

UNIT-1(CRYSTALLOGRAPHY)

Thursday, August 7, 2025

1. INTRODUCTION TO CRYSTALLOGRAPHY

What is Crystallography?

Crystallography is the study of how atoms are arranged in solid materials, especially crystals.

- It uses special tools like **X-ray diffraction** to look inside crystals and see how the atoms are organized.
- This helps scientists learn about the **chemical bonds** and **physical properties** of different materials.
- Crystallography is very important in **science fields** like chemistry, physics, biology, and materials science.
- It has helped make big discoveries in areas like **medicine**, **nanotechnology**, and **electronics**.
- By knowing how atoms are arranged, scientists can understand **how materials behave**.
- It also helps in **creating new materials** with special features for specific uses.

Image of crystalline solid

1. MILLER INDICES (CUBIC SYSTEM)

What is a Crystalline Solid?

A crystalline solid is a type of solid where the tiny building blocks (like atoms, molecules, or ions) are arranged in a very neat and repeating pattern.

This pattern repeats in all directions (3D), which gives the solid a clear shape and strong structure.

The repeating pattern is called a crystal lattice.

Beautiful crystals like diamonds or salt look shiny and symmetric because of this special arrangement.

The fixed spots where the atoms sit in this pattern are called lattice sites.

What is a Single Crystal?

A single crystal is a solid where the atoms are arranged in a continuous and unbroken repeating pattern throughout the entire material.

The pattern extends without any breaks across the whole solid.

There are no grain boundaries (no interruptions in the pattern).

Single crystals are often transparent, shiny, and have uniform properties in specific directions.

Common examples include diamond, quartz, and silicon wafers used in electronics.

What is a Polycrystal?

A polycrystal (or polycrystalline solid) is a solid made up of many small crystals, called grains.

Each grain has a well-ordered atomic pattern, but the grains are not aligned with each other.

The areas where grains meet are called grain boundaries.

Polycrystals are usually stronger and tougher, but may not have uniform properties in all directions.

Common examples include metals like iron, copper, and ceramics.

1. Lattice

plane. This spacing is crucial for understanding crystal structures and plays a key role in techniques such as X-ray diffraction.

Derivation of the Formula

Consider a crystal plane with Miller indices (hkl). The plane intercepts the x, y, and z axes at distances OA, OB, and OC, respectively. By the definition of Miller indices, these intercepts relate to the lattice constants a, b, and c as follows:

- $OA = a / h$
- $OB = b / k$
- $OC = c / l$

Let d be the perpendicular distance from the origin to this plane. Define the direction cosines of this perpendicular line with respect to the x, y, and z axes as $\cos \alpha$, $\cos \beta$, and $\cos \gamma$, respectively.

From right triangle relationships,

- $\cos \alpha = d / OA = d / (a / h) = (d \times h) / a$
- $\cos \beta = d / OB = d / (b / k) = (d \times k) / b$
- $\cos \gamma = d / OC = d / (c / l) = (d \times l) / c$

A fundamental property of direction cosines states:

- $\cos^2 \alpha + \cos^2 \beta + \cos^2 \gamma = 1$

Substituting the above expressions gives:

- $(d \times h / a)^2 + (d \times k / b)^2 + (d \times l / c)^2 = 1$

Which simplifies to:

- $d^2 \times (h^2 / a^2 + k^2 / b^2 + l^2 / c^2) = 1$

Rearranging, the general formula for interplanar spacing is:

- $d_{hkl} = 1 / \sqrt{(h^2 / a^2) + (k^2 / b^2) + (l^2 / c^2)}$

Final Formula for Cubic Systems

In a cubic crystal system, all lattice parameters are equal, i.e., $a = b = c$. Substituting this into the general formula gives:

- $d_{hkl} = 1 / \sqrt{(h^2 / a^2) + (k^2 / a^2) + (l^2 / a^2)}$
 $= 1 / \sqrt{(h^2 + k^2 + l^2) / a^2}$
 $= a / \sqrt{h^2 + k^2 + l^2}$

This formula allows straightforward calculation of the interplanar spacing for any set of planes (hkl) in a cubic lattice, given the lattice constant a.

4. BRAGG'S LAW

What is Bragg's Law?

- Vacancy defects are found in **metals and crystals**.

What is an Interstitial Defect?

An interstitial defect is when an **extra atom gets squeezed** into a small space between atoms.

- It's like stuffing an extra chair between others.
- This makes the material **more dense**.
- It changes how hard or strong the solid is.
- Found in things like **steel**.

What is a Substitutional Defect?

A substitutional defect is when **one atom is replaced** by a different kind of atom.

- It's like swapping one person's seat with someone else.
- This changes the **properties** of the material.
- Common in **alloys**, like brass (copper + zinc).
- It helps make **stronger and rust-resistant** materials.

7. SCHOTTKY DEFECTS AND FRANKEL DEFECTS

What is a Schottky Defect?

A Schottky defect happens when **a positive and a negative ion are both missing**.

- This keeps the charge balanced.
- It makes the material **lighter** (less dense).
- Found in salts like **NaCl (table salt)**.
- It affects how the solid **melts or conducts**.

What is a Frenkel Defect?

A Frenkel defect happens when a **small ion leaves its place** and goes into a gap in the solid.

- The number of atoms stays the same.
- It doesn't change the **density**.
- Seen in materials like **silver chloride (AgCl)**.
- It helps with **electric flow** in some solids.

NOTES CREDIT: ONE AND ONLY FOUNDER "MOHD ASIM SAAD " @asimsaadz.com



What is Schrödinger's Equation?

Schrödinger's equation is a key equation in quantum mechanics. It explains how the **wave function (ψ)** of a particle changes with **time and position**.

- It is like **Newton's laws** in classical physics — but for **quantum particles**.
- It helps us calculate the **behavior and energy** of particles like electrons in atoms.

There are two main forms:

- **Time-Dependent Schrödinger Equation (TDSE)**
- **Time-Independent Schrödinger Equation (TISE)**

8. TIME-DEPENDENT SCHRÖDINGER EQUATION (TDSE)

Equation:

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x, t)}{\partial x^2} + V(x)\psi(x, t)$$

Where:

- $\psi(x, t)$ = wave function (depends on position and time)
- i = imaginary unit ($\sqrt{-1}$)
- \hbar = reduced Planck's constant ($h/2\pi$)
- m = mass of the particle
- $V(x)$ = potential energy

Meaning:

- This equation describes how the wave function **evolves over time**.
- It gives a **complete description** of a quantum system.

Derivation (Basic Idea):

- Start with **energy conservation**:

$$E = \text{K.E.} + \text{P.E.} = (p^2/2m) + V$$

- In quantum mechanics, replace:

$$E \rightarrow i\hbar(\partial/\partial t)$$

$$p \rightarrow -i\hbar(\partial/\partial x)$$

- Plug these into the classical energy equation to get Schrödinger's equation.

