indices?
13. What does an infinite intercept represent?
14. What Miller index corresponds to an infinite intercept?
15. How is a negative Miller index represented?
16. What is the difference between  $[uvw]$  and  $\langle uvw \rangle$ ?
17. What is the difference between  $(hkl)$  and  $\{hkl\}$ ?
18. In a cubic crystal, what is the normal direction to the  $(111)$  plane?
19. What is the FCC slip plane family?
20. What is the FCC slip direction family?

## 51. 2-MARK EXAMINATION QUESTIONS

1. Define point coordinates in a crystal.
2. What is meant by a crystallographic direction?
3. Define crystallographic direction indices.
4. What is a crystallographic plane?
5. Define Miller indices.
6. What is the notation used for a crystallographic direction?
7. What is the notation used for a crystallographic plane?

8. What does the notation  $[uvw]$  represent?
9. What does the notation  $(hkl)$  represent?
10. What is meant by  $\langle uvw \rangle$ ?
11. What is meant by  $\{hkl\}$ ?
12. State the difference between  $[uvw]$  and  $(hkl)$ .
13. What does an infinite intercept mean while determining Miller indices?
14. What Miller index is assigned to a plane parallel to an axis?
15. How is a negative Miller index represented?
16. State the procedure for determining direction indices.
17. State the procedure for determining Miller indices.
18. What is the crystallographic direction along the body diagonal of a cubic unit cell?
19. What is the Miller index of a plane intercepting all three cubic axes at  $a, b, c$ ?
20. State the relationship between  $(hkl)$  and  $[hkl]$  in a cubic crystal.

## **52. 5-MARK EXAMINATION QUESTIONS**

1. Explain point coordinates in a cubic unit cell with suitable examples.
2. Explain the crystallographic coordinate system and lattice axes.
3. Describe the procedure for determining crystallographic direction indices.
4. Determine the direction indices of a line joining two specified points in a cubic unit cell.
5. Explain positive and negative crystallographic directions with suitable examples.
6. Differentiate between a specific crystallographic direction and a family of directions.
7. Define Miller indices and explain their significance.
8. Explain the step-by-step procedure for determining Miller indices of a crystal plane.
9. Explain the significance of zero and negative Miller indices.
10. Determine the Miller indices of planes having specified intercepts.
11. Differentiate between  $[uvw]$ ,  $\langle uvw \rangle$ ,  $(hkl)$  and  $\{hkl\}$ .
12. Explain the significance of crystallographic planes and directions in Metallurgical Engineering.
13. Explain the relationship between a plane and its normal direction in cubic crystals.
14. Explain the  $(100)$ ,  $(110)$  and  $(111)$  planes in a cubic crystal.
15. Explain how crystallographic directions and planes are related to slip in metals.

## **53. 10-MARK EXAMINATION QUESTIONS**

**Q1.**

**Define point coordinates. Explain the crystallographic coordinate system and describe how the position of a point is represented in a cubic unit cell with suitable examples.**

**Q2.**

What are crystallographic directions? Explain the complete procedure for determining direction indices  $[uvw]$ , including the treatment of fractional and negative coordinates.

Q3.

Explain crystallographic planes and Miller indices in detail. Describe the complete step-by-step procedure for determining Miller indices from the intercepts of a plane.

Q4.

Determine the Miller indices of a plane having intercepts  $(2a)$ ,  $(3b)$ , and  $(c)$ . Explain every step of the calculation.

Q5.

Explain the meaning and significance of the following crystallographic notations with suitable examples:

$$(x, y, z), \quad [uvw], \quad \langle uvw \rangle, \quad (hkl), \quad \{hkl\}$$

Q6.

Explain the  $((100))$ ,  $((110))$  and  $((111))$  planes of a cubic crystal with neat diagrams. Also state their corresponding normal directions.

Q7.

A direction joins the points  $P_1(1/2, 0, 1/2)$  and  $P_2(1, 1, 0)$ . Determine the crystallographic direction indices of the line. Show all calculation steps.

Q8.

A crystal plane has intercepts  $(2a)$ ,  $(3b)$  and is parallel to the  $c$ -axis. Determine its Miller indices and explain the significance of the zero index.

Q9.

Differentiate between point coordinates, crystallographic directions and crystallographic planes. Explain their notation, method of determination and engineering significance.

Q10.

Discuss the importance of crystallographic directions and planes in Metallurgical Engineering. Explain their role in slip, plastic deformation, cleavage, anisotropy and crystal growth.

#### 54. NUMERICAL PRACTICE QUESTIONS

##### Problem 1 — Point Coordinates

A point is located at:

- $(0.25a)$  along  $x$ ,



- (0.50b) along y,
- (0.75c) along z.

Write its point coordinates.

**Answer:**

$$(0.25, 0.50, 0.75)$$

### Problem 2 — Direction

A direction starts at:

$$P_1 = (0, 0, 0)$$

and ends at:

$$P_2 = (1, 1, 1)$$

Determine its direction indices.

**Answer:**

$$[111]$$

### Problem 3 — Direction with Fractions

A direction joins:

$$P_1 = (0, 0, 0)$$

to:

$$P_2 = \left(\frac{1}{2}, 1, \frac{1}{2}\right)$$

Determine the direction indices.

Difference:

$$\left(\frac{1}{2}, 1, \frac{1}{2}\right)$$

Multiply by 2:

$$(1, 2, 1)$$

Therefore:

$$[121]$$

#### Problem 4 — Miller Indices

A plane has intercepts:

$$a, \quad b, \quad \infty$$

Determine its Miller indices.

Reciprocals:

$$1, 1, 0$$

Therefore:

$$\boxed{(110)}$$

---

#### Problem 5 — Miller Indices

A plane has intercepts:

$$2a, \quad 3b, \quad \infty$$

Reciprocals:

$$\frac{1}{2}, \frac{1}{3}, 0$$

Multiply by 6:

$$3, 2, 0$$

Therefore:

$$\boxed{(320)}$$

### 55. TEACHING SUMMARY FOR STUDENTS

The entire lecture can be remembered through one sequence:

## POINT → DIRECTION → PLANE

### Point

Where is it?

$$(x, y, z)$$

### Direction

Which way does it point?

$$[uvw]$$

### Plane

Which plane is it?

$$(hkl)$$

Then remember the two families:

$$\langle uvw \rangle = \text{family of directions}$$

$$\{hkl\} = \text{family of planes}$$

And the two fundamental procedures:

### Direction

$$\text{Final point} - \text{Initial point} \rightarrow \text{smallest integers}$$

### Plane

$$\text{Intercepts} \rightarrow \text{Reciprocals} \rightarrow \text{smallest integers}$$

## 56. FINAL "MUST REMEMBER" BOX

### EXAM GOLDEN RULES

$(x, y, z) = \text{Point Coordinate}$

$[uvw] = \text{Specific Direction}$

$\langle uvw \rangle = \text{Family of Directions}$

$(hkl) = \text{Specific Plane}$

$\{hkl\} = \text{Family of Planes}$

$\text{Direction} = \text{Final} - \text{Initial}$

$\text{Miller indices} = \text{Reciprocals of intercepts}$

$\infty \text{ intercept} \rightarrow 0 \text{ index}$

$\text{Negative value} \rightarrow \text{bar over index}$

For cubic crystals:

$[hkl] \perp (hkl)$

and for FCC slip:

$\{111\} \langle 110 \rangle$

## Lecture-17

### UNIT-II: THE STRUCTURE OF CRYSTALLINE SOLIDS

#### Lecture Notes: Linear Density and Planar Density

**Course:** MTPC201 – Introduction to Materials Engineering

**Semester:** 3rd Semester Diploma in Metallurgical Engineering

**Topic:** Linear Density and Planar Density

#### 1. LEARNING OBJECTIVES

After completing this topic, students will be able to:

1. Define linear density.
2. Define planar density.
3. Explain the physical significance of linear and planar densities.
4. Calculate linear density along selected crystallographic directions.
5. Calculate planar density on selected crystallographic planes.
6. Determine the number of atoms contributing to a line or plane.

7. Understand the importance of atom-sharing fractions.
8. Calculate LD for SC, BCC and FCC structures.
9. Calculate PD for SC, BCC and FCC structures.
10. Identify closely packed directions and planes.
11. Relate atomic density to plastic deformation and slip.
12. Solve numerical examination problems involving LD and PD.

## 2. INTRODUCTION

In a crystalline solid, atoms are arranged in a regular and periodic manner.

However, atoms are **not equally densely distributed in every direction or on every plane**.

For example, in an FCC crystal:

- some directions contain atoms more closely packed than others;
- some planes contain a greater number of atoms per unit area than others.

This leads to two important crystallographic quantities:

### Linear Density

Measures the number of atoms along a particular crystallographic direction.

### Planar Density

Measures the number of atoms on a particular crystallographic plane.

Therefore:

Linear Density → 1-dimensional atomic density   Planar Density → 2-dimensional atomic density

They can be considered one- and two-dimensional analogues of the **Atomic Packing Factor (APF)**.

## 3. WHY DO WE STUDY LINEAR AND PLANAR DENSITY?

Linear and planar densities are important because crystal properties are often **direction-dependent**.

They help us understand:

- slip;
- plastic deformation;
- dislocation motion;
- cleavage;
- diffusion;

- crystal growth;
- anisotropy;
- surface behaviour;
- X-ray diffraction;
- crystallographic equivalence.

Most importantly for Metallurgical Engineering:

High atomic density → important slip directions/planes

In FCC metals, for example, slip occurs predominantly on:

$\{111\}\langle 110 \rangle$

because these constitute highly packed planes and directions.

## **PART-A**

### **LINEAR DENSITY**

#### **4. DEFINITION OF LINEAR DENSITY**

**Linear density (LD)** is defined as the number of atoms whose centres lie on a specified crystallographic direction per unit length of that direction.

Mathematically:

$LD = \frac{\text{Length of the direction vector}}{\text{Number of atoms centred on the direction}}$

The standard units are:

atoms/m

or:

atoms/nm

Numerically, since "atoms" is a count, LD is often reported simply as:

m<sup>-1</sup>

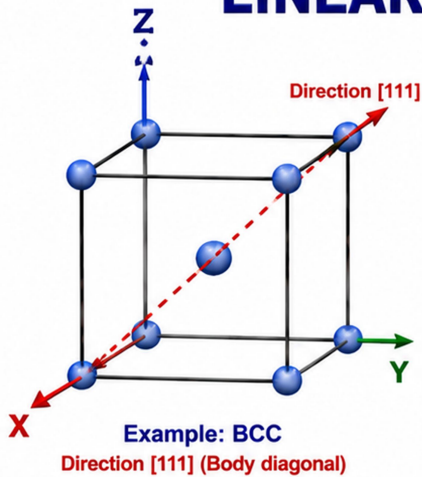
or:

nm<sup>-1</sup>

This definition follows the standard Callister treatment.

# LINEAR AND PLANAR DENSITIES

## LINEAR DENSITY (L.D.)



Linear density is the number of atom centers lying on a crystallographic direction per unit length.

### Formula

$$\text{L.D.} = \frac{\text{Number of atom centers lying on the direction}}{\text{Length of the direction (in units of } a \text{)}}$$

### For direction [111] in BCC

Atoms on [111] = 2 corner atoms (each contributes 1/2)

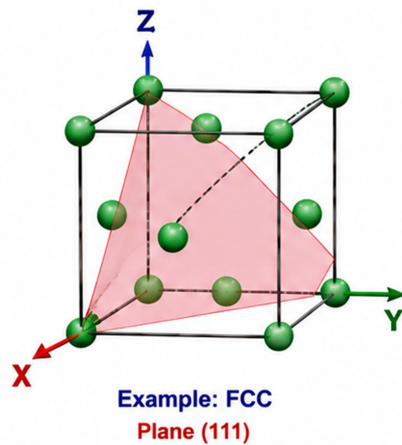
Total atoms = 1

Length of [111] =  $\sqrt{3} a$

$$\text{L.D.} = \frac{1}{\sqrt{3} a} = \frac{1}{1.732 a} = 0.577/a$$

## Linear Density in Common Directions

| Crystal | Direction | L.D. (atoms / a)       |
|---------|-----------|------------------------|
| BCC     | [100]     | 1                      |
|         | [110]     | $\sqrt{2} / 2 = 0.707$ |
|         | [111]     | $\sqrt{3} / 2 = 0.577$ |
| FCC     | [100]     | 1                      |
|         | [110]     | $\sqrt{2} = 1.414$     |
|         | [111]     | $\sqrt{3} = 1.732$     |



## PLANAR DENSITY (P.D.)

Planar density is the number of atom centers lying on a crystallographic plane per unit area of that plane.

### Formula

$$\text{P.D.} = \frac{\text{Number of atom centers lying on the plane}}{\text{Area of the plane (in units of } a^2 \text{)}}$$

### For plane (111) in FCC

Atoms on (111) plane:

• 3 corner atoms (each contributes 1/6) =  $3 \times \frac{1}{6} = \frac{1}{2}$

• 3 face center atoms (each contributes 1/2) =  $3 \times \frac{1}{2} = \frac{3}{2}$

Total atoms =  $\frac{1}{2} + \frac{3}{2} = 2$

Area of (111) plane =  $\frac{\sqrt{3}}{4} a^2$

$$\text{P.D.} = \frac{2}{(\sqrt{3}/4) a^2} = \frac{8}{\sqrt{3} a^2} = \frac{4.618}{a^2}$$

## Planar Density in Common Planes

| Crystal | Plane | P.D. (atoms / a <sup>2</sup> ) |
|---------|-------|--------------------------------|
| BCC     | (100) | 1                              |
|         | (110) | $\sqrt{2} / 2 = 0.707$         |
|         | (111) | $\sqrt{3} / 2 = 0.866$         |
| FCC     | (100) | 2                              |
|         | (110) | $\sqrt{2} = 1.414$             |
|         | (111) | $4\sqrt{3} / 3 = 2.309$        |

## KEY POINTS

- Linear density is a 1-dimensional density along a direction.
- Planar density is a 2-dimensional density on a plane.
- Consider atoms whose centers lie on the line or plane.
- Use fraction of contribution for corner, edge and face atoms.

- Corner atom (contribution: 1/8 in volume)
- Face center atom (contribution: 1/2 on face)
- Edge center atom (contribution: 1/4 on edge)

## 5. BASIC IDEA OF LINEAR DENSITY

Imagine drawing a straight line through the centres of atoms in a particular crystallographic direction.

For example:

[110]

The line may pass through:

- corner atoms;
- face-centred atoms;
- body-centred atoms,

depending on the crystal structure.

We count the **fractional contribution of atoms associated with the repeat length**, and divide by the length of that direction.

## 6. IMPORTANT POINT: COUNT ATOMS CAREFULLY

When calculating LD, do not simply count every visible atom.

Atoms at the ends of a direction vector are shared with adjacent repeat segments.

Therefore, fractional contributions must be considered.

For example, if two end atoms each contribute:

$$1/2$$

then total contribution is:

$$1/2 + 1/2 = 1$$

If an atom lies completely inside the selected line segment, its contribution is:

$$1$$

## 7. GENERAL PROCEDURE FOR LINEAR DENSITY

### Step 1

Identify the crystallographic direction.

Example:

$$[110]$$

### Step 2

Draw the direction vector through the unit cell.

### Step 3

Identify atoms whose centres lie on the direction.

### Step 4

Calculate the fractional contribution of each atom.

### Step 5

Calculate the length of the direction vector.

### Step 6

Use:

$$LD = N/L$$

where:

- $N$  = effective number of atoms;
- $L$  = length of direction vector.



## 8. IMPORTANT GEOMETRICAL LENGTHS IN A CUBIC UNIT CELL

For cubic lattice parameter  $a$ :

[100]

$$L_{100} = a$$

[110]

This is a face diagonal:

$$L_{110} = a\sqrt{2}$$

[111]

This is a body diagonal:

$$L_{111} = a\sqrt{3}$$

## 9. LINEAR DENSITY OF SC — [100]

Consider a simple cubic crystal.

The [100] direction runs along one cube edge.

At the two ends are two corner atoms.

Each contributes:

$$\frac{1}{2}$$

Therefore:

$$N = \frac{1}{2} + \frac{1}{2} = 1$$

Length:

$$L = a$$

Therefore:

$$LD_{[100]} = \frac{1}{a}$$

Hence:

$$LD_{[100]}^{SC} = \frac{1}{a}$$

## 10. LINEAR DENSITY OF BCC — [100]

For BCC, the [100] direction is still along a cube edge.

The body-centred atom does not lie on the [100] edge.

Thus:

$$N = 1$$

and:

$$L = a$$

Therefore:

$$LD_{[100]}^{BCC} = \frac{1}{a}$$

### Important observation

SC and BCC have the same [100] linear density:

$$LD_{[100]}^{SC} = LD_{[100]}^{BCC} = \frac{1}{a}$$

## 11. LINEAR DENSITY OF FCC — [100]

In FCC, the [100] direction is also along a cube edge.

The face-centred atoms are not located on the cube edge.

Therefore:

$$N = 1$$

Length:

$$L = a$$

Hence:

$$LD_{[100]}^{FCC} = \frac{1}{a}$$

Therefore:

$$LD_{[100]}^{SC} = LD_{[100]}^{BCC} = LD_{[100]}^{FCC} = \frac{1}{a}$$

## 12. LINEAR DENSITY OF SC — [110]

The [110] direction lies along a face diagonal.

Length:

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

Only the two corner atoms lie on the direction.

Their combined contribution is:

$$N = 1$$

Therefore:

$$LD = \frac{1}{a\sqrt{2}}$$

Hence:

$$LD_{[110]}^{SC} = \frac{1}{a\sqrt{2}}$$

### 13. LINEAR DENSITY OF BCC — [110]

The [110] direction lies along a face diagonal.

The body-centred atom is at:

$$\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$$

but the [110] face-diagonal direction has:

$$z = 0$$

for the selected face.

Therefore, the body-centred atom does not lie on this direction.

Effective number of atoms:

$$N = 1$$

Length:

$$a\sqrt{2}$$

Therefore:

$$LD_{[110]}^{BCC} = \frac{1}{a\sqrt{2}}$$

### 14. LINEAR DENSITY OF FCC — [110]

This is an especially important calculation.

The [110] direction is a face diagonal.

In FCC, there is a face-centred atom located directly on this diagonal.

The two corner atoms together contribute:

$$1$$

and the face-centred atom contributes:

$$1$$

Therefore:

$$N = 2$$

Length:

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

Thus:

$$LD = \frac{2}{a\sqrt{2}}$$

Therefore:

$$LD_{[110]}^{FCC} = \frac{\sqrt{2}}{a}$$

This is why  $\langle 110 \rangle$  is a highly packed direction in FCC. The standard Callister treatment similarly derives FCC [110] LD by counting the two effective atoms along the direction vector.

## 15. LINEAR DENSITY OF SC — [111]

The [111] direction is the body diagonal.

Length:

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

Only the two corner atoms lie on this line.

Their combined contribution:

$$N = 1$$

Therefore:

$$LD_{[111]}^{SC} = \frac{1}{a\sqrt{3}}$$

## 16. LINEAR DENSITY OF BCC — [111]

The [111] direction is the body diagonal.

It passes through:

- one corner atom;
- the body-centred atom;
- the opposite corner atom.

The two corner atoms together contribute:

$$1$$

The body-centred atom contributes:

$$1$$

Therefore:

$$N = 2$$

Length:

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

Thus:

$$LD_{[111]}^{BCC} = \frac{2}{a\sqrt{3}}$$

## 17. LINEAR DENSITY OF FCC — [111]

The [111] direction is the body diagonal.

The line passes through the two corner atoms but does not pass through face-centred atoms.

Thus:

$$N = 1$$

Length:

$$a\sqrt{3}$$

Therefore:

$$LD_{[111]}^{FCC} = \frac{1}{a\sqrt{3}}$$

## 18. MASTER TABLE — LINEAR DENSITY

For cubic structures:

| Direction | SC                    | BCC                   | FCC                   |
|-----------|-----------------------|-----------------------|-----------------------|
| [100]     | $\frac{1}{a}$         | $\frac{1}{a}$         | $\frac{1}{a}$         |
| [110]     | $\frac{1}{a\sqrt{2}}$ | $\frac{1}{a\sqrt{2}}$ | $\frac{\sqrt{2}}{a}$  |
| [111]     | $\frac{1}{a\sqrt{3}}$ | $\frac{2}{a\sqrt{3}}$ | $\frac{1}{a\sqrt{3}}$ |

This compact comparison is a useful examination table. Equivalent directions in a cubic structure have the same linear density.

## 19. LINEAR DENSITY IN TERMS OF ATOMIC RADIUS

For hard-sphere models:

### SC

Atoms touch along:

$$[100]$$

Therefore:

$$a = 2R$$

### BCC

Atoms touch along:

$$[111]$$

Therefore:

$$\sqrt{3}a = 4R$$

or:

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

### FCC

Atoms touch along:

$$[110]$$

Therefore:

$$\sqrt{2}a = 4R$$

or:

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

These relationships are extremely useful for converting LD expressions from  $a$  to  $R$ .

## Lecture-18

### PART-B

### PLANAR DENSITY

#### 20. DEFINITION OF PLANAR DENSITY

**Planar density (PD)** is the number of atoms whose centres lie on a specified crystallographic plane per unit area of that plane.

Mathematically:

$$PD = \frac{\text{Area of the plane}}{\text{Number of atoms centred on the plane}}$$

Units:

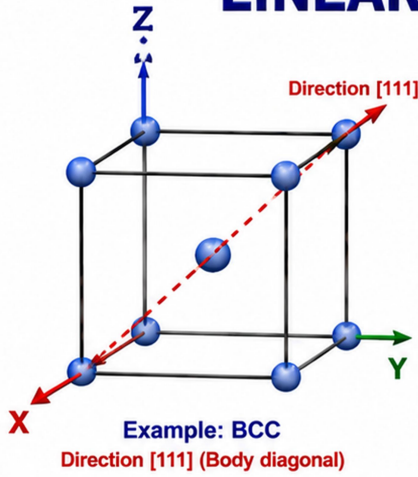
atoms/m<sup>2</sup>

or:

atoms/nm<sup>2</sup>

This is the standard crystallographic definition used in materials science.

## LINEAR AND PLANAR DENSITIES



**Example: BCC**  
Direction [111] (Body diagonal)

**LINEAR DENSITY (L.D.)**

Linear density is the number of atom centers lying on a crystallographic direction per unit length.

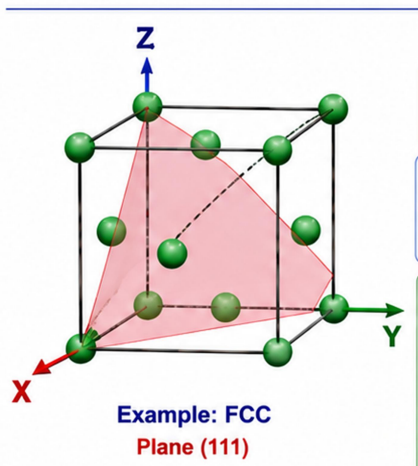
**Formula**

$$\text{L.D.} = \frac{\text{Number of atom centers lying on the direction}}{\text{Length of the direction (in units of } a\text{)}}$$

**For direction [111] in BCC**

Atoms on [111] = 2 corner atoms (each contributes 1/2)  
**Total atoms = 1**  
Length of [111] =  $\sqrt{3} a$   
$$\text{L.D.} = \frac{1}{\sqrt{3} a} = \frac{1}{1.732 a} = \mathbf{0.577/a}$$

| Crystal | Direction | L.D. (atoms / a)       |
|---------|-----------|------------------------|
| BCC     | [100]     | 1                      |
|         | [110]     | $\sqrt{2} / 2 = 0.707$ |
|         | [111]     | $\sqrt{3} / 2 = 0.577$ |
| FCC     | [100]     | 1                      |
|         | [110]     | $\sqrt{2} = 1.414$     |
|         | [111]     | $\sqrt{3} = 1.732$     |



**Example: FCC**  
Plane (111)

**PLANAR DENSITY (P.D.)**

Planar density is the number of atom centers lying on a crystallographic plane per unit area of that plane.

**Formula**

$$\text{P.D.} = \frac{\text{Number of atom centers lying on the plane}}{\text{Area of the plane (in units of } a^2\text{)}}$$

**For plane (111) in FCC**

Atoms on (111) plane:

- 3 corner atoms (each contributes 1/6) =  $3 \times \frac{1}{6} = \frac{1}{2}$
- 3 face center atoms (each contributes 1/2) =  $3 \times \frac{1}{2} = \frac{3}{2}$

**Total atoms =  $\frac{1}{2} + \frac{3}{2} = 2$**

Area of (111) plane =  $\frac{\sqrt{3}}{4} a^2$   
$$\text{P.D.} = \frac{2}{(\sqrt{3}/4) a^2} = \frac{8}{\sqrt{3} a^2} = \mathbf{\frac{4.618}{a^2}}$$

| Crystal | Plane | P.D. (atoms / a <sup>2</sup> ) |
|---------|-------|--------------------------------|
| BCC     | (100) | 1                              |
|         | (110) | $\sqrt{2} / 2 = 0.707$         |
|         | (111) | $\sqrt{3} / 2 = 0.866$         |
| FCC     | (100) | 2                              |
|         | (110) | $\sqrt{2} = 1.414$             |
|         | (111) | $4\sqrt{3} / 3 = 2.309$        |

**KEY POINTS**

- Linear density is a 1-dimensional density along a direction.
- Planar density is a 2-dimensional density on a plane.
- Consider atoms whose centers lie on the line or plane.
- Use fraction of contribution for corner, edge and face atoms.

 Corner atom (contribution: 1/8 in volume)  
 Face center atom (contribution: 1/2 on face)  
 Edge center atom (contribution: 1/4 on edge)

### 21. BASIC IDEA OF PLANAR DENSITY

Imagine selecting a particular plane inside a crystal.

For example:

(100)

Atoms whose **centres lie exactly in that plane** are counted.

The number of atoms is then divided by the area of the selected planar repeat region.



Therefore:

$$PD = N/A$$

where:

- $N$  = effective number of atoms in the plane;
- $A$  = area of the selected planar region.

## **22. IMPORTANT RULE: COUNT ONLY ATOMS ON THE PLANE**

This is one of the most common mistakes.

While calculating PD:

**Count the centres of atoms that lie in the plane, not atoms merely touching or overlapping the plane in a drawing.**

The selected plane should be treated as passing through the relevant atom centres.

## **23. ATOM SHARING IN PLANAR DENSITY**

When counting atoms on a plane, atoms may lie:

- at the corner of the planar region;
- along the edge;
- inside the planar region.

Their contributions are different.

For a rectangular planar repeat region:

### **Corner atom**

Usually contributes:

$\frac{1}{4}$

because four planar regions share it.

### **Edge atom**

Usually contributes:

$\frac{1}{2}$

### **Interior atom**

Contributes:

1

These fractions depend on the geometry of the chosen planar repeat region.

## **24. GENERAL PROCEDURE FOR PLANAR DENSITY**

### **Step 1**

Identify the plane:

(hkl)

### **Step 2**

Draw the plane through the unit cell.

### **Step 3**

Identify all atoms whose centres lie on the plane.

### **Step 4**

Determine the fractional contribution of each atom.

### **Step 5**

Calculate the area of the planar region.

### **Step 6**

Use:

$$PD = N/A$$

## **25. PLANAR DENSITY OF SC — (100)**

Consider the (100) plane of a simple cubic crystal.

It is a square plane.

Side length:

$$a$$

Area:

$$A = a^2$$

There are four corner atoms.

Each contributes:

$$\frac{1}{4}$$

Therefore:

$$N = 4 \left( \frac{1}{4} \right) = 1$$

Thus:

$$PD = \frac{1}{a^2}$$

Hence:

$$PD_{(100)}^{SC} = \frac{1}{a^2}$$

## 26. PLANAR DENSITY OF BCC — (100)

For BCC (100), the body-centred atom is not on the (100) plane.

Only the four corner atoms contribute.

Therefore:

$$N = 4 \left( \frac{1}{4} \right) = 1$$

Area:

$$a^2$$

Thus:

$$PD_{(100)}^{BCC} = \frac{1}{a^2}$$

## 27. PLANAR DENSITY OF FCC — (100)

For FCC (100):

- four corner atoms are present;
- one face-centred atom lies at the centre of the face.

Corner contribution:

$$4 \times \frac{1}{4} = 1$$

Face-centred atom:

$$1$$

Total:

$$N = 2$$

Area:

$$a^2$$

Therefore:

$$PD_{(100)}^{FCC} = \frac{2}{a^2}$$

## 28. PLANAR DENSITY OF SC — (110)

The (110) plane forms a rectangle.

Its dimensions are:

$$a$$

and:

$$a\sqrt{2}$$

Therefore:

$$A = a(a\sqrt{2})$$

$$A = a^2\sqrt{2}$$

Only corner atoms lie on the plane.

Effective number:

$$N = 1$$

Therefore:

$$PD = \frac{1}{a^2\sqrt{2}}$$

Hence:

$$PD_{(110)}^{SC} = \frac{1}{\sqrt{2}a^2}$$

## 29. PLANAR DENSITY OF BCC — (110)

This is a particularly important BCC plane.

The (110) plane contains:

- four corner atoms;
- the body-centred atom.

Corner contribution:

$$4 \times \frac{1}{4} = 1$$

Body-centred atom:

$$1$$

Total:

$$N = 2$$

Area:

$$A = a^2\sqrt{2}$$

Therefore:

$$PD = \frac{2}{a^2\sqrt{2}}$$

Hence:

$$\boxed{PD_{(110)}^{BCC} = \frac{\sqrt{2}}{a^2}}$$

This is one of the most important numerical results for BCC.

## 30. PLANAR DENSITY OF FCC — (110)

For FCC (110), the planar region contains:

- corner atoms;
- appropriate face-centred atoms lying on the plane.

The effective number of atoms is:

$$N = 2$$

and the rectangular plane area is:

$$A = a^2\sqrt{2}$$

Therefore:

$$PD = \frac{2}{a^2\sqrt{2}}$$

Hence:

$$\boxed{PD_{(110)}^{FCC} = \frac{\sqrt{2}}{a^2}}$$

Thus, the (110) planar density has the same expression for BCC and FCC when expressed in terms of the same lattice parameter  $a$ .

### 31. PLANAR DENSITY OF SC — (111)

The (111) plane forms an equilateral triangular region.

Its side length is:

$$a\sqrt{2}$$

Area of an equilateral triangle:

$$A = \frac{\sqrt{3}}{4} s^2$$

Therefore:

$$A = \frac{\sqrt{3}}{4} (a\sqrt{2})^2$$

$$A = \frac{\sqrt{3}}{4} (2a^2)$$

$$A = \frac{\sqrt{3}}{2} a^2$$

Three corner atoms lie on the triangular plane.

Each contributes:

$$\frac{1}{6}$$

Therefore:

$$N = 3 \left( \frac{1}{6} \right) = \frac{1}{2}$$

Thus:

$$PD = \frac{1/2}{(\sqrt{3}/2)a^2}$$

Therefore:

$$PD_{(111)}^{SC} = \frac{1}{\sqrt{3}a^2}$$

### 32. PLANAR DENSITY OF BCC — (111)

The BCC body-centred atom does not lie on the (111) plane selected through the three relevant corners.

Thus only three corner atoms contribute.

$$N = \frac{1}{2}$$

Area:

$$A = \frac{\sqrt{3}}{2}a^2$$

Therefore:

$$PD_{(111)}^{BCC} = \frac{1}{\sqrt{3}a^2}$$

### 33. PLANAR DENSITY OF FCC — (111)

The FCC (111) plane is particularly important because it is a **close-packed plane**.

The triangular planar region contains:

- three corner atoms;
- three face-centred atoms.

Effective number of atoms:

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

$$N = \frac{1}{2} + \frac{3}{2}$$

$$N = 2$$

Area:

$$A = \frac{\sqrt{3}}{2}a^2$$

Therefore:

$$PD = \frac{2}{(\sqrt{3}/2)a^2}$$

Hence:

$$PD_{(111)}^{FCC} = \frac{4}{\sqrt{3}a^2}$$

This is the highest planar density among the common cubic planes considered here.



34. MASTER TABLE — PLANAR DENSITY

| For the common cubic planes: |                         |                         |
|------------------------------|-------------------------|-------------------------|
| Plane                        | SC                      | BCC                     |
| (100)                        | $\frac{1}{a^2}$         | $\frac{1}{a^2}$         |
| (110)                        | $\frac{1}{\sqrt{2}a^2}$ | $\frac{\sqrt{2}}{a^2}$  |
| (111)                        | $\frac{1}{\sqrt{3}a^2}$ | $\frac{1}{\sqrt{3}a^2}$ |

### 35. COMPARISON OF LINEAR DENSITY

For a cubic crystal:

$$LD_{[100]} = \frac{1}{a}$$

$$LD_{[110]} = \frac{1}{a\sqrt{2}} \quad \text{for SC/BCC}$$

but:

$$LD_{[110]}^{FCC} = \frac{\sqrt{2}}{a}$$

For BCC:

$$LD_{[111]} = \frac{2}{a\sqrt{3}}$$

Therefore:

[111] is a highly packed direction in BCC

For FCC:

[110] is a highly packed direction

### 36. COMPARISON OF PLANAR DENSITY

For FCC:

$$PD_{(111)} = \frac{4}{\sqrt{3}a^2}$$

which is significantly larger than:

$$PD_{(100)} = \frac{2}{a^2}$$

and:

$$PD_{(110)} = \frac{\sqrt{2}}{a^2}$$

Thus:

(111) is the close-packed plane in FCC

### 37. CLOSE-

#### PACKED DIRECTIONS

A close-packed direction is a crystallographic direction having a particularly high linear density.

#### SC

No exceptionally dense direction comparable to FCC/BCC close-packed directions.

#### BCC

$\langle 111 \rangle$

is the most densely packed direction.

### **FCC**

$\langle 110 \rangle$

is the close-packed direction.

### **38. CLOSE-PACKED PLANES**

#### **FCC**

$\{111\}$

is the close-packed plane family.

#### **HCP**

The basal plane:

(0001)

is the close-packed plane.

#### **BCC**

BCC does not possess a truly close-packed plane in the same sense as FCC/HCP, although  $\{110\}$  planes are relatively dense.

### **39. RELATIONSHIP TO SLIP**

Plastic deformation of crystalline metals occurs primarily through **slip**, which involves the movement of dislocations.

A slip system consists of:

Slip plane+Slip direction

The most densely packed plane and direction combinations generally offer favourable pathways for dislocation motion.

For FCC:

$\{111\}\langle 110 \rangle$

There are 12 primary FCC slip systems.

This explains why FCC metals such as:

- aluminium;
- copper;
- nickel;

are generally quite ductile.

#### 40. LINEAR DENSITY VS PLANAR DENSITY

| Feature            | Linear Density              | Planar Density                          |
|--------------------|-----------------------------|-----------------------------------------|
| Dimension          | 1-D                         | 2-D                                     |
| Measures           | Atoms along direction       | Atoms on plane                          |
| Formula            | $N/L$                       | $N/A$                                   |
| Direction notation | $[uvw]$                     | —                                       |
| Plane notation     | —                           | $(hkl)$                                 |
| Unit               | atoms/m                     | atoms/m <sup>2</sup>                    |
| Main significance  | Atomic packing along a line | Atomic packing on a plane               |
| Application        | Slip direction, diffusion   | Slip plane, cleavage, surface behaviour |

#### 41. LINEAR DENSITY VS ATOMIC PACKING FACTOR

These terms should not be confused.

##### Linear Density

$LD = \text{atoms on direction} / \text{length}$

##### Planar Density

$PD = \text{atoms on plane} / \text{area}$

##### Atomic Packing Factor

$APF = \text{volume occupied by atoms} / \text{volume of unit cell}$

Thus:

- $LD \rightarrow$  one-dimensional;
- $PD \rightarrow$  two-dimensional;
- $APF \rightarrow$  three-dimensional.

## 42. IMPORTANT NUMERICAL CONCEPT

Suppose:

$$a = 0.4 \text{ nm}$$

For FCC [110]:

$$LD = \frac{\sqrt{2}}{a}$$

Therefore:

$$LD = \frac{1.414}{0.4}$$

$$LD \approx 3.535 \text{ atoms/nm}$$

This means that, on average according to the crystallographic counting convention, approximately 3.535 atom-centres occur per nanometre along that direction.

### 43. SOLVED NUMERICAL EXAMPLE 1

#### Question

Calculate the linear density along the [111] direction for BCC crystal having:

$$a = 0.2866 \text{ nm}$$

#### Solution

For BCC:

$$LD_{[111]} = \frac{2}{a\sqrt{3}}$$

Substitute:

$$LD = \frac{2}{0.2866\sqrt{3}}$$

$$LD \approx 4.03 \text{ atoms/nm}$$

Therefore:

|                                            |
|--------------------------------------------|
| $LD_{[111]} \approx 4.03 \text{ atoms/nm}$ |
|--------------------------------------------|

---

### 44. SOLVED NUMERICAL EXAMPLE 2

#### Question

Calculate the linear density along [110] in an FCC crystal with:

$$a = 0.3615 \text{ nm}$$

#### Solution

For FCC:

$$LD_{[110]} = \frac{\sqrt{2}}{a}$$

Therefore:

$$LD = \frac{1.414}{0.3615}$$

|                                    |
|------------------------------------|
| $LD \approx 3.91 \text{ atoms/nm}$ |
|------------------------------------|

## 45. SOLVED NUMERICAL EXAMPLE 3

### Question

Calculate the planar density of the FCC (111) plane for:

$$a = 0.3615 \text{ nm}$$

### Solution

For FCC (111):

$$PD_{(111)} = \frac{4}{\sqrt{3}a^2}$$

Substituting:

$$PD = \frac{4}{\sqrt{3}(0.3615)^2}$$

$$PD \approx 17.68 \text{ atoms/nm}^2$$

## 46. SOLVED NUMERICAL EXAMPLE 4

### Question

Calculate the planar density of BCC (110) plane when:

$$a = 0.2866 \text{ nm}$$

### Solution

For BCC (110):

$$PD_{(110)} = \frac{\sqrt{2}}{a^2}$$

Therefore:

$$PD = \frac{1.414}{(0.2866)^2}$$

$$PD \approx 17.22 \text{ atoms/nm}^2$$

## 47. VERY IMPORTANT EXAMINATION TECHNIQUE

When solving LD or PD problems, **always write the following three things first:**

### 1. Structure

SC / BCC / FCC

### 2. Direction or plane

Example:

[110]

or:

(111)

### **3. General formula**

For example:

$$LD=N/a$$

or:

$$PD=N/A$$

Then substitute numerical values.

This makes the calculation easy to follow and reduces errors.

### **48. COMMON MISTAKES**

#### **Mistake 1**

Counting every visible atom as one atom.

**Correction:** Apply appropriate fractional sharing.

#### **Mistake 2**

Using cube edge  $a$  for every direction.

Incorrect for:

[110],[111]

Remember:

[110]→ $a/2$  [111]→ $a/3$

#### **Mistake 3**

Confusing LD and PD.

LD:

Atoms/length

PD:

atoms/area

#### **Mistake 4**

Counting atoms that are near the plane but whose centres are not in it.

#### **Mistake 5**

Confusing plane notation with direction notation.



$$[110] = (110)$$

#### 49. HIGH-YIELD FORMULA SHEET

##### Linear Density

$$LD = \frac{N}{L}$$

##### Direction lengths

$$L_{100} = a$$

$$L_{110} = a\sqrt{2}$$

$$L_{111} = a\sqrt{3}$$

---

##### Planar Density

$$PD = \frac{N}{A}$$

##### Common plane areas

For (100):

$$A = a^2$$

For (110):

$$A = a^2\sqrt{2}$$

For (111):

$$A = \frac{\sqrt{3}}{2}a^2$$

#### 50. MASTER FORMULA TABLE

| Linear Density |                 |                         |                         |
|----------------|-----------------|-------------------------|-------------------------|
| Structure      | [100]           | [110]                   | [111]                   |
| SC             | $\frac{1}{a}$   | $\frac{1}{\sqrt{2}a}$   | $\frac{1}{\sqrt{3}a}$   |
| BCC            | $\frac{1}{a}$   | $\frac{1}{\sqrt{2}a}$   | $\frac{2}{\sqrt{3}a}$   |
| FCC            | $\frac{1}{a}$   | $\frac{\sqrt{2}}{a}$    | $\frac{1}{\sqrt{3}a}$   |
| Planar Density |                 |                         |                         |
| Structure      | (100)           | (110)                   | (111)                   |
| SC             | $\frac{1}{a^2}$ | $\frac{1}{\sqrt{2}a^2}$ | $\frac{1}{\sqrt{3}a^2}$ |
| BCC            | $\frac{1}{a^2}$ | $\frac{\sqrt{2}}{a^2}$  | $\frac{1}{\sqrt{3}a^2}$ |
| FCC            | $\frac{2}{a^2}$ | $\frac{\sqrt{2}}{a^2}$  | $\frac{4}{\sqrt{3}a^2}$ |

## 51. ENGINEERING SIGNIFICANCE

Linear and planar density provide a quantitative way to describe the atomic packing of a crystal.

They help explain:

### 1. Plastic deformation

Dislocations tend to move along favourable crystallographic systems.

### 2. Slip

FCC:

$\{111\}\langle 110 \rangle$

### 3. Cleavage

Fracture may preferentially occur along planes of particular atomic bonding/packing characteristics.

### 4. Diffusion

Atomic movement may vary with crystallographic direction.

### 5. Anisotropy

Properties of single crystals can depend on orientation.

### 6. Surface behaviour

Surface energy and chemical activity may vary with crystallographic plane.

### 7. Crystal growth

Growth rates can depend on crystallographic orientation.

## 52. RELATION TO THE NEXT TOPIC: CLOSE-PACKED STRUCTURES

Linear and planar density provide the mathematical foundation for understanding **close-packed crystal structures**.

The important sequence is:

Crystal Structure → Direction/Plane → Atomic Density → Close Packing → Slip

For FCC:

$\langle 110 \rangle$  = close-packed directions

and:

$\{111\}$  = close-packed planes

For HCP:

(0001) = basal close-packed plane

This connects directly with the next Unit-II topic in the syllabus, **Close-Packed Crystal Structures**.

## 53. VIVA QUESTIONS

1. What is linear density?
2. What is planar density?
3. What are the units of linear density?
4. What are the units of planar density?
5. Write the formula for linear density.
6. Write the formula for planar density.
7. What is the length of the  $[110]$  direction in a cubic unit cell?
8. What is the length of the  $[111]$  direction?
9. Which is the close-packed direction in FCC?
10. Which is the close-packed direction in BCC?
11. Which is the close-packed plane in FCC?
12. Why are fractional atoms counted in LD and PD calculations?
13. What is the linear density of FCC  $[110]$ ?
14. What is the planar density of FCC  $(111)$ ?
15. Why is FCC  $(111)$  called a close-packed plane?
16. What is the difference between LD and PD?

17. What is the relationship between LD and crystal anisotropy?
18. What is the FCC slip system?
19. What is meant by a slip system?
20. Why are LD and PD important in Metallurgical Engineering?

#### **54. 2-MARK EXAMINATION QUESTIONS**

**Q1.**

Define linear density and write its mathematical expression.

**Q2.**

Define planar density and write its mathematical expression.

**Q3.**

State the units of linear density and planar density.

**Q4.**

What is the length of the  $[110]$  direction in a cubic unit cell?

**Q5.**

What is the length of the  $[111]$  direction in a cubic unit cell?

**Q6.**

What is the linear density of the  $[100]$  direction in a cubic crystal?

**Q7.**

Which is the close-packed direction in FCC?

**Q8.**

Which is the close-packed direction in BCC?

**Q9.**

Which is the close-packed plane in FCC?

**Q10.**

What is the planar density of the FCC  $(111)$  plane?

**Q11.**

Why are fractional atom contributions considered in linear and planar density calculations?

**Q12.**

Differentiate between linear density and planar density.

**Q13.**

Write the expressions for the linear density of  $[111]$  in BCC.

**Q14.**

Write the expression for the linear density of  $[110]$  in FCC.

**Q15.**

Write the expression for the planar density of  $(110)$  in BCC.

**Q16.**

What is meant by a close-packed direction?

**Q17.**

What is meant by a close-packed plane?

**Q18.**

State the FCC slip system.

**Q19.**

Why is the FCC  $(111)$  plane important in plastic deformation?

**Q20.**

What is the relationship between atomic density and slip?

## **55. 5-MARK EXAMINATION QUESTIONS**

**Q1.**

Define linear density. Explain the procedure for calculating linear density for a crystallographic direction.

**Q2.**

Define planar density. Explain the procedure for calculating planar density of a crystallographic plane.

**Q3.**

Derive the linear density of the  $[110]$  direction for an FCC crystal.

**Q4.**

Derive the linear density of the  $[111]$  direction for a BCC crystal.

**Q5.**

Calculate the linear densities of  $[100]$ ,  $[110]$  and  $[111]$  directions for a simple cubic crystal.

**Q6.**

Calculate the linear densities of [100], [110] and [111] directions for a BCC crystal.

**Q7.**

Calculate the linear densities of [100], [110] and [111] directions for an FCC crystal.

**Q8.**

Derive the planar density of the (110) plane for BCC.

**Q9.**

Derive the planar density of the (111) plane for FCC.

**Q10.**

Calculate the planar densities of (100), (110) and (111) planes for an FCC crystal.

**Q11.**

Explain why  $\langle 110 \rangle$  is the close-packed direction in FCC.

**Q12.**

Explain why  $\{111\}$  is the close-packed plane family in FCC.

**Q13.**

Differentiate between linear density, planar density and atomic packing factor.

**Q14.**

Explain the significance of linear and planar densities in plastic deformation of metals.

**Q15.**

Explain the importance of atomic density in determining slip systems.

## **56. 10-MARK EXAMINATION QUESTIONS**

**Q1.**

**Define linear density and explain in detail the method of calculating linear density along crystallographic directions. Derive the expressions for [100], [110] and [111] directions for SC, BCC and FCC crystals.**

**Q2.**

**Define planar density. Explain the method of calculating planar density and derive the expressions for (100), (110) and (111) planes for SC, BCC and FCC crystals.**

**Q3.**

Derive the linear density of the [110] direction in an FCC crystal and the [111] direction in a BCC crystal. Explain why these directions are considered highly packed directions.

**Q4.**

Derive the planar density of the FCC (111) plane. Explain why the (111) plane is called a close-packed plane and discuss its importance in plastic deformation.

**Q5.**

Prepare a comparative table of linear densities for [100], [110] and [111] directions in SC, BCC and FCC structures. Identify the most densely packed direction for BCC and FCC.

**Q6.**

Prepare a comparative table of planar densities for (100), (110) and (111) planes in SC, BCC and FCC structures. Identify the most densely packed plane in FCC.

**Q7.**

Explain linear density and planar density with neat diagrams. Discuss atom-sharing rules and geometrical calculations involved in their determination.

**Q8.**

A BCC metal has a lattice parameter of 0.2866 nm. Calculate the linear density along the [111] direction and planar density of the (110) plane. Show all steps clearly.

**Q9.**

An FCC metal has a lattice parameter of 0.3615 nm. Calculate:

- (a) Linear density along [110]
- (b) Planar density of (111)
- (c) Explain the significance of these values in relation to slip.

**Q10.**

Discuss the engineering significance of linear and planar densities. Explain their relationship with close-packed directions, close-packed planes, dislocation motion, slip and plastic deformation in crystalline metals.

## **57. IMPORTANT NUMERICALS FOR STUDENTS TO PRACTICE**

Students should practice at least these problems:

1. Find LD of SC [100].
2. Find LD of BCC [111].
3. Find LD of FCC [110].
4. Find LD of FCC [111].

5. Find PD of SC (100).
6. Find PD of BCC (110).
7. Find PD of FCC (111).
8. Calculate LD when lattice parameter is given in nm.
9. Calculate PD when lattice parameter is given in nm.
10. Convert LD from  $\text{nm}^{-1}$  to  $\text{m}^{-1}$ .
11. Compare LD of BCC [111] and FCC [110].
12. Compare PD of BCC (110) and FCC (111).
13. Identify the most densely packed direction from LD values.
14. Identify the most densely packed plane from PD values.
15. Explain how the densest plane/direction relates to slip.

## **58. ONE-PAGE REVISION SHEET**

### **LINEAR DENSITY**

$$\text{LD} = N/L$$

#### **Cubic direction lengths**

$$[100] \rightarrow a \quad [110] \rightarrow a\sqrt{2} \quad [111] \rightarrow a\sqrt{3}$$

#### **Important directions**

$$\text{FCC: } \langle 110 \rangle \quad \text{BCC: } \langle 111 \rangle$$

### **PLANAR DENSITY**

$$\text{PD} = N/A$$

#### **Common planar areas**

$$(100) \rightarrow a^2 \quad (110) \rightarrow a^2\sqrt{2} \quad (111) \rightarrow \frac{\sqrt{3}}{2}a^2$$

#### **Important planes**

$$\text{FCC: } \{111\} \quad \text{HCP: } (0001)$$

## **59. ★EXAM GOLDEN RULES**

Remember these six statements:

### **1. Linear density = atoms per unit length.**

$$\text{LD} = N/L$$

### **2. Planar density = atoms per unit area.**



PD=N/A

3.  $[110]$  length =  $a\sqrt{2}$ .

4.  $[111]$  length =  $a\sqrt{3}$ .

5. FCC close-packed direction =  $\langle 110 \rangle$ .

6. FCC close-packed plane =  $\{111\}$ .

And the most important conceptual sequence is:

Crystal Structure → Atomic Arrangement → Linear/Planar Density → Close Packing → Slip → Plastic Deformation

## Lecture 21

### UNIT-II: THE STRUCTURE OF CRYSTALLINE SOLIDS

Detailed Lecture Notes: Close-Packed Crystal Structures, Crystal Planes & Directions, Coordination Number, APF, Density and Crystal Imperfections

#### PART-A

#### CLOSE-PACKED CRYSTAL STRUCTURES

##### 1. Introduction

Atoms in crystalline solids arrange themselves in patterns that minimize the total energy of the system.

When identical atoms are considered as hard spheres of the same radius, there is a limit to how closely they can be packed.

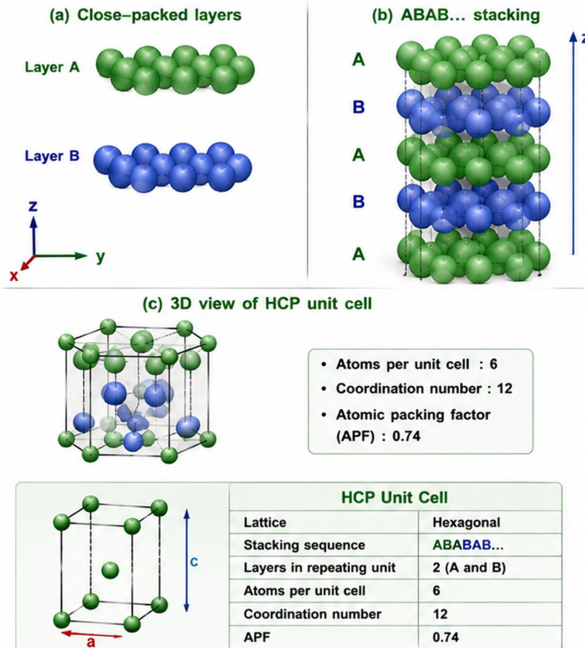
The two most important **close-packed crystal structures** are:

# STACKING SEQUENCE IN CLOSE-PACKED STRUCTURES

Close-packed structures are built by stacking layers of atoms in close-packed planes.

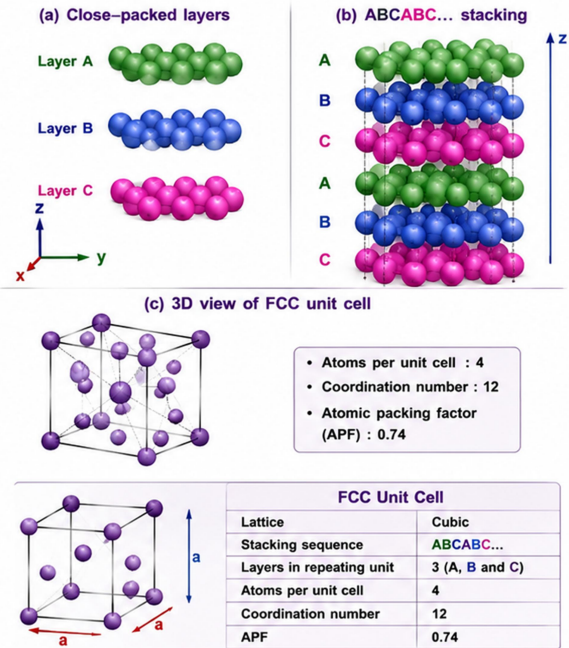
## 1. HEXAGONAL CLOSE-PACKED (HCP)

Stacking sequence : **ABABAB...**



## 2. CUBIC CLOSE-PACKED (FCC)

Stacking sequence : **ABCABC...**



### KEY POINTS

- In close-packed structures, each atom has 12 nearest neighbors.
- HCP has two distinct layers (A and B) → stacking : ABABAB...
- FCC (CCP) has three distinct layers (A, B and C) → stacking : ABCABC...
- Both have the same packing efficiency (APF = 0.74) and coordination number (12).

-  A layer atoms
-  B layer atoms
-  C layer atoms

HCP = Hexagonal Close-Packed  
FCC = Cubic Close-Packed

1. Face-Centred Cubic (FCC)
2. Hexagonal Close-Packed (HCP)

Both structures have:

Coordination Number=12

and:

Atomic Packing Factor=0.74

or approximately:

74%

Thus FCC and HCP are equally efficient in terms of ideal sphere packing.

## 2. WHAT IS CLOSE PACKING?

Consider identical spherical atoms.

If the spheres are arranged randomly, considerable empty space remains.

If they are arranged so that each sphere touches as many neighbouring spheres as geometrically possible, a **close-packed arrangement** is obtained.

For three-dimensional close packing:

CN<sub>max</sub>=12

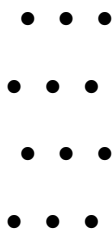
Therefore, an atom can have a maximum of **12 nearest neighbours** in an ideal close-packed structure.

### 3. CLOSE PACKING IN TWO DIMENSIONS

Imagine placing identical spherical atoms on a flat surface.

The most efficient arrangement is obtained when each atom touches six surrounding atoms.

A simplified arrangement is:



Each interior atom has:

6 nearest neighbours

in the same layer.

This arrangement is called a **close-packed layer**.

### 4. FORMATION OF THE SECOND LAYER

After forming the first close-packed layer, the next atoms can be placed in the depressions between three atoms of the first layer.

The second layer therefore does not lie directly above the atoms of the first layer.

It occupies alternate triangular holes.

We can call:

- first layer = **A**
- second layer = **B**

Thus:

AB

has been formed.

### 5. FORMATION OF THE THIRD LAYER

There are two possibilities for placing the third layer.

### **Possibility 1**

Place the third layer directly above the first layer:

A–B–A

Repeating gives:

ABABAB...

This produces:

**HCP**

### **Possibility 2**

Place the third layer in the other set of triangular sites:

A–B–C

Repeating gives:

ABCABCABC...

This produces:

**FCC**

## **6. STACKING SEQUENCES**

This is one of the most important concepts to remember.

**HCP**

ABABABAB...

**FCC**

ABCABCABC...

Therefore:

| <b>Structure</b> | <b>Stacking sequence</b> |
|------------------|--------------------------|
| HCP              | ABABAB...                |
| FCC              | ABCABC...                |

## **7. FCC AS A CLOSE-PACKED STRUCTURE**

FCC is a cubic crystal structure in which atoms occupy:

- eight corners;
- six face centres.

Effective number of atoms:

$$8(81)+6(21) = 1+3 \quad n=4$$

FCC can also be understood as a three-dimensional close-packed arrangement with:

ABCABC...

stacking.

## 8. HCP AS A CLOSE-PACKED STRUCTURE

HCP consists of close-packed hexagonal layers stacked in:

ABABAB...

The conventional HCP unit cell contains:

6 atoms

effective atoms.

The HCP unit cell is a hexagonal prism.

## 9. COORDINATION NUMBER

### Definition

The **coordination number (CN)** is the number of nearest-neighbour atoms surrounding a given atom.

It is an important measure of how closely atoms are packed.

### Major crystal structures

| Structure | Coordination Number |
|-----------|---------------------|
| SC        | 6                   |
| BCC       | 8                   |
| FCC       | 12                  |
| HCP       | 12                  |

Thus:

$$\text{FCC} = \text{HCP} = 12$$

## 10. WHY FCC AND HCP HAVE CN = 12

Consider one atom in a close-packed layer.

It has:

6

nearest neighbours in the same layer.

In the layer above:

3

nearest neighbours.

In the layer below:

3

nearest neighbours.

Therefore:

$$CN=6+3+3 \quad CN=12$$

## CRYSTAL PLANES, DIRECTIONS AND CO-ORDINATION NUMBER

### 1. CRYSTAL PLANES

Crystal planes are specified by Miller indices (h k l). They represent a family of parallel planes with intercepts on the axes.

**(100) PLANE**

Intercepts: a, ∞a, ∞a

**(010) PLANE**

Intercepts: ∞a, a, ∞a

**(001) PLANE**

Intercepts: ∞a, ∞a, a

**(111) PLANE**

Intercepts: a, a, a

### 2. CRYSTAL DIRECTIONS

Crystal directions are specified by Miller direction indices [u v w]. They represent a vector parallel to a line joining lattice points.

| Direction                 | Miller Direction [u v w] |
|---------------------------|--------------------------|
| Along +x axis             | [100]                    |
| Along +y axis             | [010]                    |
| Along +z axis             | [001]                    |
| Along face diagonal (xy)  | [110]                    |
| Along face diagonal (xz)  | [101]                    |
| Along body diagonal (xyz) | [111]                    |

### 3. CO-ORDINATION NUMBER

Co-ordination number (C.N.) is the number of nearest neighbor atoms surrounding a particular atom.

**SC (Simple Cubic)**

**C.N. = 6**  
(Atoms at the 6 faces are nearest neighbors)

**BCC (Body Centered Cubic)**

**C.N. = 8**  
(8 corner atoms are nearest neighbors)

**FCC (Face Centered Cubic)**

**C.N. = 12**  
(12 atoms: 4 in the same face + 8 in adjacent faces)

**KEY POINTS**

- Planes are represented by (h k l) using Miller indices.
- Directions are represented by [u v w] using Miller direction indices.
- Co-ordination number indicates the number of nearest neighbors.
- SC: 6, BCC: 8, FCC: 12

## 11. COMPARISON OF SC, BCC, FCC AND HCP

| Property                  | SC   | BCC  | FCC  | HCP  |
|---------------------------|------|------|------|------|
| Effective atoms/unit cell | 1    | 2    | 4    | 6*   |
| Coordination number       | 6    | 8    | 12   | 12   |
| APF                       | 0.52 | 0.68 | 0.74 | 0.74 |

| Property           | SC  | BCC | FCC    | HCP    |
|--------------------|-----|-----|--------|--------|
| Packing efficiency | 52% | 68% | 74%    | 74%    |
| Close-packed?      | No  | No  | Yes    | Yes    |
| Stacking           | —   | —   | ABCABC | ABABAB |

\*For the conventional HCP unit cell.

## 12. FCC AND HCP: SIMILARITIES

FCC and HCP both have:

- coordination number = 12;
- APF = 0.74;
- 74% ideal packing efficiency;
- close-packed atomic layers;
- three-dimensional dense atomic arrangements.

## 13. FCC AND HCP: DIFFERENCES

### FCC

Cubic

ABCABC stacking

Conventional cell: 4 atoms

Close-packed plane: {111}

More close-packed slip systems in many cases

### HCP

Hexagonal

ABABAB stacking

Conventional cell: 6 atoms

Basal close-packed plane: (0001)

Fewer easy slip systems at ordinary conditions

## 14. EXAMPLES OF FCC METALS

Important FCC metals include:

- Aluminium
- Copper
- Nickel
- Silver
- Gold
- Lead

FCC metals are generally known for good ductility because they possess favourable slip systems.

## **15. EXAMPLES OF HCP METALS**

Important HCP metals include:

- Magnesium
- Titanium
- Zinc
- Cobalt
- Zirconium

Their deformation behaviour is strongly influenced by the limited number of easily activated slip systems compared with FCC metals.

## **PART-B**

### **CRYSTAL PLANES AND DIRECTIONS**

#### **16. REVIEW: CRYSTALLOGRAPHIC DIRECTIONS**

A crystallographic direction represents an orientation in a crystal.

It is represented by:

$[uvw]$

A family of equivalent directions is represented by:

$\langle uvw \rangle$

Examples:

$[100], [110], [111]$

#### **17. CRYSTALLOGRAPHIC PLANES**

A crystallographic plane is represented by:

$(hkl)$

A family of equivalent planes is represented by:

$\{hkl\}$

Examples:

$(100), (110), (111)$

and:

$\{100\}, \{110\}, \{111\}$



## 18. CLOSE-PACKED DIRECTIONS

The most densely packed crystallographic directions are:

**FCC**

$\langle 110 \rangle$

**BCC**

$\langle 111 \rangle$

**HCP**

Close-packed directions within the basal plane belong to the:

$\langle 112\bar{0} \rangle$

family in the four-index hexagonal notation.

## 19. CLOSE-PACKED PLANES

**FCC**

$\{111\}$

**HCP**

$(0001)$

The HCP basal plane is the close-packed plane.

BCC does not have a truly close-packed plane equivalent to FCC  $\{111\}$ , although  $\{110\}$  planes are relatively densely populated.

## 20. CRYSTALLOGRAPHY AND SLIP

A **slip system** consists of:

Slip plane+Slip direction

For FCC:

$\{111\}\langle 110 \rangle$

is the primary slip system.

This is a very important metallurgical concept because plastic deformation occurs largely through dislocation movement on slip systems.

**PART–C**

**ATOMIC PACKING FACTOR**

## 21. DEFINITION OF APF

The Atomic Packing Factor (APF) is the fraction of the volume of a unit cell that is actually occupied by atoms, assuming atoms behave as hard spheres.

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

Therefore:

$$APF = \frac{n \left( \frac{4}{3} \pi r^3 \right)}{V_c}$$

where:

- $n$  = number of effective atoms/unit cell;
- $r$  = atomic radius;
- $V_c$  = unit-cell volume.

## 22. SIGNIFICANCE OF APF

APF tells us how efficiently atoms occupy space.

For example:

APF=0.74

means approximately:

74%

of the unit-cell volume is occupied by atoms in the ideal hard-sphere model.

The remaining:

26%

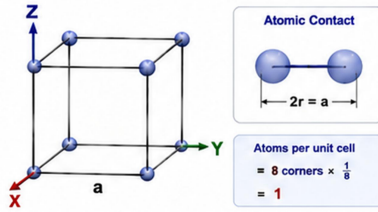
represents interstitial space.

# CALCULATION OF APF (ATOMIC PACKING FACTOR) AND DENSITY

$$\text{APF} = \frac{\text{Volume occupied by atoms in a unit cell}}{\text{Total volume of the unit cell}}$$

$$\text{Density, } \rho = \frac{\text{Mass of atoms in a unit cell}}{\text{Volume of the unit cell}}$$

## 1. SIMPLE CUBIC (SC)



**APF**

Volume of atoms in unit cell =  $1 \times \left(\frac{4}{3}\right) \pi r^3$

Volume of unit cell =  $a^3$

Since  $a = 2r$

$$\text{APF} = \frac{\left(\frac{4}{3}\right) \pi r^3}{(a^3)} = \frac{\left(\frac{4}{3}\right) \pi r^3}{(2r)^3} = \frac{\left(\frac{4}{3}\right) \pi r^3}{8r^3} = \frac{\pi}{6}$$

**APF = 0.52**

**Density**

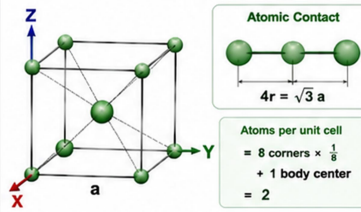
Mass of atoms in unit cell =  $1 \times \frac{M}{N_A}$

Volume of unit cell =  $a^3 = (2r)^3$

$$\text{Density, } \rho = \frac{M/N_A}{(2r)^3} = \frac{M}{8N_A r^3}$$

**SC : APF = 0.52**  
Coordination Number (C.N.) = 6

## 2. BODY CENTERED CUBIC (BCC)



**APF**

Volume of atoms in unit cell =  $2 \times \left(\frac{4}{3}\right) \pi r^3$

Volume of unit cell =  $a^3$

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

$$\text{APF} = \frac{2 \left(\frac{4}{3}\right) \pi r^3}{a^3} = \frac{\frac{8}{3} \pi r^3}{\left(\frac{4}{\sqrt{3}}\right)^3} = \frac{\frac{8}{3} \pi r^3}{\frac{64}{3\sqrt{3}}} = \frac{\sqrt{3} \pi}{8}$$

**APF = 0.68**

**Density**

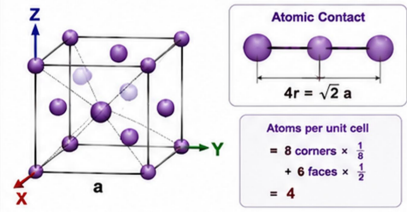
Mass of atoms in unit cell =  $2 \times \frac{M}{N_A}$

Volume of unit cell =  $a^3 = \left(\frac{4}{\sqrt{3}}\right)^3$

$$\text{Density, } \rho = \frac{2M/N_A}{\left(\frac{4}{\sqrt{3}}\right)^3} = \frac{3\sqrt{3}M}{32N_A r^3}$$

**BCC : APF = 0.68**  
Coordination Number (C.N.) = 8

## 3. FACE CENTERED CUBIC (FCC)



**APF**

Volume of atoms in unit cell =  $4 \times \left(\frac{4}{3}\right) \pi r^3$

Volume of unit cell =  $a^3$

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

$$\text{APF} = \frac{4 \left(\frac{4}{3}\right) \pi r^3}{a^3} = \frac{\frac{16}{3} \pi r^3}{(2\sqrt{2}r)^3} = \frac{\frac{16}{3} \pi r^3}{16\sqrt{2}r^3} = \frac{\pi}{3\sqrt{2}}$$

**APF = 0.74**

**Density**

Mass of atoms in unit cell =  $4 \times \frac{M}{N_A}$

Volume of unit cell =  $a^3 = (2\sqrt{2}r)^3$

$$\text{Density, } \rho = \frac{4M/N_A}{(2\sqrt{2}r)^3} = \frac{\sqrt{2}M}{4N_A r^3}$$

**FCC : APF = 0.74**  
Coordination Number (C.N.) = 12

### KEY POINTS

- APF indicates how efficiently atoms are packed in a crystal structure.
- Higher APF  $\Rightarrow$  more compact packing.
- Coordination number (C.N.) is the number of nearest neighbor atoms.
- For SC, BCC and FCC : APF  $\Rightarrow$  SC (0.52) < BCC (0.68) < FCC (0.74)  
C.N.  $\Rightarrow$  SC (6) < BCC (8) < FCC (12)

### Symbols

$r$  = Atomic radius  
 $a$  = Edge length of unit cell  
 $M$  = Atomic mass  
 $N_A$  = Avogadro's number ( $6.022 \times 10^{23}$  atoms/mol)  
 $\rho$  = Density

 = Corner atom  
Contribution = 1/8

 = Body center atom  
Contribution = 1

 = Face center atom  
Contribution = 1/2

### 23. APF OF SIMPLE CUBIC

For SC:

$$n = 1$$

Atoms touch along cube edge:

$$a = 2r$$

Therefore:

$$V_c = a^3 = (2r)^3 = 8r^3$$

Volume of one atom:

$$\frac{4}{3}\pi r^3$$

Therefore:

$$APF = \frac{\frac{4}{3}\pi r^3}{8r^3}$$

$$APF = \frac{\pi}{6}$$

Hence:

$$APF_{SC} = 0.52$$

or approximately:

$$52\%$$

## 24. APF OF BCC

For BCC:

$$n = 2$$

Atoms touch along body diagonal.

Therefore:

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

Thus:

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

Unit-cell volume:

$$V_c = a^3 = \left(\frac{4r}{\sqrt{3}}\right)^3$$

Volume of atoms:

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

Therefore:

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

After simplification:

$$\boxed{APF_{BCC} \approx 0.68}$$

Therefore:

$$\boxed{68\%}$$

## 25. APF OF FCC

For FCC:

$$n = 4$$

Atoms touch along face diagonal.

Therefore:

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

Thus:

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

Unit-cell volume:

$$V_c = (2\sqrt{2}r)^3$$

Volume occupied by atoms:

$$4 \left( \frac{4}{3} \pi r^3 \right)$$

Therefore:

$$\boxed{APF_{FCC} = 0.74}$$

or:

$$\boxed{74\%}$$

## Lecture 22

## 26. APF OF HCP

For ideal HCP:

$$n = 6$$

The basal-plane geometry gives:

$$a = 2r$$

The ideal axial ratio is:

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

The volume of the conventional hexagonal cell is:

$$V_c = \frac{3\sqrt{3}}{2} a^2 c$$

Volume occupied by six atoms:

$$V_{atoms} = 6 \left( \frac{4}{3} \pi r^3 \right)$$

Using:

$$a = 2r$$

and:

$$c = 1.633a$$

gives:

$$APF_{HCP} \approx 0.74$$

Thus:

$$\text{HCP and FCC have the same ideal APF}$$

## 27. MASTER APF TABLE

| Structure | APF  | Packing efficiency |
|-----------|------|--------------------|
| SC        | 0.52 | 52%                |
| BCC       | 0.68 | 68%                |
| FCC       | 0.74 | 74%                |
| HCP       | 0.74 | 74%                |

Therefore:

$$SC < BCC < FCC = HCP$$

in terms of ideal packing efficiency.

## PART-D

### THEORETICAL DENSITY

#### 28. DEFINITION OF DENSITY

Density is mass per unit volume:

$$\rho = \frac{m}{V}$$

For a crystalline material, the theoretical density can be calculated from its crystal structure.

×

☐

$$\rho = \frac{m}{V}$$

$$\rho = \frac{12 \text{ kg}}{5 \text{ L}} = 2.4 \text{ kg/L}$$

$m$

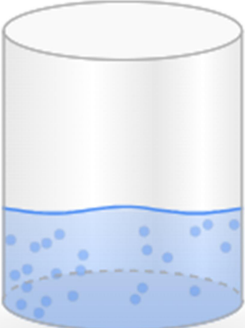
12.0

kg

$V$

5.0

L





## 29. MASS OF ONE ATOM

If the atomic weight is:

$$A \text{ g/mol}$$

then the mass of one atom is:

$$m_{atom} = \frac{A}{N_A}$$

where:

$$N_A = 6.022 \times 10^{23} \text{ atoms/mol}$$

## 30. MASS OF ONE UNIT CELL

If there are  $n$  effective atoms per unit cell:

$$m_{cell} = \frac{nA}{N_A}$$

## 31. THEORETICAL DENSITY EQUATION

Since:

$$\rho = \frac{m}{V}$$

we obtain:

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

For a cubic unit cell:

$$V_c = a^3$$

Therefore:

$$\rho = \frac{nA}{N_A a^3}$$



This is one of the most important numerical equations in Unit-II.

### 32. THEORETICAL DENSITY OF FCC

For FCC:

$$n = 4$$

Therefore:

$$\rho_{FCC} = \frac{4A}{N_A a^3}$$

---

### 33. THEORETICAL DENSITY OF BCC

For BCC:

$$n = 2$$

Therefore:

$$\rho_{BCC} = \frac{2A}{N_A a^3}$$

---

### 34. THEORETICAL DENSITY OF SC

For SC:

$$n = 1$$

Therefore:

$$\rho_{SC} = \frac{A}{N_A a^3}$$

### 35. DENSITY OF HCP

For conventional HCP:

$$n = 6$$

and:

$$V_c = \frac{3\sqrt{3}}{2}a^2c$$

Therefore:

$$\rho_{HCP} = \frac{6A}{N_A \left( \frac{3\sqrt{3}}{2}a^2c \right)}$$

or equivalently:

$$\rho_{HCP} = \frac{4A}{\sqrt{3}N_A a^2c}$$

---

### 36. IMPORTANT UNIT CONVERSION

When calculating density, lattice parameter must be converted to **cm** if the desired density is in  $g/cm^3$ .

Remember:

$$1 \text{ nm} = 10^{-7} \text{ cm}$$

Therefore:

$$1 \text{ nm}^3 = 10^{-21} \text{ cm}^3$$

Also:

$$1 \text{ \AA} = 10^{-8} \text{ cm}$$

### 37. SOLVED NUMERICAL — FCC DENSITY

Suppose an FCC metal has:

$$A = 63.5 \text{ g/mol}$$

and:

$$a = 0.3615 \text{ nm}$$

**Step 1: Convert  $a$**

$$a = 0.3615 \times 10^{-7} \text{ cm}$$

**Step 2**

FCC:

$$n = 4$$

**Step 3**

Use:

$$\rho = \frac{nA}{N_A a^3}$$

Thus:

$$\rho = \frac{4(63.5)}{(6.022 \times 10^{23})(0.3615 \times 10^{-7})^3}$$

This gives approximately:

$$\boxed{\rho \approx 8.94 \text{ g/cm}^3}$$

### 38. EXPERIMENTAL VS THEORETICAL DENSITY

#### Theoretical density

Calculated from:

- crystal structure;
- atomic weight;
- lattice parameter.

#### Experimental density

Measured experimentally.

The experimental density may be lower than theoretical density because real materials contain:

- vacancies;

- pores;
- cracks;
- inclusions;
- other defects.

Thus:

$$\rho_{\text{real}} \leq \rho_{\text{ideal}}$$

in many practical situations.

## **PART-E**

### **IMPERFECTIONS IN SOLIDS**

#### **39. INTRODUCTION**

A perfect crystal would contain atoms arranged exactly according to an ideal periodic lattice.

Real engineering materials are never perfectly crystalline.

They contain various types of imperfections.

These are called:

Crystal defects

or:

Imperfections in solids

#### **40. ARE CRYSTAL DEFECTS ALWAYS BAD?**

No.

This is an extremely important concept.

Some defects are undesirable because they can reduce:

- strength;
- fatigue life;
- corrosion resistance;
- density;
- toughness.

But controlled defects are essential for:

- plastic deformation;
- diffusion;

- alloy strengthening;
- semiconductor operation;
- precipitation hardening;
- heat treatment;
- ionic conductivity.

Therefore:

Defects are not simply "bad"; they control material behaviour.

#### **41. CLASSIFICATION OF CRYSTAL DEFECTS**

Crystal imperfections can be classified according to their dimensionality.

##### **0-D**

Point defects

##### **1-D**

Linear defects/dislocations

##### **2-D**

Interfacial defects

##### **3-D**

Bulk/volume defects

Thus:

0D→1D→2D→3D

# IMPERFECTIONS IN SOLIDS

Imperfections (defects) are irregularities in the orderly arrangement of atoms in a crystal. They strongly influence the mechanical, electrical, optical and chemical properties of materials.

### 1. POINT DEFECTS (Zero-Dimensional)

**(a) VACANCIES**  
An atom is missing from its normal lattice site.

● Normal atom  
○ Vacant site

**(b) SELF-INTERSTITIALS**  
An extra atom occupies an interstitial site.

● Normal atom  
● Self-interstitial atom

### 2. DISLOCATIONS (LINEAR DEFECTS) (One-Dimensional)

**(a) EDGE DISLOCATION**

Extra half-plane of atoms  
⊥ Dislocation line

**(b) SCREW DISLOCATION**

Dislocation line  
↱ Dislocation line

### 3. INTERFACIAL DEFECTS (Two-Dimensional)

**(a) GRAIN BOUNDARY**  
Boundary between two grains of different orientations.

Grain 1 Grain Boundary Grain 2

**(b) PHASE BOUNDARY**  
Boundary between two different phases in the same material.

Phase A Phase Boundary Phase B

### 4. BULK OR VOLUME DEFECTS (Three-Dimensional)

**(a) VOIDS (CAVITIES)**  
Empty spaces or cavities within the crystal.

**(b) INCLUSIONS**  
Foreign atoms or particles trapped in the crystal.

**(c) PRECIPITATES**  
Second phase particles within the matrix.

**SUMMARY**

- Point defects involve disturbance at a single lattice site (vacancy, interstitial).
- Linear defects are dislocations along a line in the crystal.
- Interfacial defects are boundaries between different regions (grain or phase).
- Bulk defects exist within the volume of the material.

**LEGEND**

- Host (normal) atom
- Extra atom / interstitial
- Foreign atom / particle
- Vacant site / void

**KEY EFFECTS OF DEFECTS**

- Affect strength and ductility.
- Influence electrical and thermal conductivity.
- Control diffusion processes.
- Play a vital role in phase transformations and material behavior.

## 42. MASTER CLASSIFICATION TABLE

| Type                | Dimension | Examples                                                      |
|---------------------|-----------|---------------------------------------------------------------|
| Point defects       | 0-D       | Vacancy, self-interstitial                                    |
| Linear defects      | 1-D       | Edge, screw, mixed dislocation                                |
| Interfacial defects | 2-D       | Grain boundary, twin boundary, stacking fault, phase boundary |
| Bulk defects        | 3-D       | Voids, pores, cracks, inclusions, precipitates                |

## PART-F

### POINT DEFECTS

## 43. DEFINITION

Point defects are localized imperfections associated with one or a few atomic sites.

They are essentially:

## 0-dimensional defects

The syllabus specifically identifies:

- vacancies;
- self-interstitials.

### 44. VACANCY DEFECT

A vacancy is formed when an atom is missing from its normal lattice position.

Ideal lattice:

• • • •

• • • •

• • • •

With vacancy:

• • • •

• • ○ •

• • • •

where:

○=vacant lattice site

### 45. CAUSES OF VACANCIES

Vacancies can arise due to:

- thermal agitation;
- solidification;
- plastic deformation;
- irradiation;
- heat treatment.

Vacancy concentration increases strongly with temperature.

The equilibrium vacancy fraction can be represented approximately by:

$$\frac{N_v}{N} = \exp \left( -\frac{Q_v}{kT} \right)$$

where:



- $N_v$  = number of vacancies;
- $N$  = total number of atomic sites;
- $Q_v$  = vacancy formation energy;
- $k$  = Boltzmann constant;
- $T$  = absolute temperature.

#### 46. IMPORTANCE OF VACANCIES

Vacancies are extremely important because they facilitate:

##### Diffusion

Atoms can move from one lattice site to another by jumping into vacant sites.

##### Heat treatment

Vacancy-assisted diffusion is essential during many metallurgical processes.

##### Solid-state reactions

Vacancies facilitate atomic redistribution.

Therefore:

Vacancies → Atomic diffusion

#### 47. SELF-INTERSTITIAL DEFECT

A self-interstitial occurs when an extra atom of the same type as the host occupies a normally unoccupied interstitial position.

For example:

• • • •

• • • •

•

• • • •

The additional atom is located between normal lattice sites.

#### 48. CHARACTERISTICS OF SELF-INTERSTITIALS

Self-interstitials:

- distort the surrounding lattice;
- produce local strain;
- have relatively high formation energy;

- are generally less numerous than vacancies in equilibrium;
- can influence diffusion and defect interactions.

#### 49. VACANCY VS SELF-INTERSTITIAL

##### Vacancy

Atom missing

Normal site is empty

Produces local distortion

Important for diffusion

Relatively common equilibrium point defect

##### Self-interstitial

Extra atom present

Atom occupies interstitial site

Usually produces stronger local distortion

Also contributes to defect transport

Generally much less common in equilibrium

#### Lecture 23

#### PART-G

#### LINEAR DEFECTS — DISLOCATIONS

##### 50. DEFINITION

A **dislocation** is a linear or one-dimensional crystal defect around which there is a localized lattice distortion.

Dislocations are fundamental to understanding plastic deformation of crystalline materials.

##### 51. TYPES OF DISLOCATIONS

The major types are:

1. Edge dislocation
2. Screw dislocation
3. Mixed dislocation

##### 52. EDGE DISLOCATION

An edge dislocation can be visualized as an extra half-plane of atoms inserted into the crystal.

Simplified:

• • • • •

• • • • •

• • •

• • •

• • • • •

• • • • •

The termination of the extra half-plane represents the dislocation line.

### 53. CHARACTERISTICS OF EDGE DISLOCATION

At the edge dislocation:

- atoms above/below the dislocation experience lattice distortion;
- compressive strain exists near the extra half-plane;
- tensile strain exists on the opposite side;
- the Burgers vector is perpendicular to the dislocation line.

Therefore:

$b \perp$  dislocation line

for a pure edge dislocation.

### 54. SCREW DISLOCATION

A screw dislocation results from shear displacement of one portion of the crystal relative to another.

The atomic planes form a helical or spiral arrangement around the dislocation line.

For a pure screw dislocation:

$b \parallel$  dislocation line

### 55. MIXED DISLOCATION

Most real dislocations are neither purely edge nor purely screw.

They contain both components.

Therefore:

Mixed dislocation = edge component + screw component

### 56. BURGERS VECTOR

The **Burgers vector** describes the magnitude and direction of lattice distortion associated with a dislocation.

It is represented by:

$b$

It is fundamental to dislocation theory.

For an ideal crystal:

$$b=0$$

For a crystal containing a dislocation:

$$b \neq 0$$

## 57. EDGE VS SCREW DISLOCATION

| Feature          | Edge                              | Screw                                      |
|------------------|-----------------------------------|--------------------------------------------|
| Basic picture    | Extra half-plane                  | Helical distortion                         |
| Burgers vector   | Perpendicular to dislocation line | Parallel to dislocation line               |
| Main deformation | Lattice compression/tension       | Shear                                      |
| Slip             | Can move under shear stress       | Can also glide under suitable shear stress |

## 58. DISLOCATIONS AND PLASTIC DEFORMATION

This is one of the most important metallurgical concepts.

If an entire plane of atoms had to slide simultaneously, an enormous stress would be required.

Dislocations make plastic deformation much easier.

Instead of moving an entire plane at once, the dislocation moves through the crystal.

Thus:

Dislocation motion → Slip → Plastic deformation

## 59. DISLOCATION MOTION

Two important modes are:

### Glide

Movement of a dislocation through its slip plane.

### Climb

Movement of an edge dislocation out of its slip plane, involving vacancy diffusion.

Climb is therefore strongly temperature-dependent.

## **60. WHY DISLOCATIONS ARE IMPORTANT TO METALLURGISTS**

Control of dislocation motion is central to:

- strengthening;
- annealing;
- cold working;
- recovery;
- recrystallization;
- grain refinement;
- alloy design.

Many strengthening mechanisms work by making dislocation motion more difficult.

Examples include:

- solid-solution strengthening;
- grain-boundary strengthening;
- precipitation strengthening;
- work hardening.

## **PART-H**

### **INTERFACIAL DEFECTS**

#### **61. DEFINITION**

Interfacial defects are two-dimensional imperfections associated with boundaries between regions of a material.

They are:

2D defects

Important examples include:

1. External surfaces
2. Grain boundaries
3. Twin boundaries
4. Stacking faults
5. Phase boundaries

#### **62. EXTERNAL SURFACE**

An external surface is the boundary between the crystal and its surroundings.

Atoms at the surface have fewer nearest neighbours than atoms inside the crystal.

Therefore, surface atoms have higher energy than interior atoms.

This contributes to:

- surface energy;
- adsorption;
- corrosion;
- oxidation;
- catalytic behaviour;
- surface reactions.

### **63. GRAIN BOUNDARY**

Engineering metals are usually **polycrystalline**.

A polycrystalline material consists of many small crystals or grains.

Each grain has its own crystallographic orientation.

The boundary between two grains is called a:

Grain boundary

### **64. GRAIN BOUNDARY STRUCTURE**

Simplified:

Grain A    Grain B

////////|\\\\\\\\\\

////////|\\\\\\\\\\

////////|\\\\\\\\\\

////////|\\\\\\\\\\

The vertical region represents the grain boundary.

Atoms at the boundary cannot maintain perfect periodicity with both neighbouring grains.

### **65. IMPORTANCE OF GRAIN BOUNDARIES**

Grain boundaries can:

- impede dislocation motion;

- influence strength;
- influence diffusion;
- act as preferred sites for precipitation;
- affect corrosion;
- influence recrystallization.

The relationship between grain size and strength is commonly expressed by the Hall–Petch relation:

$$\sigma_y = \sigma_0 + k_y d^{-1/2}$$

where:

- $\sigma_y$  = yield stress;
- $d$  = average grain diameter;
- $k_y$  = Hall–Petch constant.

Thus, smaller grains generally increase yield strength.

## **66. TWIN BOUNDARY**

A twin boundary separates two regions that are mirror-related crystallographically.

The two sides have a specific symmetrical relationship.

Twin boundaries may form during:

- deformation;
- annealing;
- crystal growth.

## **67. STACKING FAULT**

A stacking fault is an interruption in the normal stacking sequence of close-packed planes.

For FCC:

Normal:

ABCABCABC

A stacking fault can locally disturb this sequence.

Because FCC and HCP differ primarily in stacking sequence, stacking faults are closely related to local changes between FCC- and HCP-like arrangements.

## **68. PHASE BOUNDARY**

A phase boundary separates two different phases.

For example:

$\alpha|\beta$

The two phases differ in:

- composition;
- crystal structure;
- properties;
- sometimes chemical bonding.

Phase boundaries are extremely important in:

- steels;
- aluminium alloys;
- precipitation-hardened alloys;
- composites;
- ceramics.

## **69. INTERFACIAL DEFECTS SUMMARY**

| <b>Defect</b>  | <b>Description</b>                           |
|----------------|----------------------------------------------|
| Surface        | Boundary between material and environment    |
| Grain boundary | Boundary between differently oriented grains |
| Twin boundary  | Mirror-related crystallographic boundary     |
| Stacking fault | Error in close-packed layer sequence         |
| Phase boundary | Boundary between different phases            |

## **PART-I**

## **BULK OR VOLUME DEFECTS**

## **70. DEFINITION**

Bulk or volume defects are three-dimensional imperfections that occupy a finite volume of the material.

They are:

3D defects

## **71. EXAMPLES OF BULK DEFECTS**



Important examples include:

- pores;
- voids;
- cracks;
- inclusions;
- precipitate particles;
- large second-phase particles;
- shrinkage cavities.

## **72. POROSITY**

Porosity refers to the presence of pores or voids within a material.

It can result from:

- gas entrapment;
- solidification shrinkage;
- powder processing;
- inadequate compaction.

Porosity generally reduces:

- density;
- strength;
- fatigue resistance;
- ductility.

## **73. CRACKS**

A crack is a sharp discontinuity in a material.

Cracks are especially dangerous because they can act as stress concentrators.

A crack may initiate and propagate under:

- tensile loading;
- fatigue;
- thermal stresses;
- residual stresses;
- corrosion-assisted conditions.

## 74. INCLUSIONS

An inclusion is a foreign or non-metallic particle embedded in a matrix.

In steels, common inclusions include:

- oxides;
- sulfides;
- silicates.

Depending on their size, morphology and distribution, inclusions can influence:

- machinability;
- fatigue;
- toughness;
- fracture;
- cleanliness of steel.

## 75. PRECIPITATES

A precipitate is a particle of a second phase that forms within a matrix.

Controlled precipitates can be beneficial.

For example, precipitation hardening uses finely dispersed particles to impede dislocation motion.

Therefore:

Fine precipitates → Dislocation obstruction → Higher strength

This is an important example showing that a "defect" or microstructural discontinuity can be deliberately engineered to improve properties.

## Lecture 24

## 76. DEFECTS AND MATERIAL PROPERTIES

Different defects affect different properties.

| Defect            | Major effect                   |
|-------------------|--------------------------------|
| Vacancy           | Diffusion                      |
| Self-interstitial | Lattice distortion             |
| Dislocation       | Plastic deformation            |
| Grain boundary    | Strength, diffusion, corrosion |

| <b>Defect</b>  | <b>Major effect</b>                    |
|----------------|----------------------------------------|
| Stacking fault | Deformation behaviour                  |
| Twin boundary  | Deformation/crystallographic behaviour |
| Porosity       | Density, strength, fatigue             |
| Crack          | Fracture                               |
| Inclusion      | Fatigue, toughness, machinability      |
| Precipitate    | Strengthening                          |

## **77. DEFECTS AND STRENGTH**

A key principle in Metallurgy is:

**Plastic deformation occurs through dislocation motion; strengthening is often achieved by obstructing dislocation motion.**

Important obstacles include:

- solute atoms;
- grain boundaries;
- precipitates;
- other dislocations;
- particles.

Therefore:

Obstacle to dislocation motion → Higher strength

## **78. DEFECTS AND DIFFUSION**

Diffusion is strongly associated with point defects.

### **Vacancy diffusion**

An atom jumps into a neighbouring vacancy.

### **Interstitial diffusion**

A small atom moves between interstitial positions.

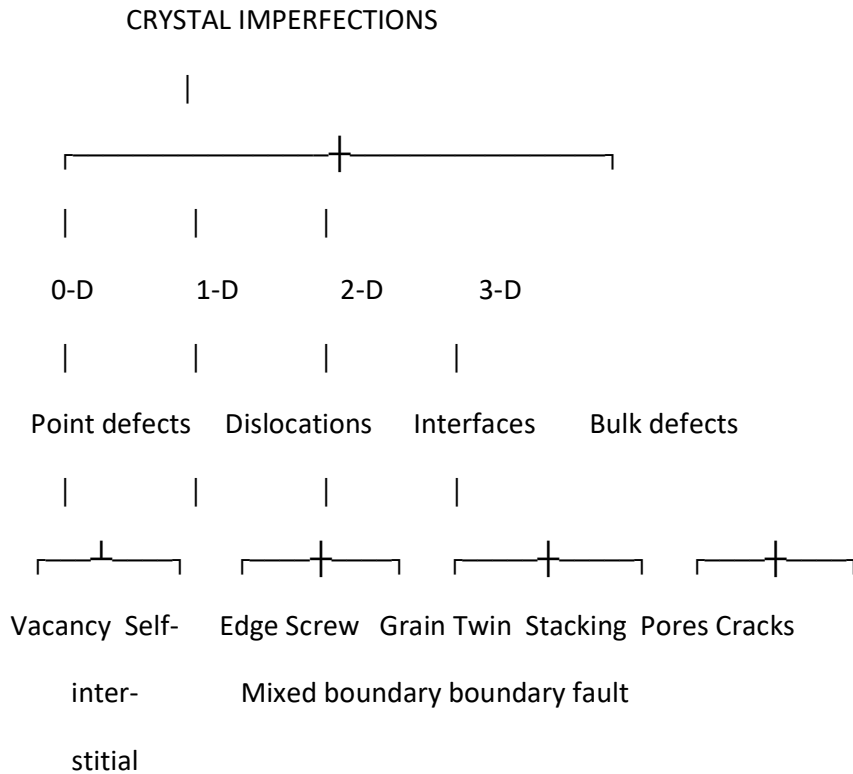
Therefore:

Point defects → Atomic mobility → Diffusion

This is particularly important in:

- carburizing;
- nitriding;
- homogenization;
- sintering;
- precipitation;
- heat treatment.

## 79. COMPLETE DEFECT CLASSIFICATION



## 80. IMPORTANT COMPARISON: 0D, 1D, 2D, 3D

| Dimensionality | Defect      | Examples                                      |
|----------------|-------------|-----------------------------------------------|
| 0-D            | Point       | Vacancy, self-interstitial                    |
| 1-D            | Linear      | Edge, screw, mixed dislocations               |
| 2-D            | Interfacial | Grain boundary, twin boundary, stacking fault |
| 3-D            | Volume      | Pores, cracks, inclusions, precipitates       |

## 81. CLOSE PACKING → DEFECTS → PROPERTIES

The entire topic can be connected through:

Atomic Arrangement → Packing → Defects → Dislocation Motion → Properties

This is exactly the type of structure–property understanding expected from a Materials Engineering course. The syllabus identifies material structure and crystal defects as explicit course outcomes.

## 82. HIGH-YIELD FORMULA SHEET

|                       |                                      |
|-----------------------|--------------------------------------|
| Atomic Packing Factor | $APF = \frac{n(4/3)\pi r^3}{V_c}$    |
| Cubic cell volume     | $V_c = a^3$                          |
| Theoretical density   | $\rho = \frac{nA}{N_A V_c}$          |
| For cubic crystals:   | $\rho = \frac{nA}{N_A a^3}$          |
| HCP cell volume       | $V_c = \frac{3\sqrt{3}}{2} a^2 c$    |
| HCP ideal ratio       | $\frac{c}{a} = 1.633$                |
| Vacancy concentration | $\frac{N_v}{N} = e^{-Q_v/kT}$        |
| Hall–Petch relation   | $\sigma_y = \sigma_0 + k_y d^{-1/2}$ |

## 83. MASTER REVISION TABLE

| Parameter       | SC   | BCC  | FCC  | HCP  |
|-----------------|------|------|------|------|
| Atoms/unit cell | 1    | 2    | 4    | 6*   |
| CN              | 6    | 8    | 12   | 12   |
| APF             | 0.52 | 0.68 | 0.74 | 0.74 |
| Packing         | 52%  | 68%  | 74%  | 74%  |

| Parameter              | SC | BCC                   | FCC                   | HCP                           |
|------------------------|----|-----------------------|-----------------------|-------------------------------|
| Close-packed direction | —  | $\langle 111 \rangle$ | $\langle 110 \rangle$ | basal $\langle 11-20 \rangle$ |
| Close-packed plane     | —  | —                     | $\{111\}$             | (0001)                        |
| Stacking               | —  | —                     | ABCABC                | ABABAB                        |

\*Conventional HCP cell.

#### 84. IMPORTANT CONCEPTUAL QUESTIONS FOR CLASS DISCUSSION

##### Why are FCC and HCP both called close-packed?

Because both achieve the maximum ideal packing efficiency for equal spheres:

$$APF=0.74$$

##### Why do FCC and HCP have the same APF but different properties?

Because their **stacking sequences differ**:

$$FCC=ABCABC \quad HCP=ABABAB$$

The difference in crystallographic symmetry and available slip systems leads to different deformation behaviour.

##### Why are vacancies important?

Because they provide sites through which atoms can migrate.

##### Why are dislocations important?

Because they make plastic deformation possible at stresses much lower than would be required for simultaneous movement of an entire atomic plane.

##### Why can grain boundaries strengthen a metal?

They interrupt the continuity of slip and act as obstacles to dislocation motion.

#### 85. COMMON STUDENT MISTAKES

##### Mistake 1

Thinking:

HCP and FCC have different packing efficiency.

**Correct:**

$$FCC=HCP=0.74$$

##### Mistake 2

Thinking:

FCC has ABCD stacking.

**Correct:**

ABCABC...

**Mistake 3**

Thinking:

HCP has ABC stacking.

**Correct:**

ABAB...

**Mistake 4**

Using  $n=4$  for HCP.

For the conventional HCP cell:

$n=6$

**Mistake 5**

Confusing coordination number and number of atoms per unit cell.

For FCC:

$CN=12$

but:

$n=4$

**Mistake 6**

Calling all defects harmful.

Some defects are deliberately introduced to improve properties.

## **86. 2-MARK EXAMINATION QUESTIONS**

1. Define a close-packed crystal structure.
2. Name the two important close-packed crystal structures.
3. State the stacking sequence of FCC.
4. State the stacking sequence of HCP.
5. What is the coordination number of FCC?
6. What is the coordination number of HCP?
7. Define coordination number.

8. What is the APF of FCC?
9. What is the APF of HCP?
10. State the APF of SC and BCC.
11. What is meant by atomic packing factor?
12. Define theoretical density.
13. Write the theoretical density equation for a cubic crystal.
14. How many effective atoms are present in an FCC unit cell?
15. How many effective atoms are present in a conventional HCP unit cell?
16. What is the ideal  $c/a$  ratio of HCP?
17. What is a crystal defect?
18. Define vacancy defect.
19. Define self-interstitial defect.
20. What is a dislocation?
21. Name the three types of dislocations.
22. What is an edge dislocation?
23. What is a screw dislocation?
24. Define Burgers vector.
25. What is an interfacial defect?
26. What is a grain boundary?
27. What is a stacking fault?
28. What is a twin boundary?
29. Define bulk defect.
30. Give two examples of bulk defects.
31. What is porosity?
32. What is an inclusion?
33. Which defect is primarily associated with diffusion?
34. Which defect is primarily responsible for plastic deformation?
35. What is the close-packed plane of FCC?
36. What is the close-packed plane of HCP?



37. What is the close-packed direction of FCC?

38. What is the close-packed direction of BCC?

### **87. 5-MARK EXAMINATION QUESTIONS**

1. Explain the formation of close-packed atomic layers.
2. Explain the stacking sequence of FCC and HCP.
3. Compare FCC and HCP crystal structures.
4. Explain coordination number and determine the CN of SC, BCC, FCC and HCP.
5. Define APF and explain its physical significance.
6. Derive the APF of the SC structure.
7. Derive the APF of the BCC structure.
8. Derive the APF of the FCC structure.
9. Explain the calculation of theoretical density of a crystalline material.
10. Calculate the theoretical density of a cubic metal when atomic weight, lattice parameter and crystal structure are given.
11. Define point defects and explain vacancy and self-interstitial defects.
12. Explain vacancy formation and its importance in diffusion.
13. Explain edge, screw and mixed dislocations.
14. Differentiate between edge and screw dislocations.
15. Explain the role of dislocations in plastic deformation.
16. Explain grain boundaries and their effect on mechanical properties.
17. Explain stacking faults and twin boundaries.
18. Explain bulk defects with suitable examples.
19. Classify crystal imperfections according to dimensionality.
20. Explain the relationship between crystal defects and material properties.

### **88. 10-MARK EXAMINATION QUESTIONS**

**Q1.**

**Explain close-packed crystal structures in detail. Describe the formation of close-packed layers and derive the ABAB and ABCABC stacking sequences for HCP and FCC respectively.**

**Q2.**

Compare FCC and HCP structures with respect to atomic arrangement, stacking sequence, number of atoms/unit cell, coordination number, APF, packing efficiency and important engineering metals.

**Q3.**

Define Atomic Packing Factor. Derive the APF of SC, BCC and FCC structures and compare their packing efficiencies.

**Q4.**

Derive the theoretical density equation for a cubic crystal. Explain each term and solve a suitable numerical problem involving atomic weight, lattice parameter and crystal structure.

**Q5.**

Explain crystallographic planes and directions in close-packed structures. Discuss the close-packed planes and directions of FCC, BCC and HCP and explain their significance in slip and plastic deformation.

**Q6.**

Define crystal imperfections and classify them according to dimensionality. Explain point, linear, interfacial and bulk defects with neat diagrams and examples.

**Q7.**

Explain point defects in crystalline solids. Describe vacancy and self-interstitial defects, their formation, characteristics and importance in diffusion.

**Q8.**

What are dislocations? Explain edge, screw and mixed dislocations with suitable diagrams. Define Burgers vector and discuss the role of dislocations in plastic deformation.

**Q9.**

Explain interfacial defects in crystalline materials. Discuss external surfaces, grain boundaries, twin boundaries, stacking faults and phase boundaries, and explain their effects on material properties.

**Q10.**

Explain bulk or volume defects. Discuss pores, voids, cracks, inclusions and precipitates and explain their effects on mechanical properties and engineering performance.

#### **89. INTEGRATED 10-MARK QUESTION**

**Q11.**

A metal has an FCC crystal structure with atomic weight 63.5g/mol and lattice parameter 0.3615nm.

Calculate:

1. Number of atoms per unit cell.
2. Coordination number.
3. Atomic packing factor.
4. Theoretical density.
5. Identify the close-packed plane.
6. Identify the close-packed direction.
7. State the primary slip system.

**Expected answers**

$n=4$   $CN=12$   $APF=0.74$   $\rho \approx 8.94 \text{ g/cm}^3$  Close-packed plane= $\{111\}$  Close-packed direction= $\langle 110 \rangle$   
Slip system= $\{111\}\langle 110 \rangle$

**90. INTEGRATED DEFECT QUESTION**

**Q12.**

**A metallurgical engineer observes that a cold-worked metal becomes stronger but less ductile. Explain this behaviour using crystal defects and dislocations.**

**Key answer**

Cold working increases the density of dislocations.

The dislocations interact and obstruct one another.

Therefore:

Cold work  $\rightarrow$  Increased dislocation density  $\rightarrow$  Greater resistance to dislocation motion  $\rightarrow$  Higher strength/hardness

but generally:

Higher strength  $\rightarrow$  Reduced ductility

This phenomenon is called:

Work hardening / strain hardening

**91. FINAL ONE-PAGE REVISION SHEET**

**CLOSE PACKING**

FCC=ABCABC... HCP=ABABAB...  $CN_{\text{FCC}}=CN_{\text{HCP}}=12$ ,  $APF_{\text{FCC}}=APF_{\text{HCP}}=0.74$

**APF**

SC=0.52 BCC=0.68 FCC=0.74 HCP=0.74

## DENSITY

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

For cubic:

$$\rho = \frac{nA}{N_A a^3}$$

For HCP:

$$V_c = \frac{3\sqrt{3}}{2} a^2 c$$

## CLOSE-PACKED SYSTEMS

### FCC

{111}<110>

### HCP

(0001)

basal close-packed plane.

## DEFECTS

0D→Point 1D→Dislocation 2D→Interface 3D→Bulk

### POINT DEFECTS

Vacancy Self-interstitial

### DISLOCATIONS

Edge Screw Mixed

Edge:

$b \perp$  dislocation line

Screw:

$b \parallel$  dislocation line

## Lecture 25

Lecture Notes: Mechanical, Electrical, Magnetic and Optical Properties of Materials

**UNIT–3: PROPERTIES OF ENGINEERING MATERIALS**

**1. Learning Objectives**

After completing these 15 lectures, students should be able to:

1. Define stress, strain and elastic deformation.
2. Explain different types of mechanical deformation.
3. State and apply Hooke's law.
4. Distinguish elastic and plastic deformation.
5. Define electrical resistivity and conductivity.
6. Explain electronic and ionic conduction.
7. Explain energy-band formation in solids.
8. Differentiate conductors, semiconductors and insulators.
9. Explain intrinsic and extrinsic semiconductivity.
10. Explain factors affecting carrier mobility.
11. Describe piezoelectricity and its applications.
12. Classify materials according to magnetic behaviour.
13. Explain superconductivity and its important characteristics.
14. Explain electromagnetic radiation and its interaction with solids.
15. Explain reflection, refraction, absorption and transmission.
16. Describe applications of optical phenomena including luminescence, photoconductivity, LEDs, lasers and optical fibres.

**BASIC CONCEPTS OF STRESS AND STRAIN**

**1.1 What is a Mechanical Property?**

A **mechanical property** describes how a material responds when an external mechanical force is applied.

Important mechanical properties include:

- Strength
- Elasticity
- Plasticity

- Stiffness
- Ductility
- Malleability
- Toughness
- Hardness
- Brittleness
- Resilience
- Creep resistance
- Fatigue resistance

For this unit, the fundamental concepts are **stress, strain and deformation**.

### **1.2 Force**

A force is an external action that tends to change the state of rest, motion or shape of a body.

SI unit:

F=Newton (N)

When force acts on a material, it may produce:

- Change in length
- Change in shape
- Change in volume
- Permanent deformation
- Fracture

### **1.3 Stress**

**Stress** is the internal resisting force developed per unit original cross-sectional area when an external force is applied.

$$\sigma = \frac{F}{A_0}$$

Where:

- $\sigma$  = stress
- F = applied force
- $A_0$  = original cross-sectional area

SI unit:

$$\text{N/m}^2 = \text{Pa}$$

Engineering stress is generally expressed in:

$$\text{MPa} = 10^6 \text{Pa}$$

### **Example**

A rod has an original cross-sectional area of  $100\text{mm}^2$  and is subjected to a tensile load of  $10\text{kN}$ .

$$\sigma = 10,000 / 100$$

Since  $1\text{N/mm}^2 = 1\text{MPa}$ ,

$$\sigma = 100\text{MPa}$$

## **1.4 Types of Stress**

### **A. Tensile Stress**

Produced when forces pull the material apart.

Examples:

- Tie rods
- Crane cables
- Suspension wires

### **B. Compressive Stress**

Produced when forces push the material together.

Examples:

- Columns
- Building pillars
- Compression members

### **C. Shear Stress**

Produced when forces act parallel to the cross-sectional plane.

$$\tau = AF$$

Examples:

- Rivets
- Bolts
- Punching operations

### **D. Bending Stress**

Developed when a component is subjected to bending.

Examples:

- Beams
- Shafts
- Machine frames

### **E. Torsional Stress**

Developed when a component is subjected to twisting.

Examples:

- Transmission shafts
- Drive shafts

### **1.5 Strain**

**Strain** is the deformation produced per unit original dimension.

For longitudinal deformation:

$$\epsilon = \Delta L / L_0$$

Where:

- $\epsilon$  = strain
- $\Delta L$  = change in length
- $L_0$  = original length

Strain has **no unit** because it is a ratio of two lengths.

It may be expressed as percentage:

$$\% \text{ strain} = \Delta L / L_0 \times 100$$

### **1.6 Types of Strain**



Longitudinal strain

$$\epsilon_L = \frac{\Delta L}{L_0}$$

Lateral strain

$$\epsilon_{lat} = \frac{\Delta d}{d_0}$$

Shear strain

$$\gamma = \frac{\Delta x}{L}$$

Volumetric strain

$$\epsilon_v = \frac{\Delta V}{V_0}$$

## LECTURE 26 — DEFORMATION AND ITS TYPES

### 2.1 Deformation

**Deformation** is the change in dimensions or shape of a material caused by an applied force or other external stimulus.

It may be:

1. Elastic
2. Plastic

### 2.2 Elastic Deformation

Elastic deformation is **recoverable deformation**.

When the applied load is removed:

Material returns approximately to original shape

Examples:

- Small extension of a steel spring
- Slight bending of a metal ruler

#### Characteristics

- Temporary
- Reversible
- Usually occurs at low stresses
- Associated with atomic bond stretching

### 2.3 Plastic Deformation

Plastic deformation is **permanent deformation**.

After removing the load:

Original shape is not completely recovered

Plastic deformation is particularly important in:

- Rolling
- Forging
- Extrusion
- Drawing
- Sheet-metal forming

### 2.4 Elastic vs Plastic Deformation

#### Elastic

Temporary

Reversible

Occurs at lower stress

Atoms return approximately to original positions

Useful in springs

#### Plastic

Permanent

Irreversible

Occurs after yield

Atoms undergo permanent rearrangement

Useful in metal forming

### 2.5 Factors Affecting Deformation

Deformation depends on:

- Applied stress
- Temperature
- Loading rate
- Material composition
- Crystal structure
- Grain size
- Defects
- Heat treatment
- Previous deformation history

## 2.6 Engineering Significance

A component must be designed so that deformation remains within acceptable limits.

For example:

A bridge beam may not fracture but excessive deflection can still make the structure unsafe.

Therefore:

**Strength and stiffness are not the same thing.**

- **Strength** → ability to resist failure.
- **Stiffness** → resistance to deformation.

## LECTURE 27 — HOOKE'S LAW

### 3.1 Hooke's Law

Within the elastic limit:

$$\sigma \propto \epsilon$$

Therefore,

$$\sigma = E\epsilon$$

where E is **Young's modulus**.

Thus:

$$E = \epsilon \sigma$$

### 3.2 Young's Modulus

Young's modulus is a measure of the stiffness of a material under tensile or compressive loading.

$$E = \frac{\text{stress}}{\text{strain}}$$

Unit:

Pa

Usually expressed in GPa.

Approximate values:

- Aluminium: ~69 GPa
- Copper: ~110 GPa
- Steel: ~200 GPa

Therefore, steel is considerably stiffer than aluminium.

### 3.3 Stress–Strain Curve

A typical ductile metal exhibits:

1. Linear elastic region
2. Elastic limit
3. Yield region
4. Plastic deformation
5. Strain hardening
6. Ultimate tensile strength
7. Necking
8. Fracture

### **Important points**

#### **Proportionallimit:**

Stress is proportional to strain.

#### **Elasticlimit:**

Maximum stress from which the material can return approximately to its original dimensions.

#### **Yieldstrength:**

Stress at which significant plastic deformation begins.

#### **Ultimate tensile strength (UTS):**

$UTS = A_0 \text{maximum load}$

#### **Fracturestrength:**

Stress corresponding approximately to final fracture.

### **3.4 Other Elastic Constants**

#### **Shear modulus**

$$G = \tau / \gamma$$

#### **Bulk modulus**

$K = \text{hydrostatic stress} / \text{volumetric strain}$

#### **Poisson's ratio**

When a tensile load is applied, the material generally becomes longer and thinner.

$$\nu = - \text{lateral strain} / \text{longitudinal strain}$$

For isotropic materials:

$$E = 2G(1 + \nu)$$

and

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

## LECTURE 28 — ELECTRICAL RESISTIVITY, CONDUCTIVITY AND OHM'S LAW

The syllabus specifically includes **electrical resistivity of metals, Ohm's law and electrical conductivity**.

### 4.1 Electric Current

Electric current is the rate of flow of electric charge.

$$I=Q/t$$

Unit:

Ampere(A)

### 4.2 Electrical Resistance

Resistance is the opposition offered by a material to current flow.

$$R=V/I$$

Unit:

$\Omega$

### 4.3 Ohm's Law

At constant physical conditions:

$$V=IR$$

Therefore:

$$I=V/R$$

### 4.4 Resistivity

Resistance depends on the dimensions of the conductor.

$$R=\rho L/A$$

Therefore:

$$\rho=RA/L$$

where:

- $\rho$  = resistivity
- $R$  = resistance
- $A$  = cross-sectional area

- $L$  = length

SI unit:

$\Omega\text{m}$

**Important concept**

**Resistance is a property of a particular conductor.**

**Resistivity is an intrinsic property of the material.**

#### 4.5 Electrical Conductivity

Electrical conductivity is the ability of a material to conduct electric current.

$\sigma = 1 / \rho$

Unit:

$\text{S/m}$

Thus:

- High resistivity  $\rightarrow$  low conductivity
- Low resistivity  $\rightarrow$  high conductivity

#### 4.6 Effect of Temperature on Metals

For most metallic conductors:

$$R_T = R_0[1 + \alpha(T - T_0)]$$

where  $\alpha$  is the temperature coefficient of resistance.

As temperature increases:

Metal resistivity generally increases

because increased lattice vibration interferes with electron movement.

### LECTURE 28 — ELECTRONIC AND IONIC CONDUCTION

#### 5.1 Electronic Conduction

Electronic conduction occurs due to the movement of **electrons**.

It is particularly important in:

- Metals
- Semiconductors
- Electronic materials

Metals contain relatively mobile conduction electrons.

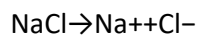
## 5.2 Ionic Conduction

Ionic conduction occurs through movement of positively or negatively charged ions.

It is important in:

- Ionic solids
- Molten salts
- Electrolytes
- Solid electrolytes

For example:



In an electric field, the ions migrate and contribute to electrical conduction.

## 5.3 Electronic vs Ionic Conduction

### Electronic conduction

Electrons are charge carriers

Common in metals

Usually no mass transport of material

High conductivity possible in metals

Important in wires

### Ionic conduction

Ions are charge carriers

Common in ionic materials/electrolytes

Ionic movement occurs

Strongly affected by temperature and defects

Important in batteries, fuel cells and electrochemical devices

## 5.4 Factors Affecting Electrical Conductivity

Conductivity depends on:

- Carrier concentration
- Carrier mobility
- Temperature
- Crystal defects
- Impurities
- Alloying

- Microstructure

A useful conceptual relation is:

$$\sigma = nq\mu$$

where:

- $n$  = carrier concentration
- $q$  = charge
- $\mu$  = carrier mobility

## LECTURE 29 — ENERGY BAND STRUCTURES IN SOLIDS

### 6.1 Why Energy Bands Form

An isolated atom has discrete electron energy levels.

When many atoms come together to form a solid, their atomic orbitals interact.

The discrete energy levels split into a large number of closely spaced levels, producing **energy bands**.

Important bands:

- Valence band
- Conduction band
- Forbidden energy gap

### 6.2 Valence Band

The valence band contains electrons associated with bonding and valence states.

### 6.3 Conduction Band

The conduction band contains energy states in which electrons can move relatively freely and contribute to electrical conduction.

### 6.4 Forbidden Energy Gap

The energy difference between the valence band and conduction band is called the **band gap**:

$$E_g = E_C - E_V$$

where:

- $E_C$  = conduction-band energy
- $E_V$  = valence-band energy

### 6.5 Conductors



In conductors:

- Valence and conduction bands overlap, or
- The conduction band is partially occupied.

Therefore electrons can move easily.

Examples:

- Copper
- Aluminium
- Silver

## 6.6 Insulators

Insulators have a large forbidden energy gap.

Therefore very few electrons can reach the conduction band at ordinary temperatures.

Examples:

- Glass
- Ceramics
- Many polymers

## 6.7 Semiconductors

Semiconductors have a relatively small band gap.

Their conductivity lies between conductors and insulators.

Examples:

- Silicon
- Germanium

## 6.8 Comparison

| Property           | Conductor                               | Semiconductor          | Insulator          |
|--------------------|-----------------------------------------|------------------------|--------------------|
| Band gap           | Very small/overlap                      | Small                  | Large              |
| Conductivity       | Very high                               | Intermediate           | Very low           |
| Temperature effect | Conductivity decreases with temperature | Conductivity increases | Generally very low |
| Example            | Cu                                      | Si                     | Glass              |

## **LECTURE 30 — ELECTRICAL CHARACTERISTICS OF COMMERCIAL ALLOYS AND ALUMINIUM ELECTRICAL WIRES**

The syllabus specifically identifies **electrical characteristics of commercial alloys** and **aluminium electrical wires** as part of Unit–3.

### **7.1 Electrical Characteristics of Alloys**

Pure metals generally provide high electrical conductivity.

However, alloying introduces:

- Solute atoms
- Lattice distortion
- Scattering centres

These interfere with electron movement and generally increase resistivity.

Thus:

Alloying usually decreases electrical conductivity

### **7.2 Why Are Some Alloys Used as Resistance Materials?**

A resistance material should ideally possess:

- High resistivity
- Stable electrical properties
- High melting point
- Good oxidation resistance
- Low temperature coefficient
- Adequate mechanical strength

Examples include resistance-alloy systems such as:

- Nichrome
- Constantan
- Manganin

Applications:

- Heating elements
- Resistance wires
- Electrical measuring instruments

### 7.3 Aluminium as Electrical Wire Material

Aluminium is widely used as an electrical conductor because it offers:

- Good electrical conductivity
- Low density
- Relatively low cost
- Good corrosion resistance due to its oxide film
- Ease of processing

A major advantage is its low density compared with copper.

#### Applications

- Overhead transmission lines
- Distribution conductors
- Electrical cables
- Power transmission

### 7.4 Aluminium vs Copper

| Property                      | Aluminium       | Copper                               |
|-------------------------------|-----------------|--------------------------------------|
| Electrical conductivity       | High            | Very high                            |
| Density                       | Low             | High                                 |
| Weight for transmission lines | Advantageous    | Less advantageous                    |
| Cost                          | Generally lower | Generally higher                     |
| Applications                  | Overhead lines  | Wiring, cables, electrical equipment |

#### Important examination point

#### Why is aluminium preferred for overhead electrical transmission lines?

Because it combines **good electrical conductivity with low density**, making long-span conductors lighter and economically attractive.

## LECTURE 31 — SEMICONDUCTIVITY

The syllabus explicitly requires **intrinsic and extrinsic semiconduction**.

### 8.1 Semiconductor

A semiconductor is a material whose electrical conductivity lies between that of a conductor and an insulator and whose conductivity can be significantly modified by temperature, impurities, light or electric fields.

Examples:

- Silicon
- Germanium

## 8.2 Intrinsic Semiconductor

A pure semiconductor without intentional impurity addition is called an **intrinsic semiconductor**.

At absolute zero:

Very few free charge carriers

At higher temperature, some covalent bonds break and electron–hole pairs are generated.

Thus:

$$n=p$$

where:

- $n$  = electron concentration
- $p$  = hole concentration

## 8.3 Electron–Hole Pair

When an electron gains sufficient energy to move from the valence band to the conduction band:

- A free electron is created in the conduction band.
- A vacancy called a **hole** is left in the valence band.

Both contribute to electrical conduction.

## 8.4 Extrinsic Semiconductor

A semiconductor whose conductivity is deliberately modified by adding controlled impurities is called an **extrinsic semiconductor**.

The process is called **doping**.

Two types:

1. n-type
2. p-type

## 8.5 n-Type Semiconductor

A semiconductor doped with a donor impurity that contributes additional electrons.

For silicon, typical donor elements belong to Group V, such as:

- Phosphorus
- Arsenic
- Antimony

The additional electrons become majority carriers.

Majority carrier = electrons Minority carrier = holes

### 8.6 p-Type Semiconductor

A semiconductor doped with an acceptor impurity.

Typical Group III dopants include:

- Boron
- Aluminium
- Gallium

The major charge carriers are holes.

Majority carrier = holes Minority carrier = electrons

### 8.7 Intrinsic vs Extrinsic

#### Intrinsic

Pure semiconductor

Electron and hole concentrations approximately equal

Lower conductivity

Temperature-dependent

#### Extrinsic

Doped semiconductor

One carrier type dominates

Higher controlled conductivity

Controlled by dopant concentration and temperature

## LECTURE 32 — FACTORS AFFECTING CARRIER MOBILITY AND PIEZOELECTRICITY

The syllabus includes both **carrier mobility** and **piezoelectricity and its applications**.

### 9.1 Carrier Mobility

Carrier mobility indicates how easily a charge carrier moves through a material under an applied electric field.

$$v_d = \mu E$$

where:

- $v_d$  = drift velocity
- $\mu$  = carrier mobility
- $E$  = electric field

## 9.2 Factors Affecting Carrier Mobility

### 1. Temperature

In many materials, increased temperature increases lattice vibrations, resulting in more scattering. Therefore mobility may decrease.

### 2. Impurities

Impurity atoms act as scattering centres.

Higher impurity concentration can reduce mobility.

### 3. Crystal defects

Vacancies, dislocations and other defects can scatter carriers.

### 4. Phonons

Lattice vibrations interact with charge carriers.

### 5. Carrier concentration

At high carrier concentrations, carrier–carrier and impurity interactions can influence mobility.

### 6. Crystal structure

The arrangement of atoms affects the ease with which carriers move.

## 9.3 Piezoelectricity

**Piezoelectricity** is the property of certain materials to develop electric charge on their surfaces when mechanical stress is applied.

This is called the **direct piezoelectric effect**.

Conversely, an applied electric field can produce mechanical deformation.

This is called the **converse piezoelectric effect**.

## 9.4 Principle

Mechanical stress → Electrical charge

and

Electrical field → Mechanical deformation

## 9.5 Examples of Piezoelectric Materials

- Quartz
- Rochelle salt
- PZT (lead zirconate titanate)
- Certain ceramic materials
- Certain polymeric materials such as PVDF

## **9.6 Applications**

### **Sensors**

Mechanical pressure can be converted into an electrical signal.

### **Ultrasonic devices**

Piezoelectric elements generate and receive ultrasonic waves.

### **Ignition systems**

Mechanical force produces a high electrical potential.

### **Microphones**

Sound-induced mechanical vibration is converted into electrical signals.

### **Actuators**

Electrical signals produce controlled mechanical displacement.

### **Medical ultrasound**

Piezoelectric transducers generate and detect ultrasonic waves.

## **LECTURE 33 — MAGNETIC PROPERTIES**

The syllabus requires five major magnetic classifications: **diamagnetism, paramagnetism, ferromagnetism, antiferromagnetism and ferrimagnetism.**

### **10.1 Magnetism**

Magnetism originates primarily from:

- Electron orbital motion
- Electron spin
- Magnetic moments associated with electrons

Materials respond differently to an applied magnetic field.

### **10.2 Diamagnetism**

Diamagnetic materials develop a magnetic moment opposite to an applied magnetic field.

They are weakly repelled by a magnetic field.

### **Characteristics**

- Weak negative magnetic susceptibility
- No permanent magnetic moment in the absence of field
- Weak magnetic response

Examples:

- Copper
- Silver
- Gold
- Bismuth

### **10.3 Paramagnetism**

Paramagnetic materials contain atoms/ions with unpaired electrons.

Their magnetic moments tend to align partially with an applied magnetic field.

They are weakly attracted to the magnetic field.

Examples:

- Aluminium
- Platinum
- Magnesium

### **10.4 Ferromagnetism**

Ferromagnetic materials exhibit strong magnetic interaction between neighbouring atomic moments.

Magnetic moments can align parallel.

Examples:

- Iron
- Cobalt
- Nickel

Characteristics:

- Strong attraction to magnetic field
- Magnetic domains



- Can retain magnetization
- Exhibits hysteresis

### 10.5 Magnetic Domains

A ferromagnetic material consists of regions called **magnetic domains**.

Within a domain:

Magnetic moments are strongly aligned

In an unmagnetized material, domains may have different orientations.

An applied field causes domain alignment, producing magnetization.

## LECTURE 34 — ANTIFERROMAGNETISM, FERRIMAGNETISM AND SUPERCONDUCTIVITY

### 11.1 Antiferromagnetism

In antiferromagnetic materials, neighbouring magnetic moments align in opposite directions with approximately equal magnitude.

Thus:

$\uparrow\downarrow\uparrow\downarrow$

The net magnetic moment is approximately zero.

Example:

- Manganese oxide (MnO)

### 11.2 Ferrimagnetism

In ferrimagnetic materials, neighbouring magnetic moments are aligned oppositely but have **unequal magnitudes**.

Therefore:

Net magnetic moment  $\neq 0$

Ferrites are important ferrimagnetic materials.

Applications:

- Transformer cores
- High-frequency magnetic components
- Permanent magnets
- Electronic devices

### 11.3 Comparison of Magnetic Materials

| Type              | Magnetic moment arrangement                        | Response               |
|-------------------|----------------------------------------------------|------------------------|
| Diamagnetic       | Induced opposite moment                            | Weak repulsion         |
| Paramagnetic      | Random without field; partial alignment with field | Weak attraction        |
| Ferromagnetic     | Parallel                                           | Strong magnetism       |
| Antiferromagnetic | Opposite, approximately equal                      | Nearly zero net moment |
| Ferrimagnetic     | Opposite, unequal                                  | Net magnetization      |

### 11.4 Superconductivity

The syllabus includes **superconductivity** under magnetic properties.

A **superconductor** is a material that, below a characteristic critical temperature, exhibits extremely low electrical resistance and expels magnetic flux under appropriate conditions.

### 11.5 Critical Temperature

The temperature below which superconductivity appears is called the:

Critical temperature  $T_c$

Above  $T_c$ , the material returns to its normal state.

### 11.6 Meissner Effect

A defining characteristic of superconductivity is the **Meissner effect**.

When a material enters the superconducting state, magnetic flux is expelled from its interior under appropriate conditions.

Thus superconductivity is not merely the absence of electrical resistance.

### 11.7 Critical Magnetic Field

A sufficiently strong magnetic field can destroy superconductivity.

The limiting magnetic field is called the **critical magnetic field**.

### 11.8 Applications of Superconductors

- MRI systems
- High-field magnets
- Particle accelerators
- Sensitive magnetic sensors

- Magnetic levitation
- High-performance electrical systems
- Quantum technologies

## LECTURE 35 — ELECTROMAGNETIC RADIATION

The optical-property portion of the syllabus begins with **electromagnetic radiation** and its interactions with solids.

### 12.1 Electromagnetic Radiation

Electromagnetic radiation consists of oscillating electric and magnetic fields propagating through space.

Important parameters:

- Wavelength  $\lambda$
- Frequency  $\nu$
- Speed  $c$
- Photon energy  $E$

Relationship:

$$c = \lambda \nu$$

For electromagnetic radiation in vacuum:

$$c \approx 3 \times 10^8 \text{ m/s}$$

### 12.2 Photon Energy

According to quantum theory:

$$E = h\nu$$

where:

- $E$  = photon energy
- $h$  = Planck's constant
- $\nu$  = frequency

Using:

$$c = \lambda \nu$$

we get:

$$E = hc / \lambda$$

Therefore:

Shorter wavelength → higher photon energy

### **12.3 Electromagnetic Spectrum**

From low to high frequency:

1. Radio waves
2. Microwaves
3. Infrared
4. Visible light
5. Ultraviolet
6. X-rays
7. Gamma rays

As frequency increases:

$\lambda \downarrow$

and

$E \uparrow$

### **12.4 Visible Light**

The visible region is approximately:

400–700nm

approximately.

It contains different colours according to wavelength.

## **LECTURE 36 — LIGHT INTERACTIONS WITH SOLIDS**

When light strikes a solid, several processes may occur:

1. Reflection
2. Refraction
3. Absorption
4. Transmission
5. Scattering

The syllabus specifically emphasizes **atomic and electronic interactions**.

### **13.1 Atomic Interaction**

Electromagnetic radiation can interact with atoms through processes involving:

- Electron excitation
- Electron transitions
- Vibrational transitions
- Rotational transitions

The exact interaction depends on photon energy.

### **13.2 Electronic Interaction**

If photon energy is sufficient, electrons can move between energy states.

For example:

Valence band → Conduction band

If:

$$h\nu \geq E_g$$

a photon may generate an electron–hole pair in a semiconductor.

This principle is important in:

- Photodetectors
- Photovoltaic devices
- Photoconductors
- LEDs

### **13.3 Absorption**

Absorption occurs when incident electromagnetic energy is taken up by the material.

The absorbed energy can produce:

- Electronic excitation
- Vibrational excitation
- Heating
- Electron–hole pairs

### **13.4 Scattering**

Light may change its direction because of interaction with:

- Atoms
- Defects

- Grain boundaries
- Particles
- Microstructural features

Scattering strongly affects the transparency and appearance of materials.

## LECTURE 36 — REFLECTION, REFRACTION, ABSORPTION AND TRANSMISSION

### 14.1 Reflection

Reflection occurs when light returns into the original medium after striking a surface.

The law of reflection states:

$$\theta_i = \theta_r$$

where:

- $\theta_i$  = angle of incidence
- $\theta_r$  = angle of reflection

### 14.2 Refraction

Refraction is the change in direction of light as it passes from one medium to another because its velocity changes.

Snell's law:

$$n_1 \sin \theta_1 = n_2 \sin \theta_2$$

where  $n$  is the refractive index.

For a medium:

$$n = c/v$$

where:

- $c$  = velocity of light in vacuum
- $v$  = velocity in material

### 14.3 Absorption

If incident light intensity is  $I_0$ , the intensity after passing through a material may decrease according to an exponential relationship:

$$I = I_0 e^{-\alpha x}$$

where:

- $I$  = transmitted intensity
- $I_0$  = incident intensity
- $\alpha$  = absorption coefficient
- $x$  = thickness

#### **14.4 Transmission**

Transmission refers to passage of light through a material.

Transparent materials transmit much of the incident visible light.

Examples:

- Optical glass
- Certain polymers
- High-purity transparent ceramics

#### **14.5 Transparent, Translucent and Opaque**

##### **Transparent**

Allows most incident visible light to pass through with relatively little scattering.

Example:

- Window glass

##### **Translucent**

Allows light to pass but scatters it strongly.

Example:

- Frosted glass

##### **Opaque**

Does not transmit significant visible light.

Examples:

- Metals
- Thick ceramics
- Wood

#### **14.6 Optical Properties and Material Structure**

Optical behaviour depends on:

- Electronic structure

- Band gap
- Defects
- Grain boundaries
- Impurities
- Porosity
- Surface condition
- Microstructure

Thus:

Structure→Optical properties

## LECTURE 37 — APPLICATIONS OF OPTICAL PHENOMENA

The syllabus specifically lists:

- Luminescence
- Photoconductivity
- Light-emitting diodes
- Lasers
- Optical fibres in communications.

### 15.1 Luminescence

**Luminescence** is the emission of light by a material that is not primarily caused by heating.

An electron absorbs energy and moves to a higher energy state.

It subsequently returns to a lower energy state and releases energy as light.

Simplified:

Energy absorption→Excited state→Lower energy state→Photon emission

### 15.2 Photoluminescence

When light causes a material to emit light, the process is called **photoluminescence**.

Two important forms:

#### Fluorescence

Emission occurs rapidly and usually stops quickly after excitation is removed.

#### Phosphorescence

Emission can continue for a longer time after excitation.



### 15.3 Photoconductivity

Photoconductivity is the increase in electrical conductivity of a material when light is absorbed.

For a semiconductor:

$$h\nu \geq E_g$$

may generate electron–hole pairs.

Therefore:

Light intensity  $\uparrow \rightarrow$  Carrier concentration  $\uparrow \rightarrow$  Conductivity  $\uparrow$

Applications:

- Light sensors
- Automatic street-light controls
- Photodetectors
- Imaging systems
- Security systems

### 15.4 Light-Emitting Diode — LED

An LED is a semiconductor device that emits light when electrical current passes through it under forward-bias conditions.

The basic mechanism involves electron–hole recombination.

Energy is released as photons.

Approximately:

$$E_{\text{photon}} \approx E_g$$

and:

$$\lambda \approx \frac{hc}{E_g}$$

Therefore the semiconductor band gap

strongly influences the emitted wavelength/colour.

### 15.5 Advantages of LEDs

- High efficiency
- Long service life
- Small size
- Fast response

- Low operating power
- Low heat generation compared with conventional incandescent sources

Applications:

- Displays
- Indicators
- Lighting
- Automotive lamps
- Communication systems

### **15.6 LASER**

LASER stands for:

#### **Light Amplification by Stimulated Emission of Radiation**

A laser produces light through stimulated emission.

### **15.7 Characteristics of Laser Light**

Laser light is generally:

- Highly directional
- Highly coherent
- Nearly monochromatic
- High intensity

### **15.8 Basic Laser Principle**

1. Atoms/electrons are excited.
2. Population inversion is established.
3. Stimulated emission occurs.
4. Photons are amplified.
5. A coherent laser beam emerges.

### **15.9 Applications of Lasers**

- Optical communication
- Welding
- Cutting
- Drilling

- Medical surgery
- Barcode scanners
- Measurement
- Material processing
- Data storage

### **15.10 Optical Fibre**

An optical fibre is a thin, flexible transparent waveguide used to transmit light signals.

It generally consists of:

1. Core
2. Cladding
3. Protective coating

The core has a higher refractive index than the cladding.

$n_{\text{core}} > n_{\text{cladding}}$

This permits light guidance through **total internal reflection**.

### **15.11 Total Internal Reflection**

When light travels from a higher refractive-index medium to a lower refractive-index medium and the incidence angle exceeds the critical angle, total internal reflection occurs.

Critical angle:

$\sin C = n_2 / n_1$

for:

$n_1 > n_2$

### **15.12 Optical Fibre Communication**

Basic communication sequence:

Electrical signal → Light source → Optical fibre → Photodetector → Electrical signal

Typical components:

- LED or laser source
- Optical fibre
- Photodetector

### **15.13 Advantages of Optical Fibre**

- Very high bandwidth
- Low signal attenuation
- Lightweight
- Small diameter
- Immune to electromagnetic interference
- Electrical isolation
- Suitable for long-distance communication

Applications:

- Internet
- Telephone networks
- Cable television
- Data centres
- Medical endoscopy
- Industrial communication

## Mechanical Properties

Normal stress

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

Strain

$$\epsilon = \frac{\Delta L}{L_0}$$

Hooke's law

$$\sigma = E\epsilon$$

Young's modulus

$$E = \frac{\sigma}{\epsilon}$$

Shear modulus

$$G = \frac{\tau}{\gamma}$$

Poisson's ratio

$$\nu = - \frac{\epsilon_{lateral}}{\epsilon_{longitudinal}}$$

## Electrical Properties

## Electrical Properties

Ohm's law

$$V = IR$$

Resistance

$$R = \rho \frac{L}{A}$$

Resistivity

$$\rho = \frac{RA}{L}$$

Conductivity

$$\sigma = \frac{1}{\rho}$$

Carrier conductivity

$$\sigma = nq\mu$$

Drift velocity

$$v_d = \mu E$$

---

## Optical Properties

Wave equation

$$c = \lambda\nu$$

Photon energy

$$E = h\nu = \frac{hc}{\lambda}$$

Refractive index

$$n = \frac{c}{v}$$

Snell's law

$$n_1 \sin \theta_1 = n_2 \sin \theta_2$$

Absorption

$$I = I_0 e^{-\alpha x}$$

## VERY IMPORTANT DIFFERENCES FOR EXAMINATION

### 1. Stress vs Strain

#### Stress

Internal resisting force per unit area

#### Strain

Deformation per unit original dimension

| Stress                                 | Strain                  |
|----------------------------------------|-------------------------|
| $\sigma = F/A$                         | $\epsilon = \Delta L/L$ |
| Unit: Pa                               | Dimensionless           |
| Represents intensity of internal force | Represents deformation  |

## 2. Elastic vs Plastic Deformation

| Elastic              | Plastic                    |
|----------------------|----------------------------|
| Recoverable          | Permanent                  |
| Below elastic limit  | Beyond yield               |
| Temporary            | Permanent                  |
| Important in springs | Important in metal forming |

## 3. Resistance vs Resistivity

| Resistance                         | Resistivity                 |
|------------------------------------|-----------------------------|
| Depends on dimensions and material | Intrinsic material property |
| $R = \rho L/A$                     | $\rho = RA/L$               |
| Unit: $\Omega$                     | Unit: $\Omega m$            |

## 4. Conductor vs Semiconductor vs Insulator

| Conductor                      | Semiconductor             | Insulator             |
|--------------------------------|---------------------------|-----------------------|
| Very high conductivity         | Intermediate conductivity | Very low conductivity |
| Bands overlap/partially filled | Small band gap            | Large band gap        |
| Cu, Al                         | Si, Ge                    | Glass                 |

## 5. Intrinsic vs Extrinsic Semiconductor

| Intrinsic          | Extrinsic                      |
|--------------------|--------------------------------|
| Pure               | Doped                          |
| $n = p$            | $n \neq p$ generally           |
| Lower conductivity | Controlled higher conductivity |

**Intrinsic**

No intentional dopant

**Extrinsic**

Donor/acceptor added

**6. n-Type vs p-Type****n-Type**

Donor impurity

Extra electrons

Electrons are majority carriers

P, As, Sb

**p-Type**

Acceptor impurity

Holes

Holes are majority carriers

B, Al, Ga

**7. Ferromagnetism vs Ferrimagnetism****Ferromagnetic:**

↑↑↑↑

Moments are predominantly parallel.

**Ferrimagnetic:**

↑↓↑↓

but opposing moments are unequal, giving a net magnetic moment.

**8. LED vs LASER****LED**

Spontaneous/recombination-based emission dominates

Broad spectrum relative to laser

Less directional

Lower coherence

Simple and economical

**LASER**

Stimulated emission

Highly narrow spectral output

Highly directional

Highly coherent

More specialized

**IMPORTANT ENGINEERING APPLICATION MAP****Property****Material/Device****Application**

Elasticity

Steel spring

Energy storage

Strength

Steel

Structures



| Property                   | Material/Device    | Application            |
|----------------------------|--------------------|------------------------|
| Conductivity               | Copper             | Electrical wiring      |
| Low density + conductivity | Aluminium          | Transmission lines     |
| High resistivity           | Nichrome           | Heating elements       |
| Semiconductivity           | Silicon            | Electronic devices     |
| Piezoelectricity           | PZT                | Sensors/actuators      |
| Ferromagnetism             | Fe-based materials | Motors/transformers    |
| Ferrimagnetism             | Ferrites           | High-frequency devices |
| Superconductivity          | Superconductors    | MRI/high-field magnets |
| Photoconductivity          | Semiconductor      | Light sensors          |
| Electroluminescence        | LED                | Lighting/displays      |
| Stimulated emission        | Laser              | Communication/cutting  |
| Total internal reflection  | Optical fibre      | Communication          |

### CONCEPTUAL QUESTIONS FOR CLASSROOM DISCUSSION

1. Why does a metal generally become more resistive when heated?
2. Why does adding impurities generally reduce the electrical conductivity of a pure metal?
3. Why can silicon be converted into either n-type or p-type material?
4. Why is aluminium preferred in many overhead transmission applications?
5. Why can steel be strong but still undergo plastic deformation?
6. Why does a semiconductor become more conductive when its temperature increases?
7. Why is a hole treated as a positive charge carrier?
8. Why are ferrites useful at high frequencies?
9. Why does a superconductor expel magnetic flux?
10. Why can glass be transparent while metals are opaque?
11. Why is the band gap important in an LED?
12. Why is optical fibre preferred over metallic cables for very high-bandwidth communication?

### EXAMINATION QUESTION BANK

## **A. 2-MARK QUESTIONS**

1. Define stress.
2. Define strain.
3. What is elastic deformation?
4. What is plastic deformation?
5. State Hooke's law.
6. Define Young's modulus.
7. Define electrical resistivity.
8. Write the SI unit of electrical conductivity.
9. State Ohm's law.
10. Distinguish resistance and resistivity.
11. What is electronic conduction?
12. What is ionic conduction?
13. Define energy band.
14. What is a forbidden energy gap?
15. Define semiconductor.
16. What is an intrinsic semiconductor?
17. What is an extrinsic semiconductor?
18. What is an n-type semiconductor?
19. What is a p-type semiconductor?
20. What is carrier mobility?
21. Define piezoelectricity.
22. Name two piezoelectric materials.
23. What is diamagnetism?
24. What is paramagnetism?
25. Define ferromagnetism.
26. Define antiferromagnetism.
27. Define ferrimagnetism.
28. What is superconductivity?

29. What is the Meissner effect?
30. Define electromagnetic radiation.
31. Write the relationship between wavelength and frequency.
32. Write the expression for photon energy.
33. Define refractive index.
34. State Snell's law.
35. What is photoconductivity?
36. What is luminescence?
37. What is an LED?
38. Expand LASER.
39. What is an optical fibre?
40. What is total internal reflection?

#### **B. 5-MARK QUESTIONS**

##### **Mechanical Properties**

1. Explain tensile stress, compressive stress and shear stress with examples.
2. Explain elastic and plastic deformation.
3. Define stress and strain and derive their relationship according to Hooke's law.
4. Explain Young's modulus, shear modulus and bulk modulus.
5. Explain the important regions of a tensile stress–strain curve.

##### **Electrical Properties**

6. Define electrical resistance, resistivity and conductivity and establish their relationship.
7. Explain Ohm's law with a suitable equation.
8. Explain electronic and ionic conduction.
9. Explain the effect of temperature on the electrical resistivity of metals.
10. Explain the energy-band structure of conductors, semiconductors and insulators.
11. Explain why alloying generally increases the resistivity of metals.
12. Explain the advantages of aluminium as an electrical conductor.

##### **Semiconductors**

13. Explain intrinsic semiconductivity.

14. Explain extrinsic semiconductivity.
15. Differentiate n-type and p-type semiconductors.
16. Explain electron–hole pair formation.
17. Discuss factors affecting carrier mobility.
18. Explain piezoelectricity and mention its applications.

### **Magnetic Properties**

19. Explain diamagnetism and paramagnetism.
20. Explain ferromagnetism with the concept of magnetic domains.
21. Differentiate ferromagnetic, antiferromagnetic and ferrimagnetic materials.
22. Explain the Meissner effect.

### **Optical Properties**

23. Explain electromagnetic radiation and photon energy.
24. Explain reflection and refraction.
25. Explain absorption and transmission of light by solids.
26. Explain photoconductivity.
27. Explain luminescence and distinguish fluorescence from phosphorescence.
28. Explain the working principle of an LED.
29. Explain the basic principle of laser operation.
30. Explain the construction and working principle of optical fibre.

## **C. 10-MARK QUESTIONS**

### **Mechanical Properties**

1. **Explain the mechanical behaviour of engineering materials in detail. Define stress and strain, discuss different types of stress and strain, and explain elastic and plastic deformation with Hooke's law.**
2. **Draw and explain the engineering stress–strain curve for a ductile metal. Discuss proportional limit, elastic limit, yield strength, ultimate tensile strength, necking and fracture.**

### **Electrical Properties**

3. **Explain electrical conduction in materials. Define resistance, resistivity and conductivity, derive their relationships and discuss Ohm's law and the effect of temperature on metallic conductivity.**

4. Explain energy-band theory of solids. Using appropriate band structures, differentiate conductors, semiconductors and insulators.
5. Explain electronic and ionic conduction in materials. Discuss the factors affecting electrical conductivity and carrier mobility.
6. Explain the electrical characteristics of commercial alloys and discuss the reasons for using aluminium in electrical transmission wires.

#### **Semiconductors**

7. Explain intrinsic and extrinsic semiconductor in detail. Discuss electron-hole generation, n-type and p-type semiconductors, majority and minority carriers.
8. Explain the factors affecting carrier mobility and discuss the importance of mobility in determining the electrical conductivity of semiconductor materials.
9. Explain piezoelectricity, its direct and converse effects, important piezoelectric materials and engineering applications.

#### **Magnetic Properties**

10. Explain the magnetic behaviour of materials and classify them into diamagnetic, paramagnetic, ferromagnetic, antiferromagnetic and ferrimagnetic materials with suitable examples.
11. Explain ferromagnetism using the concept of magnetic domains. Discuss magnetization and the significance of domain alignment.
12. What is superconductivity? Explain critical temperature, critical magnetic field and Meissner effect. Discuss important engineering applications of superconductors.

#### **Optical Properties**

13. Explain electromagnetic radiation and its interaction with solids. Discuss reflection, refraction, absorption, transmission and scattering.
14. Explain the optical behaviour of solids from the viewpoint of atomic and electronic interactions. Discuss the role of electronic energy levels and band gap.
15. Explain luminescence, photoconductivity, LED and LASER. Discuss the basic principle and engineering applications of each.
16. Explain the construction, working principle and applications of optical fibre communication. Discuss the role of total internal reflection.

#### **NUMERICAL PROBLEMS FOR PRACTICE**

##### **Problem 1 — Stress**

A steel rod of cross-sectional area  $250\text{mm}^2$  is subjected to a tensile load of  $50\text{kN}$ . Calculate the tensile stress.

**Answer:**

$$\sigma = 50,000 / 250 \quad \sigma = 200 \text{MPa}$$

### **Problem 2 — Strain**

A specimen of original length 100mm elongates by 0.2mm. Calculate strain.

$$\epsilon = 0.2 / 100 \quad \epsilon = 0.002$$

Percentage strain:

$$0.2\%$$

### **Problem 3 — Young's Modulus**

A material experiences a stress of 200MPa and a strain of 0.001. Calculate Young's modulus.

$$E = \sigma / \epsilon \quad E = 200 / 0.001 \quad E = 200 \text{GPa}$$

### **Problem 4 — Resistance**

A wire has:

- Length = 2m
- Cross-sectional area =  $1 \text{mm}^2$
- Resistivity =  $1.7 \times 10^{-8} \Omega \text{m}$

Calculate its resistance.

$$R = \rho L / A \quad R = 1.7 \times 10^{-8} \times 2 / 1 \times 10^{-6} \quad R = 0.034 \Omega$$

### **Problem 5 — Conductivity**

If the resistivity of a material is:

$$2 \times 10^{-8} \Omega \text{m}$$

then:

$$\sigma = 1 / \rho \quad \sigma = 5 \times 10^7 \text{S/m}$$

### **Problem 6 — Photon Energy**

For electromagnetic radiation of frequency  $\nu$ :

$$E = h\nu$$

Thus, increasing frequency increases photon energy.

This relationship is fundamental to understanding:

- Photoconductivity
- Luminescence
- LEDs

- Lasers
- Optical detectors

## **LAST-MINUTE REVISION — ONE-PAGE CONCEPT CHAIN**

### **Mechanical**

Force→Stress→Strain→Deformation  $\sigma=E\epsilon$

### **Electrical**

Voltage→Current→Resistance  $V=IR$   $\rho=RA/L$   $\sigma=1/\rho$

### **Semiconductor**

Energy Band→Electron/Hole→Conductivity  $\sigma=nq\mu$

### **Magnetic**

Electron magnetic moment→Magnetic response Dia→Para→Ferro→Antiferro→Ferri

### **Optical**

$c=\lambda\nu$   $E=h\nu=hc/\lambda$  Light→Reflection/Refraction/Absorption/Transmission

### **Optical Devices**

Photon interaction→Luminescence      Light→Carrier generation→Photoconductivity      Electron-hole recombination→LED Stimulated emission→LASER Total Internal Reflection→Optical Fibre

For classroom delivery, I would therefore emphasize:

**Concept → simple diagram → equation → real engineering material → application → short numerical → exam question.**

For example:

**Copper wire → electron conduction → low resistivity → high conductivity → electrical wiring**

and

**Silicon → band gap → electron–hole pair → doping → n-type/p-type → electronic device**

and

**Light → semiconductor → electron–hole generation → recombination → LED/photodetector**

## **UNIT-4: ENGINEERING MATERIALS**

**Course: Introduction to Materials Engineering (MTPC201)**

**Total Lecture Period: 5 Hours**

### **1. Introduction**

Engineering materials are materials that are selected, processed and used to manufacture components, machines, structures, tools, electronic devices and other engineering products.

The syllabus for **Unit-4: Engineering Materials** allocates **5 hours** and covers three major areas:

1. Fundamentals of Engineering Materials
2. Classification of Engineering Materials:
  - Metals
  - Polymers
  - Ceramics
  - Composites
  - Electronic materials
3. Material Selection

The overall objective of the course is to develop a foundational understanding of materials, their properties and their behaviour so that students can understand how materials are selected and utilized in engineering applications.

## **LECTURE 38 — FUNDAMENTALS OF ENGINEERING MATERIALS**

### **1.1 What is an Engineering Material?**

An **engineering material** is a material having suitable physical, chemical, mechanical, electrical, thermal or optical properties that enable it to be used in an engineering application.

Examples:

- Steel for bridges
- Aluminium for aircraft structures
- Copper for electrical wires
- Polymers for insulation
- Ceramics for high-temperature applications
- Composites for lightweight structures
- Silicon for electronic devices

The important point is:

A material is not selected simply because it is "strong"; it is selected because its overall combination of properties satisfies the requirements of a particular application.

### **1.2 Why Are Engineering Materials Important?**



Almost every engineering product is made from one or more materials.

Examples:

#### **Automobile**

- Steel
- Aluminium
- Polymers
- Rubber
- Glass
- Composites

#### **Electrical equipment**

- Copper
- Aluminium
- Polymers
- Ceramics
- Semiconductor materials

#### **Building**

- Steel
- Cement-based materials
- Glass
- Aluminium
- Polymers
- Ceramics

#### **Aircraft**

- Aluminium alloys
- Titanium alloys
- Composites
- Polymers
- Superalloys

Therefore, engineering design and materials engineering are closely connected.

### **1.3 Fundamental Requirements of an Engineering Material**

Depending on the application, a material may need:

#### **Mechanical properties**

- Strength
- Stiffness
- Hardness
- Toughness
- Ductility
- Wear resistance
- Fatigue resistance
- Creep resistance

#### **Thermal properties**

- Thermal conductivity
- Thermal expansion
- Thermal stability
- Heat resistance

#### **Electrical properties**

- Electrical conductivity
- Electrical resistivity
- Dielectric behaviour
- Semiconductor behaviour

#### **Magnetic properties**

- Permeability
- Magnetic susceptibility
- Retentivity
- Coercivity

#### **Optical properties**

- Transparency
- Reflectivity

- Absorptivity
- Refractive behaviour

### **Chemical properties**

- Corrosion resistance
- Chemical stability
- Oxidation resistance

### **Manufacturing properties**

- Castability
- Weldability
- Machinability
- Formability
- Forgability
- Joinability

## **1.4 Material Structure**

The properties of a material are strongly influenced by its structure.

Material structure can be considered at several levels:

### **Atomic level**

Arrangement of atoms and type of bonding.

Examples:

- Metallic bonding
- Ionic bonding
- Covalent bonding
- Secondary bonding

### **Crystal level**

Arrangement of atoms in crystalline materials.

Examples:

- BCC
- FCC
- HCP

## **Microstructural level**

Features visible under microscopes:

- Grains
- Grain boundaries
- Phases
- Inclusions
- Precipitates
- Porosity

## **Macroscopic level**

Features visible without a microscope:

- Cracks
- Voids
- Surface defects
- Component geometry

## **Processing**

Processing means the method used to manufacture or modify the material.

Examples:

- Casting
- Forging
- Rolling
- Welding
- Heat treatment
- Sintering
- Polymerization
- Composite fabrication

## **Structure**

Processing changes the internal structure.

For example, heat treatment can change:

- Grain structure

- Phase distribution
- Precipitation
- Dislocation density

### **1.6 Example: Steel**

Consider a steel component.

#### **Processing**

Heat treatment is applied.

↓

#### **Structure**

Microstructure changes.

↓

#### **Properties**

Hardness and strength change.

↓

#### **Performance**

Wear resistance and service life change.

Thus, materials engineering connects manufacturing with final engineering performance.

### **1.7 Material Properties vs Material Performance**

These terms should not be confused.

#### **Property**

A measurable characteristic of the material.

Examples:

- Young's modulus
- Yield strength
- Density
- Electrical resistivity

#### **Performance**

How effectively the material performs in a particular application.

For example:

Two materials may have adequate strength, but one may perform better because it has:

- Lower density
- Better corrosion resistance
- Lower cost
- Better manufacturability

## **LECTURE 39 — METALS AND ALLOYS**

### **2.1 Metals**

Metals are one of the most widely used groups of engineering materials.

Typical characteristics include:

- High strength
- Good stiffness
- Good electrical conductivity
- Good thermal conductivity
- Ductility
- Toughness
- Ability to undergo plastic deformation
- Relatively high density compared with polymers

Examples:

- Iron
- Aluminium
- Copper
- Magnesium
- Titanium
- Nickel
- Zinc

### **2.2 Metallic Bonding**

Metallic bonding involves positively charged atomic cores surrounded by relatively mobile electrons.

This helps explain important metallic characteristics such as:

- Electrical conductivity

- Thermal conductivity
- Ductility
- Plastic deformability

## **2.3 Classification of Metals**

Engineering metals can broadly be classified into:

### **Ferrous metals**

Iron is the principal constituent.

Examples:

- Steels
- Cast irons

### **Non-ferrous metals**

They are not primarily iron-based.

Examples:

- Aluminium
- Copper
- Magnesium
- Titanium
- Nickel
- Zinc

## **2.4 Ferrous Materials**

### **Steel**

Steel is primarily an iron–carbon alloy, with carbon content and alloying additions strongly influencing its properties.

Important characteristics:

- High strength
- Good toughness
- Good manufacturability
- Wide range of properties
- Relatively low cost

Applications:

- Buildings
- Bridges
- Automobiles
- Railway components
- Machine parts
- Tools

## **2.5 Cast Iron**

Cast irons contain relatively high carbon compared with steels.

Important properties may include:

- Good castability
- Good compressive strength
- Good wear resistance in appropriate grades
- Good machinability for some grades
- Relatively brittle behaviour for some types

Applications:

- Machine beds
- Engine blocks
- Pipes
- Housings
- Brake components

## **2.6 Non-Ferrous Materials**

### **Aluminium**

Important characteristics:

- Low density
- Good corrosion resistance
- Good electrical conductivity
- Good thermal conductivity
- Good formability



Applications:

- Aircraft
- Electrical conductors
- Automobile components
- Packaging
- Building components

## **Copper**

Important characteristics:

- Very high electrical conductivity
- High thermal conductivity
- Good ductility
- Good corrosion resistance

Applications:

- Electrical wires
- Electrical contacts
- Heat exchangers
- Plumbing

## **Magnesium**

Important characteristics:

- Very low density
- Good machinability
- Useful strength-to-weight ratio

Applications:

- Automotive components
- Aerospace components
- Electronic housings

## **Titanium**

Important characteristics:

- High strength-to-weight ratio

- Excellent corrosion resistance
- Good high-temperature capability compared with many lightweight metals

Applications:

- Aerospace
- Chemical processing
- Biomedical implants

## **2.7 Advantages of Metals**

1. High strength
2. High stiffness
3. Good toughness
4. Good thermal conductivity
5. Good electrical conductivity for many metals
6. Good manufacturability
7. Recyclability
8. Wide range of available alloys

## **2.8 Limitations of Metals**

1. Corrosion can occur.
2. Many metals have relatively high density.
3. Some metals are expensive.
4. Some high-strength alloys may be difficult to process.
5. Electrical conductivity may be undesirable in certain applications.
6. Some metals lose strength at high temperatures.

# **LECTURE 40 — POLYMERS AND CERAMICS**

## **PART A — POLYMERS**

### **3.1 What is a Polymer?**

A **polymer** is a material consisting of very large molecules formed from repeating structural units called monomers.

The word polymer comes from:

- Poly = many

- Mer = units

A simplified representation is:

$(-M-M-M-M-M-)n$

where (M) represents a repeating unit.

### **3.2 Examples of Engineering Polymers**

- Polyethylene (PE)
- Polypropylene (PP)
- Polyvinyl chloride (PVC)
- Polystyrene (PS)
- Nylon
- PTFE
- Epoxy
- Polycarbonate

### **3.3 Classification of Polymers**

Polymers may broadly be classified as:

#### **Thermoplastics**

They soften when heated and can generally be reshaped.

Examples:

- PE
- PP
- PVC
- Nylon

Applications:

- Pipes
- Containers
- Automotive parts
- Packaging

#### **Thermosetting polymers**

They undergo permanent cross-linking during curing and cannot be repeatedly melted and reshaped like thermoplastics.

Examples:

- Epoxy
- Phenolic resin
- Melamine

Applications:

- Adhesives
- Electrical components
- Composite matrices
- Protective coatings

### **Elastomers**

These are polymers capable of undergoing large elastic deformation.

Examples:

- Natural rubber
- Silicone rubber
- Neoprene

Applications:

- Tyres
- Seals
- Gaskets
- Vibration isolation

## **3.4 Properties of Polymers**

### **Advantages**

- Low density
- Good corrosion resistance
- Good electrical insulation
- Easy processing
- Good chemical resistance for many polymers

- Low cost for many applications
- Good design flexibility

### **Limitations**

- Lower stiffness than many metals
- Lower temperature capability
- Creep can be significant
- Thermal expansion is generally relatively high
- Some polymers degrade under UV exposure
- Flammability may be a concern

## **3.5 Applications of Polymers**

### **Automobile**

- Bumpers
- Dashboard components
- Interior components

### **Electrical**

- Cable insulation
- Switch housings
- Connectors

### **Medical**

- Disposable equipment
- Tubing
- Packaging

### **Construction**

- Pipes
- Insulation
- Sealants

## **PART B — CERAMICS**

### **3.6 What are Ceramics?**

Ceramics are generally inorganic, non-metallic materials formed from metallic and/or non-metallic elements.

Examples:

- Alumina ( $\text{Al}_2\text{O}_3$ )
- Silica ( $\text{SiO}_2$ )
- Silicon carbide ( $\text{SiC}$ )
- Silicon nitride ( $\text{Si}_3\text{N}_4$ )
- Glass
- Porcelain

### **3.7 Important Characteristics of Ceramics**

Ceramics generally exhibit:

- High hardness
- High compressive strength
- High temperature resistance
- Good wear resistance
- Good chemical stability
- Good corrosion resistance
- Low ductility
- Brittleness
- Often good electrical insulation

### **3.8 Advantages of Ceramics**

1. High-temperature capability
2. High hardness
3. Excellent wear resistance
4. Good corrosion resistance
5. Good dimensional stability
6. Low electrical conductivity for many ceramics
7. Useful thermal properties

### **3.9 Limitations**

1. Brittleness
2. Low tensile toughness
3. Difficulty in machining
4. Sensitivity to flaws
5. Manufacturing can be complex

### 3.10 Applications

#### Refractories

Used in furnaces and high-temperature equipment.

#### Cutting tools

Hard ceramics such as alumina and silicon nitride can be used in appropriate cutting applications.

#### Electrical insulators

Ceramic insulators are used in electrical systems.

#### Biomedical

Certain ceramics are used for biomedical applications.

#### Construction

Bricks, tiles, sanitary ware and cement-based ceramic-related systems are widely used.

### 3.11 Metals vs Polymers vs Ceramics

| Property                | Metals         | Polymers      | Ceramics         |
|-------------------------|----------------|---------------|------------------|
| Strength                | High           | Low–moderate  | High compressive |
| Stiffness               | High           | Low–moderate  | High             |
| Density                 | Moderate–high  | Low           | Moderate         |
| Ductility               | Usually good   | Variable      | Very low         |
| Toughness               | Generally good | Variable      | Generally low    |
| Temperature resistance  | Good           | Generally low | Excellent        |
| Electrical conductivity | Usually high   | Usually low   | Usually low      |
| Corrosion resistance    | Variable       | Often good    | Generally good   |
| Processing              | Many methods   | Often easy    | Often difficult  |

### PART A — COMPOSITE MATERIALS

#### 4.1 What is a Composite?

A **composite material** is formed by combining two or more distinct constituents so that the resulting material provides a useful combination of properties.

The major constituents are commonly:

1. Matrix
2. Reinforcement

#### 4.2 Matrix

The matrix is the continuous phase.

Functions include:

- Holds reinforcement together
- Transfers load
- Protects reinforcement
- Provides shape

#### 4.3 Reinforcement

The reinforcement improves selected properties.

It may improve:

- Strength
- Stiffness
- Wear resistance
- Thermal stability
- Fatigue behaviour

#### 4.4 Types of Composites

##### Fibre-reinforced composites

Reinforcement is in fibre form.

Examples:

- Glass-fibre reinforced polymer (GFRP)
- Carbon-fibre reinforced polymer (CFRP)



Applications:

- Aircraft
- Wind turbine blades
- Automobile components
- Sports equipment

### **Particle-reinforced composites**

Particles are dispersed in the matrix.

Examples:

- Concrete
- Metal matrix composites containing ceramic particles

### **Laminated composites**

Multiple layers are bonded together.

Examples:

- Laminated glass
- Laminated structural composites

## **4.5 Advantages of Composites**

1. High strength-to-weight ratio
2. High stiffness-to-weight ratio
3. Properties can be tailored
4. Good corrosion resistance for many polymer-matrix systems
5. Good fatigue performance in suitable designs
6. Possibility of directional properties

## **4.6 Limitations**

1. Higher manufacturing cost for some composites
2. Difficult repair in some applications
3. Recycling can be difficult
4. Properties may be anisotropic
5. Manufacturing defects can strongly affect performance
6. Joining may require specialized methods

## **PART B — ELECTRONIC MATERIALS**

### **4.7 What are Electronic Materials?**

Electronic materials are materials whose electrical, semiconductor, dielectric, magnetic, optical or related properties enable them to be used in electronic and electrical devices.

Examples include:

- Silicon
- Germanium
- Gallium-based semiconductor materials
- Dielectric ceramics
- Conductive materials
- Magnetic materials

### **4.8 Conductors**

Conductors have high electrical conductivity.

Examples:

- Copper
- Aluminium
- Silver

Applications:

- Electrical wires
- Busbars
- Electrical contacts

### **4.9 Semiconductors**

Semiconductors have conductivity between conductors and insulators and can be controlled through:

- Doping
- Temperature
- Light
- Electric fields

Examples:

- Silicon

- Germanium

Applications:

- Diodes
- Transistors
- Integrated circuits
- Sensors
- Solar cells

#### **4.10 Dielectric Materials**

Dielectric materials are electrical insulators that can become electrically polarized in an electric field.

Examples:

- Ceramics
- Glass
- Polymers

Applications:

- Capacitors
- Electrical insulation
- Electronic packaging

#### **4.11 Magnetic Electronic Materials**

Magnetic materials are used in:

- Transformers
- Inductors
- Motors
- Magnetic storage
- Sensors

Examples include ferrites and ferromagnetic alloys.

#### **4.12 Optical Electronic Materials**

Materials with controlled optical properties are used in:

- LEDs
- Lasers

- Optical detectors
- Optical fibres
- Displays

A useful engineering comparison is:

| Class                | Main Strength                            | Typical Limitation               | Examples                |
|----------------------|------------------------------------------|----------------------------------|-------------------------|
| Metals               | Strength, toughness, conductivity        | Density/corrosion                | Steel, Al, Cu           |
| Polymers             | Low density, corrosion resistance        | Temperature/stiffness            | PE, PVC, epoxy          |
| Ceramics             | Hardness, temperature resistance         | Brittleness                      | Alumina, SiC            |
| Composites           | Tailored high specific properties        | Cost/recycling                   | CFRP, GFRP              |
| Electronic materials | Controlled electrical/optical properties | Application-specific limitations | Si, dielectric ceramics |

## LECTURE 42 — MATERIAL SELECTION

### 5.1 What is Material Selection?

**Material selection** is the systematic process of choosing the most appropriate material for a particular engineering application.

The correct material must satisfy:

- Functional requirements
- Safety requirements
- Manufacturing requirements
- Economic requirements
- Environmental requirements
- Service-life requirements

### 5.2 Why is Material Selection Important?

Poor material selection can result in:

- Component failure
- Excessive deformation
- Corrosion
- Wear
- Fatigue failure

- Excessive weight
- High manufacturing cost
- Reduced service life

A successful design requires:

Geometry + Material + Manufacturing + Service Conditions

### 5.3 Basic Steps in Material Selection

#### Step 1 — Define the Function

Ask:

What must the component do?

Examples:

- Carry a load
- Conduct electricity
- Resist heat
- Store energy
- Provide insulation
- Resist wear

#### Step 2 — Identify Constraints

What conditions must the material satisfy?

Examples:

- Minimum strength
- Maximum density
- Maximum operating temperature
- Corrosion resistance
- Electrical conductivity
- Dimensional stability

#### Step 3 — Identify the Objective

What are we trying to optimize?

Examples:

- Minimum mass

- Minimum cost
- Maximum stiffness
- Maximum strength
- Maximum life
- Minimum energy consumption

#### **Step 4 — Identify Material Properties**

Select the relevant properties.

For a beam:

- Young's modulus
- Yield strength
- Density

For electrical wire:

- Electrical conductivity
- Density
- Strength
- Cost

For a furnace lining:

- Refractoriness
- Thermal stability
- Thermal conductivity
- Chemical stability

#### **Step 5 — Shortlist Materials**

Candidate materials may be selected from:

- Metals
- Polymers
- Ceramics
- Composites
- Electronic materials

#### **Step 6 — Compare Candidates**

Compare:

- Performance
- Cost
- Processing
- Availability
- Reliability
- Environmental impact

### **Step 7 — Select Manufacturing Process**

The selected material must be compatible with the manufacturing process.

Examples:

- Casting
- Forging
- Rolling
- Machining
- Injection moulding
- Powder processing
- Composite lay-up

### **Step 8 — Evaluate Economic and Environmental Factors**

Consider:

- Raw-material cost
- Processing cost
- Maintenance
- Service life
- Recycling
- Energy consumption
- Environmental impact

## **5.4 Material Selection Triangle**

An excellent classroom way to remember material selection is:

{Performance}  
{Manufacturing}  
{Cost}

A material is suitable only when all three are reasonably satisfied.

## **5.5 Material Selection for Different Applications**

### **Example 1 — Electrical Wire**

Requirements:

- High electrical conductivity
- Low resistivity
- Reasonable mechanical strength
- Low density
- Economical

Possible candidates:

- Copper
- Aluminium

For overhead transmission:

Aluminium is highly attractive because of its low density and good conductivity

### **Example 2 — Cooking Utensil**

Requirements:

- Thermal conductivity
- Corrosion resistance
- Appropriate strength
- Food compatibility
- Ease of fabrication

Possible materials:

- Aluminium
- Stainless steel
- Copper-based materials with appropriate lining

### **Example 3 — Cutting Tool**



Requirements:

- High hardness
- Wear resistance
- High-temperature capability
- Adequate toughness

Possible candidates:

- Tool steel
- Cemented carbide
- Ceramics
- Superhard materials for specialized applications

#### **Example 4 — Aircraft Component**

Requirements:

- Low density
- High strength
- High stiffness
- Fatigue resistance
- Corrosion resistance

Possible candidates:

- Aluminium alloys
- Titanium alloys
- Fibre-reinforced composites

#### **Example 5 — Furnace Lining**

Requirements:

- High-temperature resistance
- Thermal stability
- Chemical stability
- Wear resistance

Ceramics/refractories become strong candidates.

### **5.6 Specific Strength**

For lightweight structural applications, strength alone is not sufficient.

A useful comparison is:

$\text{Specific strength} = \frac{\text{Strength}}{\text{Density}}$

A material with high specific strength can carry significant load with relatively low mass.

This is important in:

- Aerospace
- Automobile
- Transportation
- Sports equipment

### **5.7 Specific Stiffness**

Similarly:

where:

- $(E)$  = Young's modulus
- $(\rho)$  = density

This is important when both stiffness and low mass are important.

### **5.8 Material Selection and Safety**

The selected material should not merely satisfy normal operating conditions.

It should also account for:

- Maximum load
- Temperature variations
- Corrosive environment
- Fatigue
- Impact
- Manufacturing defects
- Unexpected loading
- Service life

Therefore a suitable **factor of safety** may be required.

## **.9 Material Selection and Environment**

Modern material selection should consider environmental impact.

Questions include:

1. Can the material be recycled?
2. How much energy is required for production?
3. Does it contain hazardous substances?
4. How long will it last?
5. Can it be repaired?
6. What happens at the end of its service life?

### **5.10 Important Material Selection Criteria**

A good material-selection decision considers:

#### **Functional properties**

- Strength
- Stiffness
- Conductivity
- Hardness
- Toughness

#### **Service properties**

- Corrosion resistance
- Wear resistance
- Fatigue resistance
- Creep resistance
- Temperature capability

#### **Manufacturing properties**

- Castability
- Machinability
- Weldability
- Formability

- Mouldability

### **Economic factors**

- Material cost
- Processing cost
- Maintenance cost
- Availability

### **Environmental factors**

- Recyclability
- Energy consumption
- Toxicity
- Life-cycle impact

## **7. MATERIAL SELECTION — COMMON MISTAKES**

Students should remember that material selection is **not** simply:

"Choose the strongest material."

For example:

A very strong material may be unsuitable because it is:

- Too expensive
- Too heavy
- Difficult to manufacture
- Difficult to weld
- Poorly corrosion resistant
- Not readily available

Therefore:

**The best material is not necessarily the material having the highest value of one property.**

It is the material that provides the **best overall solution for the specified application.**

## **8. MASTER COMPARISON OF ENGINEERING MATERIALS**

| Parameter | Metal | Polymer | Ceramic | Composite | Electronic Material |
|-----------|-------|---------|---------|-----------|---------------------|
|-----------|-------|---------|---------|-----------|---------------------|

|                         |                     |                      |                    |                           |                         |
|-------------------------|---------------------|----------------------|--------------------|---------------------------|-------------------------|
| Strength                | High                | Low–moderate         | High compressive   | High, depending on design | Application dependent   |
| Density                 | Moderate–high       | Low                  | Moderate           | Often low                 | Variable                |
| Ductility               | Usually good        | Variable             | Very low           | Direction dependent       | Variable                |
| Toughness               | Generally good      | Variable             | Generally low      | Good in selected systems  | Variable                |
| Temperature resistance  | Moderate–high       | Generally low        | Very high          | Variable                  | Variable                |
| Electrical conductivity | Often high          | Usually low          | Usually low        | Variable                  | Specifically engineered |
| Corrosion resistance    | Variable            | Often high           | High               | Often high                | Variable                |
| Processing              | Many processes      | Easy for many grades | Often difficult    | Specialized               | Highly specialized      |
| Typical applications    | Structures/machines | Packaging/insulation | Refractories/tools | Aerospace/automotive      | Electronics             |

## 9. EXAMINATION-ORIENTED SUMMARY

### Metals

#### Remember:

Strength + stiffness + toughness + conductivity + ductility

Main limitation:

Density and corrosion.

### Polymers

#### Remember:

Low density + corrosion resistance + easy processing + electrical insulation

Main limitations:

Temperature capability + stiffness + creep.

### Ceramics

#### Remember:

Hard + heat resistant + wear resistant + chemically stable

Main limitation:

Brittleness.

### **Composites**

#### **Remember:**

Matrix + reinforcement → tailored properties.

Main advantages:

High specific strength and specific stiffness.

### **Electronic Materials**

#### **Remember:**

Electrical + semiconductor + dielectric + magnetic + optical functionality.

## **10. TWO-MARK QUESTIONS**

1. Define an engineering material.
2. What is meant by material selection?
3. Name five major classes of engineering materials.
4. What is a metal?
5. What are ferrous materials?
6. Give two examples of non-ferrous metals.
7. State two important properties of aluminium.
8. State two applications of copper.
9. Define polymer.
10. What is a thermoplastic?
11. What is a thermosetting polymer?
12. What is an elastomer?
13. Give two examples of ceramics.
14. State two important properties of ceramics.
15. Why are ceramics generally brittle?
16. Define a composite material.
17. What is a matrix in a composite?

18. What is reinforcement?
19. Give two examples of fibre-reinforced composites.
20. What are electronic materials?
21. Give two examples of semiconductor materials.
22. What is a dielectric material?
23. What is meant by material property?
24. What is meant by material performance?
25. What is the processing–structure–properties–performance relationship?
26. Define specific strength.
27. Define specific stiffness.
28. State two factors considered during material selection.
29. Why is density important in aerospace material selection?
30. Why is cost considered in material selection?

#### **11. FIVE-MARK QUESTIONS**

1. Explain the importance of engineering materials in modern engineering.
2. Explain the processing–structure–properties–performance relationship with a suitable example.
3. Classify engineering materials into major groups and give examples.
4. Explain ferrous and non-ferrous materials with suitable examples.
5. Discuss the important properties and applications of aluminium.
6. Explain the classification of polymers into thermoplastics, thermosetting polymers and elastomers.
7. Discuss the advantages and limitations of polymers.
8. Explain the important properties and applications of ceramics.
9. Define composite materials and explain matrix and reinforcement.
10. Explain fibre-reinforced composites with examples and applications.
11. Explain the classification of electronic materials.
12. Compare metals, polymers and ceramics.
13. Explain the basic steps involved in material selection.
14. Discuss the factors that should be considered during material selection.
15. Explain the importance of specific strength and specific stiffness in material selection.

16. Explain material selection for an electrical wire.
17. Explain material selection for an aircraft component.
18. Discuss the role of manufacturing processes in material selection.

## **12. TEN-MARK QUESTIONS**

1. Define engineering materials and explain their importance. Discuss the processing–structure–properties–performance relationship with suitable engineering examples.
2. Classify engineering materials into metals, polymers, ceramics, composites and electronic materials. Explain the characteristics, advantages, limitations and applications of each class.
3. Explain metals as engineering materials. Classify them into ferrous and non-ferrous materials and discuss the properties and applications of steel, cast iron, aluminium, copper, magnesium and titanium.
4. What are polymers? Explain thermoplastics, thermosetting polymers and elastomers. Discuss their important properties, advantages, limitations and engineering applications.
5. What are ceramics? Explain their important mechanical, thermal, electrical and chemical characteristics. Discuss their advantages, limitations and engineering applications.
6. Define composite materials. Explain matrix and reinforcement, classify composites and discuss the advantages, limitations and applications of fibre-reinforced composites.
7. Explain electronic materials in detail. Discuss conductors, semiconductors, dielectric materials, magnetic materials and optical materials with suitable examples and applications.
8. Explain material selection as a systematic engineering process. Discuss function, constraints, objectives, required properties, manufacturing process, cost, availability, safety and environmental considerations.
9. Develop a systematic material-selection procedure for an aircraft component. Explain why density, strength, stiffness, corrosion resistance, fatigue behaviour, manufacturing and cost must be considered.
10. Compare metals, polymers, ceramics and composites with respect to density, strength, stiffness, toughness, temperature resistance, corrosion resistance, processing and applications.
11. Explain the concept of specific strength and specific stiffness. Discuss their importance in selecting materials for lightweight engineering structures.
12. A material has to be selected for an engineering component. Explain how you would proceed from identification of the component's function to final material selection, including performance, manufacturing, economic and environmental considerations.

## **13. IMPORTANT APPLICATION-BASED QUESTIONS**

These are particularly useful for classroom discussion and progressive assessment:

**Q1. Why is aluminium preferred for many overhead transmission lines?**



Expected concepts:

- Low density
- Good electrical conductivity
- Suitable strength
- Lower weight of long conductors
- Economic advantages

## **Q2. Why is ceramic preferred for furnace lining?**

Expected concepts:

- High-temperature capability
- Chemical stability
- Wear resistance
- Thermal stability

## **Q3. Why are polymers used for electrical cable insulation?**

Expected concepts:

- High electrical resistivity
- Low density
- Easy processing
- Flexibility
- Corrosion resistance

## **Q4. Why are composites used in aircraft?**

Expected concepts:

- Low density
- High specific strength
- High specific stiffness
- Tailored properties
- Corrosion resistance for suitable systems

## **Q5. Why cannot we simply select the strongest material for every application?**

Expected concepts:

- Cost

- Density
- Manufacturing
- Availability
- Corrosion
- Temperature
- Service conditions
- Environmental considerations

#### 14. QUICK REVISION TABLE

| Material Class              | Remember This                                        | Examples                |
|-----------------------------|------------------------------------------------------|-------------------------|
| <b>Metals</b>               | Strong, tough, ductile, conductive                   | Steel, Al, Cu           |
| <b>Polymers</b>             | Light, corrosion-resistant, insulating               | PE, PVC, epoxy          |
| <b>Ceramics</b>             | Hard, heat-resistant, brittle                        | Alumina, SiC            |
| <b>Composites</b>           | Matrix + reinforcement                               | CFRP, GFRP              |
| <b>Electronic materials</b> | Controlled electrical/optical functionality          | Si, dielectric ceramics |
| <b>Material selection</b>   | Function + properties + process + cost + environment | Application dependent   |