UNIT–I: Crystal Structure and Miller Indices (10 Marks)

(Advanced Engineering Physics – R25)

Introduction

In solid-state physics, understanding the **crystal structure** of materials is essential because it determines their physical, mechanical, electrical, and thermal properties. A crystal is a solid in which atoms or molecules are arranged in a **regular and periodic three-dimensional pattern**. The arrangement of atoms is described using concepts such as **lattice, unit cell, and Miller indices**.

Crystal Structure

A **crystal structure** is formed by the repetition of a basic arrangement of atoms throughout space. It can be mathematically represented as:

Crystal Structure = Lattice + Basis

Crystal Lattice

A lattice is an infinite array of points arranged periodically in three dimensions, where each point has an identical environment.

Basis

A basis is a group of atoms associated with each lattice point.

Unit Cell

A **unit cell** is the smallest repeating unit of a crystal lattice which, when repeated in all directions, generates the entire crystal.

Types of Unit Cells

1. **Simple Cubic (SC)** – atoms only at the corners
2. **Body-Centered Cubic (BCC)** – atoms at corners and one at the center
3. **Face-Centered Cubic (FCC)** – atoms at corners and faces

Atomic Packing Factor (APF)

Structure	Atoms/unit cell	Packing Factor
SC	1	0.52
BCC	2	0.68

Structure	Atoms/unit cell	Packing Factor
FCC	4	0.74

Diagram (Text Explanation)

SC → Atoms only at 8 corners

BCC → Corners + one atom at the center

FCC → Corners + one atom on each face

Miller Indices

Miller indices are a set of three integers **(h k l)** used to represent the orientation of crystal planes.

Steps to Find Miller Indices

1. Find intercepts of the plane on x, y, and z axes
2. Take reciprocals of intercepts
3. Clear fractions to get integers

Example

Intercepts = (2, ∞, 1)
Reciprocals = (½, 0, 1)
Multiply by 2 → **(1 0 2)**

Interplanar Distance

The distance between two adjacent parallel planes is called interplanar spacing.

Formula (for cubic crystals):

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

Where:

- *a* = lattice constant
- *(h k l)* = Miller indices

Importance of Miller Indices

- Used in **X-ray diffraction (XRD)**

- Helps determine **crystal orientation**
- Essential in **material characterization**

Applications of Crystal Structure

- Determination of mechanical strength
- Electrical and thermal conductivity
- Semiconductor and nanomaterial design

Conclusion

The study of crystal structure and Miller indices is fundamental in materials science. These concepts help in understanding atomic arrangement, crystal symmetry, and material behavior, making them essential tools in modern engineering and technology.

Important Keywords

Crystal lattice, unit cell, Miller indices, interplanar spacing, BCC, FCC, SC, diffraction.