4. Symmetry in Crystals

4.1 Meaning of Symmetry

Symmetry means balanced and repeated arrangement of atoms in a crystal. Symmetry is the balanced and regular repetition of identical parts in a structure. Symmetry refers to the internal arrangement of atoms in a crystal that repeats in a regular and orderly manner in three dimensions.

A crystal is said to be symmetrical if certain movements (rotation, reflection, inversion, translation) bring the crystal into a position indistinguishable from its original position. This regular repetition explains:

✔ Definite shape of crystals

✔ Uniform physical properties

✔ Predictable cleavage planes

✔ Optical and electrical behavior

Thus, symmetry connects **atomic arrangement** to **macroscopic shape**.

- **Why Symmetry is Important in Solid State Chemistry**
  - ✓ Helps classify crystals into crystal systems
  - ✓ Predicts physical properties
  - ✓ Determines crystal structure
  - ✓ Used in XRD interpretation
  - ✓ Basis of space groups

4.2 Symmetry Elements

A symmetry element is an imaginary geometric feature (point, line, or plane) about which a symmetry operation is performed that leaves the crystal unchanged in appearance.

- The element itself is the location.
- The action performed is called the symmetry operation.

Example:

Mirror plane = element

Reflection = operation

o   Plane of Symmetry (m)

o   Axis of Symmetry (Rotation Axis, n)

o   Centre of Symmetry (Inversion Centre, i)

o   Translational Symmetry

1. Plane of symmetry (σ) – divides crystal into two identical halves.

A plane of symmetry is an imaginary plane that divides a crystal into two equal halves, such that one half is the mirror image of the other.
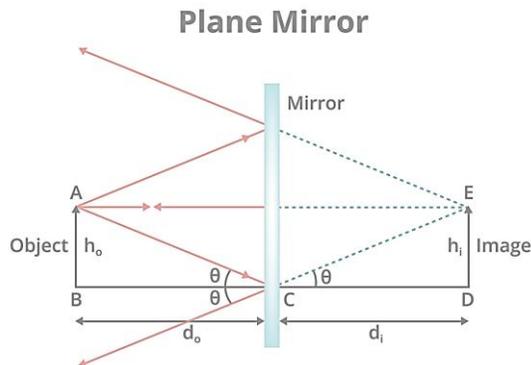
Plane Mirror

Symmetry Operation: Reflection. If a crystal is cut along this plane, the two parts look exactly alike.

- Cube has several mirror planes
- Square plate has 4 mirror planes

NOTE: If even one mirror plane exists, the crystal has plane symmetry.
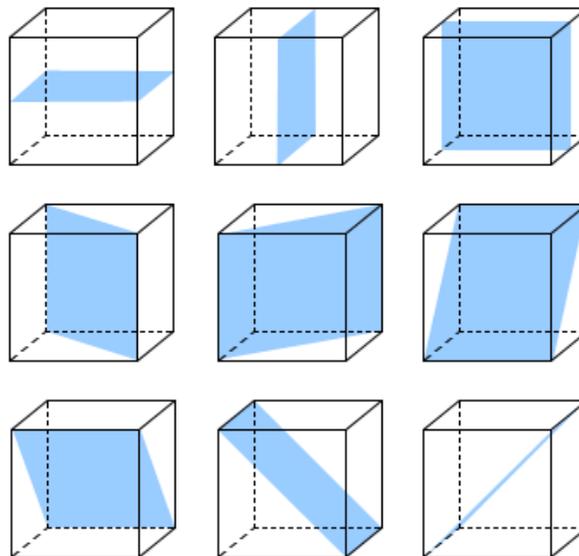
When a crystal possesses a plane of symmetry:
- Every atom on one side of the plane has a corresponding atom on the opposite side

- Both atoms are at equal distance from the plane
- The arrangement appears unchanged after reflection

This means the crystal has **bilateral symmetry**.

Types of Mirror Planes in Crystals

Mirror planes are classified based on their orientation with respect to crystal axes:

1. Vertical Mirror Plane (m_v)

- Plane is parallel to the principal axis
- Divides crystal vertically

Example: Rectangular prism

2. Horizontal Mirror Plane (m_h)

- Plane is perpendicular to principal axis
- Divides crystal into top and bottom halves

Example: Hexagonal prism

3. Diagonal Mirror Plane (m_d)

- Plane lies diagonally between axes

Example: Cube

Plane of Symmetry in Cube

A cube contains 9 mirror planes:

- 3 planes parallel to faces
- 6 diagonal planes

This is why cubic crystals are highly symmetrical.

Mathematical Expression (Atomic Position)

If a mirror plane exists: An atom at position (x, y, z) has a mirror equivalent at: (x, y, −z)
(depending on plane orientation)

2. **Axis of symmetry (C_n) – rotation gives identical appearance**

An axis of symmetry is an imaginary straight line passing through a crystal or object such that rotation of the crystal about this line by a specific angle brings it into an indistinguishable position. If a crystal looks the same after rotation about a line, that line is called an **axis of symmetry**. The symmetry element is the **axis (line)** and the symmetry operation is **rotation**. The axis of symmetry is denoted by n, where n is the order of the axis.

Example:

2-fold axis → 2

4-fold axis → 4

Order of Axis of Symmetry (n-fold Axis): If rotation by $360^\circ/n$ gives an identical appearance, then the crystal has an n-fold axis of symmetry.