

Lecture 6: Symmetry Operations in Crystal Lattices

1. Symmetry Operations

Any operation (or set of operations) that produces a crystal configuration identical to the original crystal is called a symmetry operation.

A symmetry operation is defined as a movement of the crystal or solid around a symmetry element that brings the crystal into a configuration indistinguishable from the original one before completing a full 360° rotation.

2. Symmetry Elements

Before discussing symmetry operations, it is important to recall the symmetry elements, which are:

- **Plane of symmetry:**

A plane that divides the crystal into two identical halves such that one half is the **mirror** image of the other.

- **Axis of symmetry:**

A line passing through the center of the crystal about which **rotation** causes the crystal to coincide with itself.

- **Center of symmetry:**

A crystal has a **center** of symmetry if for every point (or face) in the crystal, there exists an equivalent point (or face) at the same distance on the opposite side of the center.

3. Types of Symmetry Operations

3.1 Rotational Symmetry

Rotational symmetry is achieved by rotating the crystal about an axis passing through one of the lattice points. **After a certain number of rotations through a specific angle, the crystal coincides with itself.**

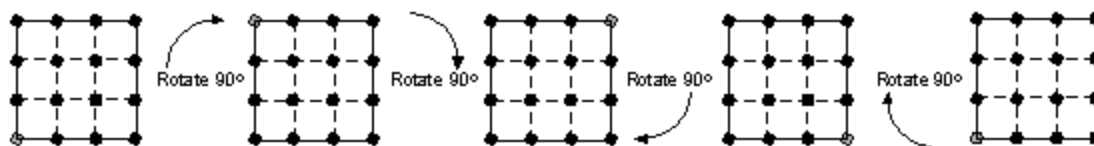
The rotational symmetry is denoted by **n**, where n is an integer representing the order of rotation.

In crystals, the allowed values of n are limited to:

$n = 1, 2, 3, 4,$ and 6

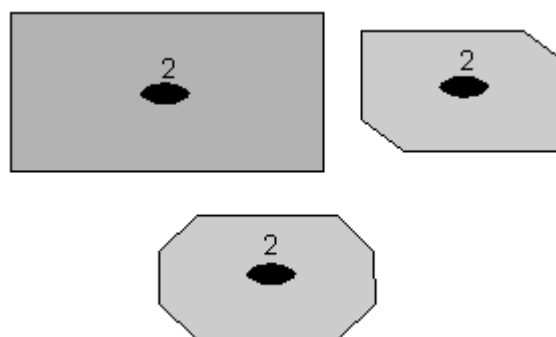
corresponding to rotation angles of:

$360^\circ, 180^\circ, 120^\circ, 90^\circ,$ and 60° , respectively.

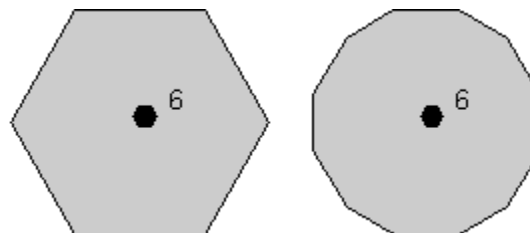


If we rotate the simple crystal by 90° , we notice that the lattice and crystal look exactly the same as they did at the start. Rotate it another 90° , and it's still the same. Another 90° rotation again results in an identical crystal, and another 90° rotation returns the crystal to its original orientation. Thus, in 1 360° rotation, the crystal has repeated itself, or looks identical 4 times. We thus say that this object has 4-fold rotational symmetry.

2-fold Rotation Axis - If an object appears identical after a rotation of 180° , that is, twice in a 360° rotation, then it is said to have a 2-fold rotation axis ($360/180 = 2$). Note that in these examples, the axes we are referring to are imaginary lines that extend toward you perpendicular to the page or blackboard. A filled oval shape represents the point where the 2-fold rotation axis intersects the page.



6-Fold Rotation Axis - If rotation of 60° about an axis causes the object to repeat itself, then it has a 6-fold axis of rotational symmetry ($360/60=6$). A filled hexagon is used as the symbol for a 6-fold rotation axis.





1 - fold



2 - fold



3 - fold

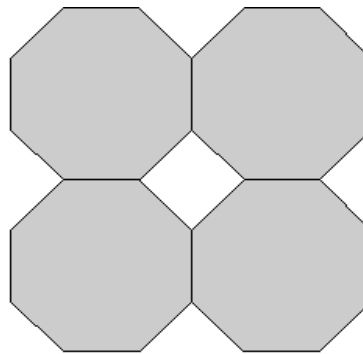
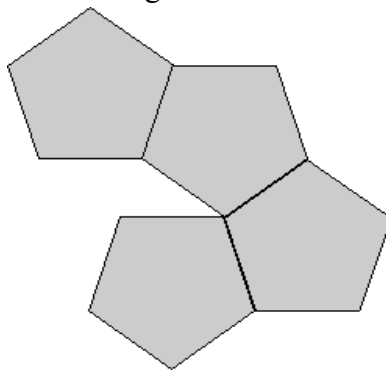


4 - fold



6 - fold

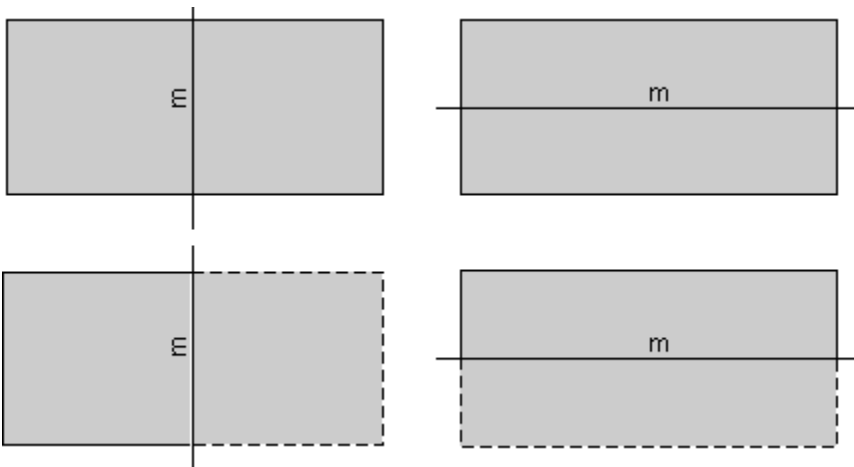
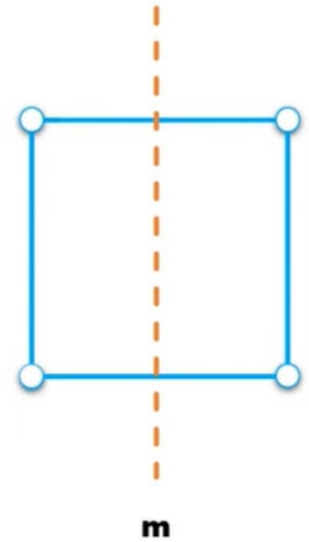
- Note that if we try to combine objects with 5-fold and 8-fold apparent symmetry, we cannot combine them in such a way that they completely fill space, as illustrated below.
- Rotations corresponding to other angles are not possible in periodic crystal lattices. This can be demonstrated by considering the geometric constraints of lattice tiling.



3.2 Mirror (Reflection) Symmetry

In mirror (or reflection) symmetry, the lattice is divided into two identical halves by a plane of symmetry passing through lattice points. The two halves are mirror images of each other.

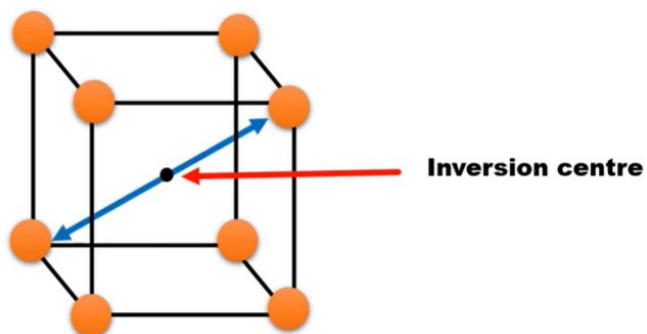
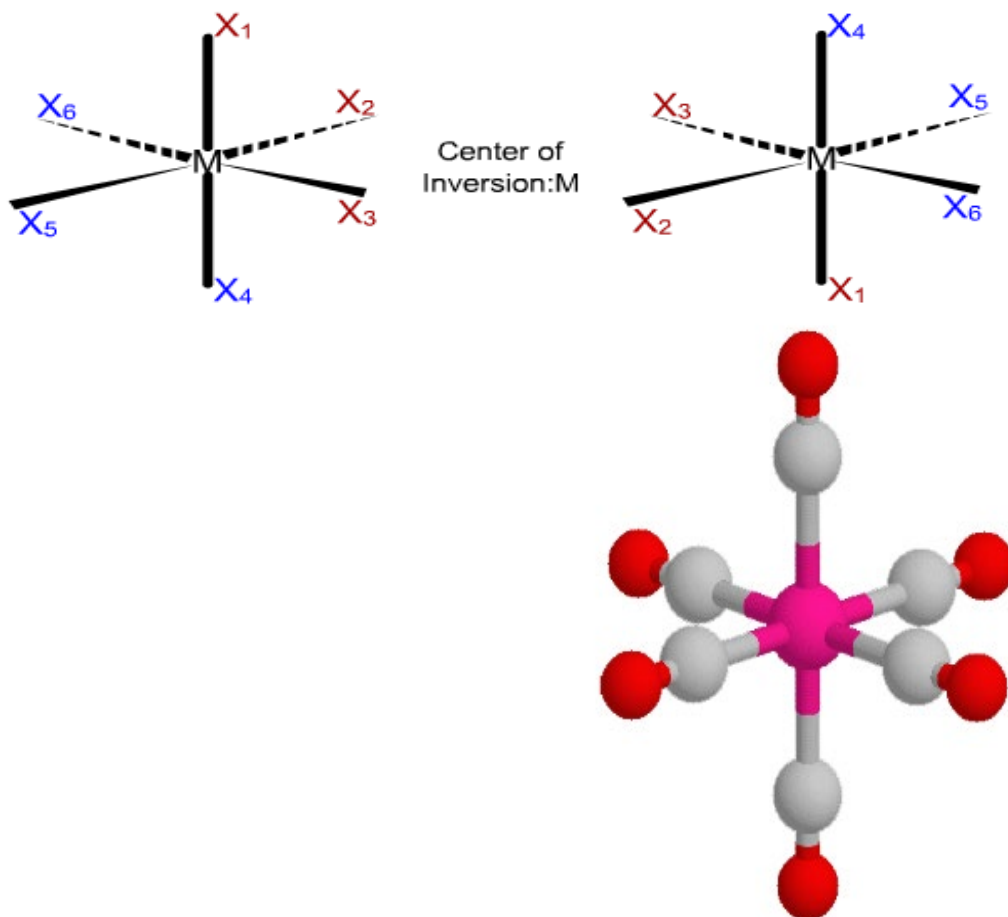
This symmetry operation is denoted by **m**.



3.3 Inversion Symmetry

In inversion symmetry, for every point located at position r relative to the **center of symmetry**, there exists an equivalent point at position $-r$.

This symmetry operation is denoted by **i**.



3.4 Rotation–Inversion Symmetry

In a rotation–inversion operation, the crystal is first rotated by an angle θ about a specific axis and then inverted through a point lying on that axis.

Rotation–inversion axes are denoted by $\bar{n}$.

Example-2:

Rotation–inversion symmetry consists of two consecutive operations:

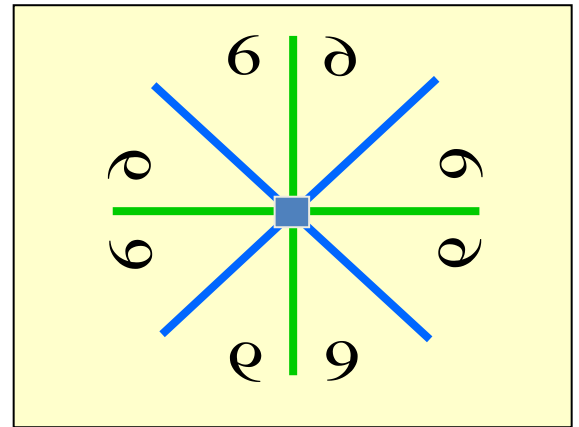
- 1) A rotation by a fixed angle about an axis.
- 2) An inversion through a point (the inversion center).

In the given figure, the green vertical and horizontal lines represent a fourfold rotation axis (90° rotation). The gray square at the center represents the inversion center.

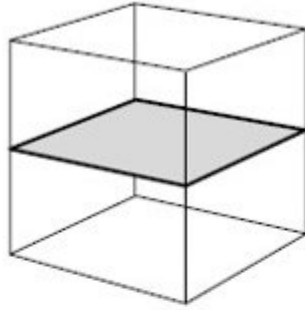
When the pattern is rotated by 90° , it does not coincide with itself. However, when this rotation is followed by inversion through the central point, every element of the figure maps onto an equivalent position. This demonstrates rotation–inversion symmetry.

Symmetry Element

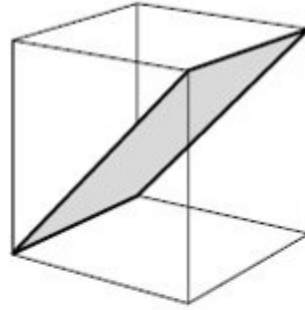
The symmetry element illustrated is a fourfold roto-inversion axis, denoted by: $\bar{4}$



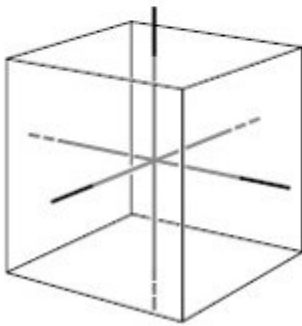
4. Examples of Symmetry Elements in Crystals



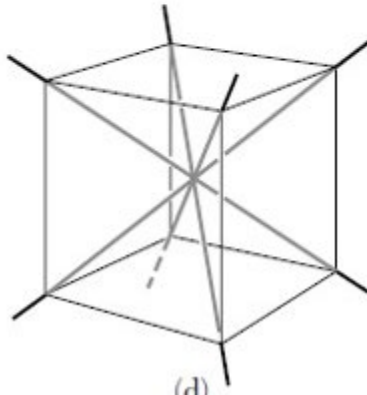
(a)



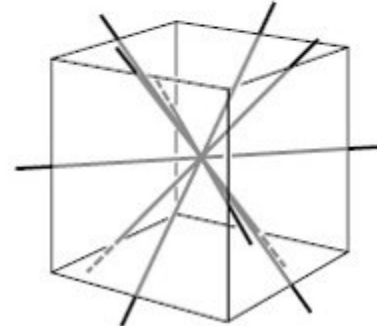
(b)



(c)



(d)



(e)

Examples of common symmetry elements include:

- (a) A mirror plane parallel to a face of a cube
- (b) A diagonal mirror plane
- (c) Three 3-fold rotation axes
- (d) Four 4-fold rotation axes
- (e) Six 6-fold rotation axes