Introduction to Solid State Physics (BSc-III)

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Why Solid state physics ?

Because solids have interesting properties like;

1. Electronic properties: Conducting wires, Transistors, FETs, ICs, etc.
2. Photonic properties: Laser Diodes, Photodiodes and CCD(Charge coupled device).
3. Superconducting properties.
4. Strength on macroscopic scale.

Major differences among solids, liquids and gases

Solids, liquids and gases all are composed of atoms and molecules

In solids and liquids the Nearest neighbor distance is of the order of a few Å
While in gases they are much far away.

The atoms may be arranged in an ordered way or disordered way, the ordered Arrangement forms crystals while the disordered one forms amorphous solids.

Crystal Structure

- An ideal crystal is a **periodic array** of atoms or molecules.

Crystal structure = Lattice + Basis

Regular periodic arrangement of points
In space looking a net-like structure with
Identical environment around every point.
Lattice may be one, two or three dimensional
1D- line lattice
2D- plane lattice
3D- space or crystal lattice

Basis may be a single atom
or a group of atoms attached to
Every point in a lattice.

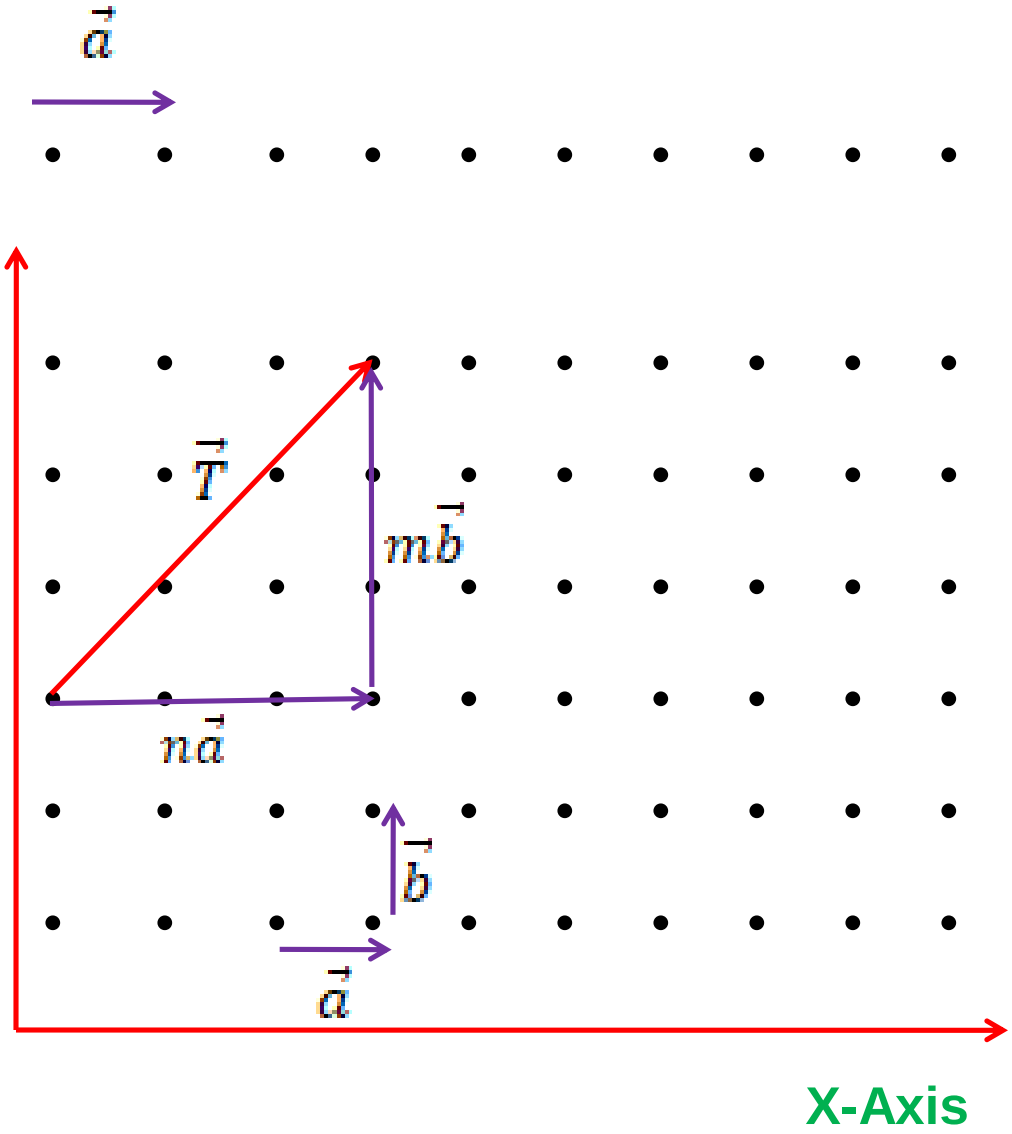
One dimensional (1D) Lattice

$$\vec{T} = n\vec{a}$$

Two dimensional (2D) Lattice

$$\vec{T} = n\vec{a} + m\vec{b}$$

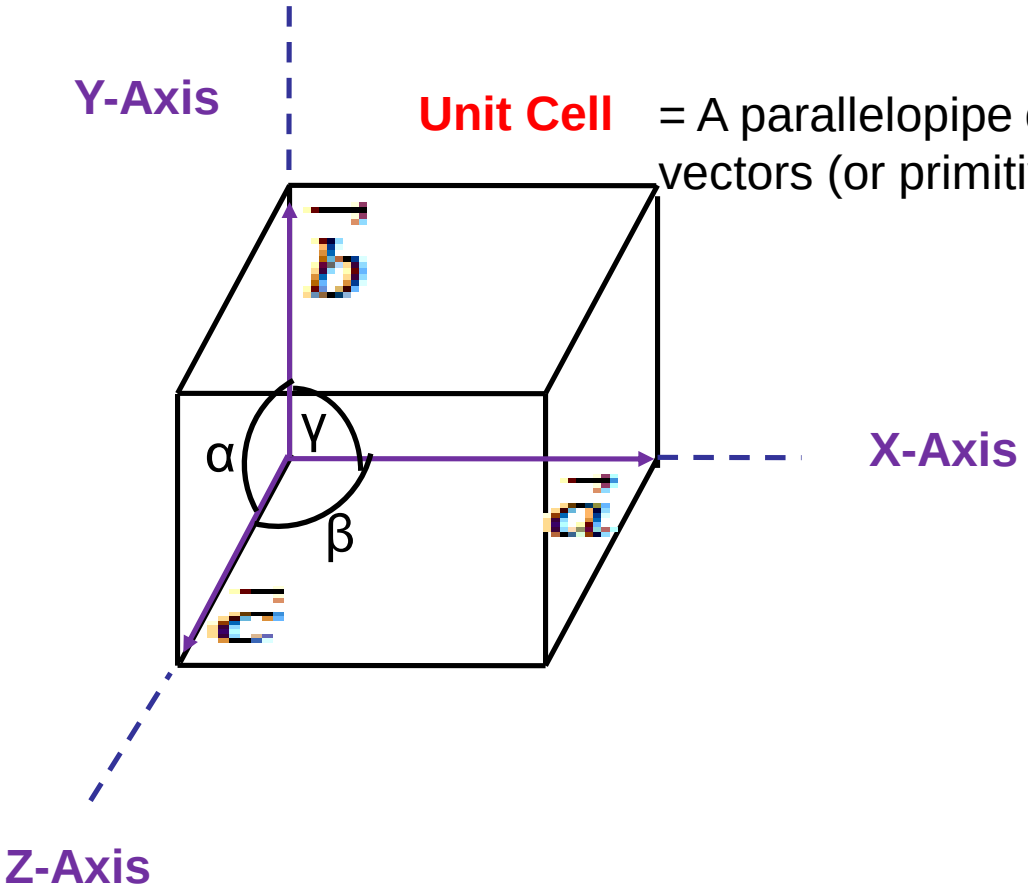
Here $\vec{T}$ is a lattice translation Vector in such a way that we can Go from one lattice point to Any other lattice point throughout The lattice.



And for a three dimensional lattice

$$\vec{T} = n\vec{a} + m\vec{b} + l\vec{c}$$

So the lattice is the collection of all such points where an atom or a group of Atom is supposed to be put in a crystal and all the lattice points are connected Through lattice translation vector T.



Unit Cell = A parallelopipe of unit vectors (or primitive vectors)

α is the angle between primitives $\vec{b}$ and $\vec{c}$
β is the angle between primitives $\vec{c}$ and $\vec{a}$
γ is the angle between primitives $\vec{a}$ and $\vec{b}$

Seven systems of Crystals

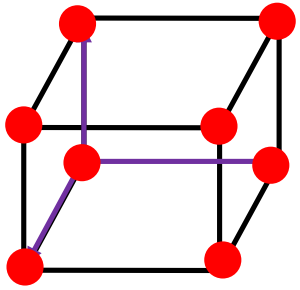
On the basis of shape of unit cell we have seven types of crystal systems

Sr. No.	Name of the system	Relation among a, b, c	Angle between axes	No. of Bravais Space Lattice
1.	Cubic	a=b=c	α=β=γ=90°	SC, FCC, BCC
2.	Trigonal	a=b=c	α=β=γ≠90°	
3.	Hexagonal	a=b≠c	α=β=90°, γ=120°	
4.	Tetragonal	a=b≠c	α=β=γ=90°	
5.	Orthorhombic	a≠b≠c	α=β=γ=90°	
6.	Monoclinic	a≠b≠c	α=γ=90°≠β	
7.	Triclinic	a≠b≠c	α≠β≠γ	

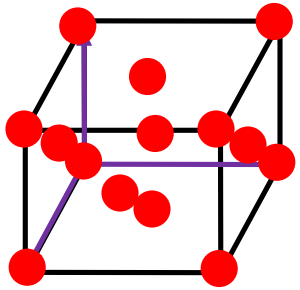
Bravais Lattice

- According to Bravais there are fourteen different types of lattices in the seven crystal systems.

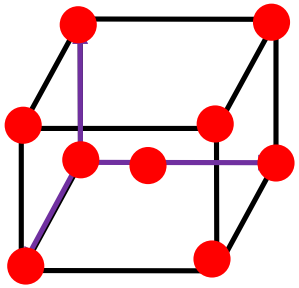
- In cubic systems there are three different types of Bravais lattices namely, SC(Simple cubic), FCC(face centered cubic) and BCC(Body centered cubic).
- **SC-** atoms at the corners of the unit cell
- **FCC-** atoms at the corners and face centers of the unit cell
- **BCC-** atoms at the corners and body centers of the unit cell



SC
P-lattice



FCC
F-lattice



BCC
I-lattice

Symmetry Operations

Any kind of translation, rotation and reflection inside a crystal lattice which leaves the Crystal and its environment unchanged after the operation are called symmetry Operations.

1. Point group symmetry operation: the symmetry operations which are performed about a point or a line are called point group operations.

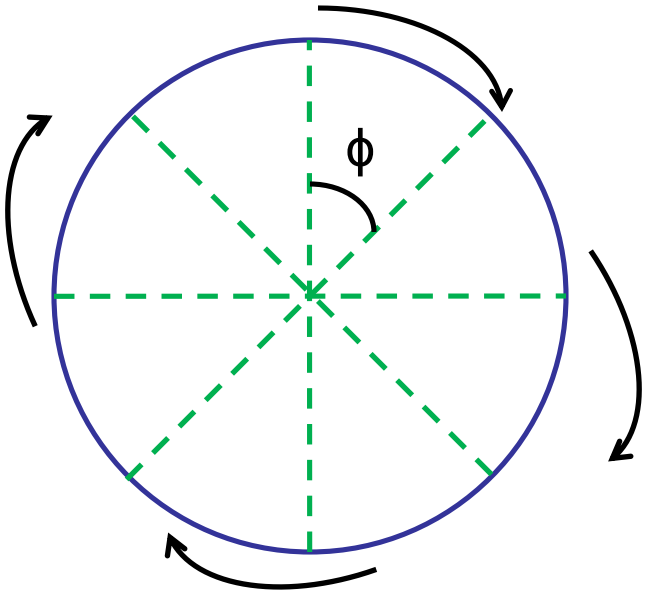
(a) Rotations
(b) Reflections
(c) inversions

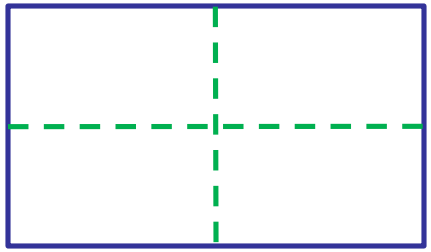
2. Space group symmetry operations: point group symmetry operations+ translation

Rotational symmetry

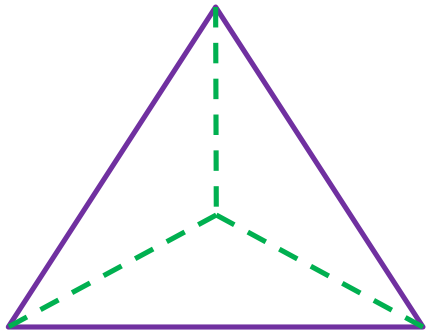
If after rotation by an angle ϕ around an axis a body remains invariant then it has rotational symmetry of n fold, where

$$n=2\pi/\phi$$

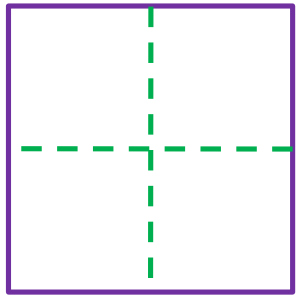




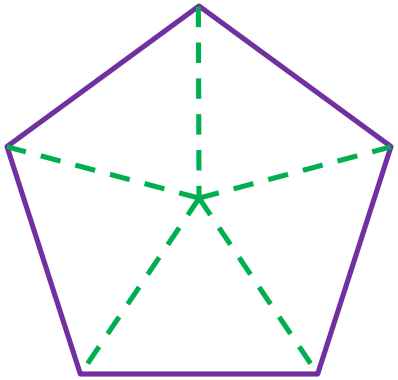
2 fold
symmetry



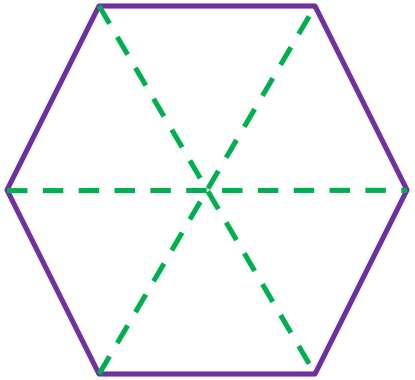
3 fold
symmetry



4 fold
symmetry



5 fold
symmetry

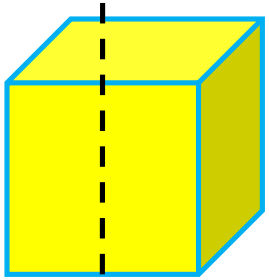


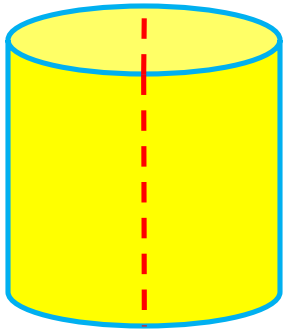
6 fold
symmetry

In a crystal 2,3,4 and 6-fold rotational symmetries occur
But 5-fold symmetry does not exist in a crystal ???

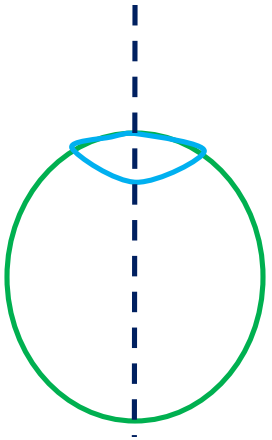
Reflection: A body has reflection symmetry if it is divided in 2 exactly similar parts by a Single plane through the body.

line of reflection symmetry





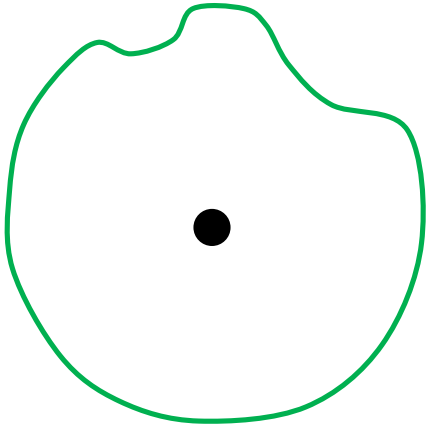
Line of reflection symmetry



The red plane divides the cube and cylinder in two similar parts which are the mirror Images of each other so they have reflection symmetry about the red plane.

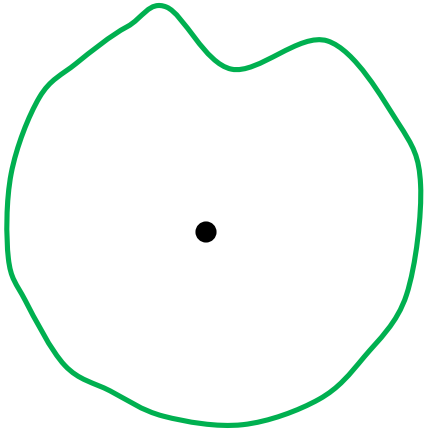
Reflection occurs in a plane about a line through the lattice point

1



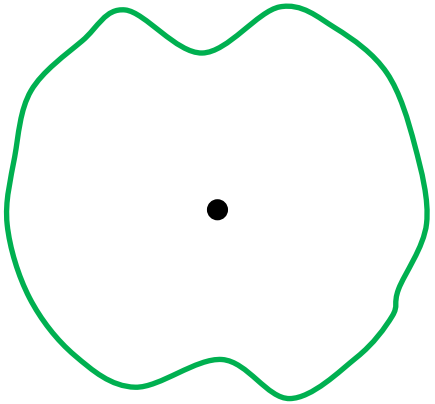
Here we have one-fold
Rotational symmetry
But not any reflection
symmetry

1m

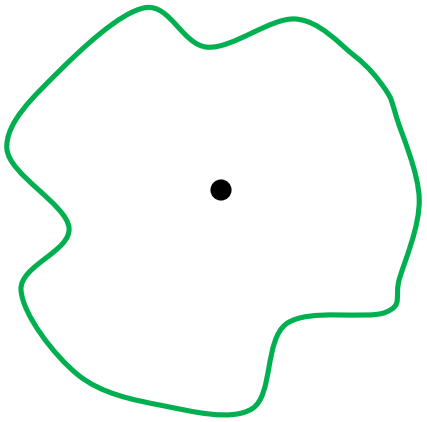


Here we have one-fold
Rotational symmetry
And also the mirror
Reflection symmetry

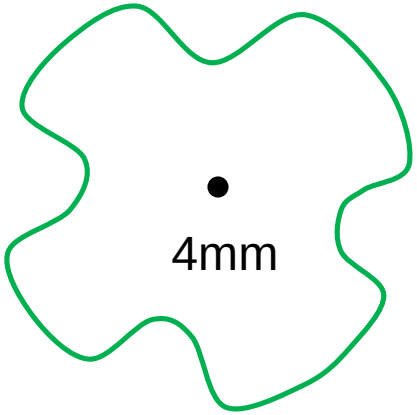
2mm



3m



Here we have 4-fold
Rotational symmetry
Plus reflection
Symmetry parallel to
Rotation axis and reflection
Perpendicular to rotation
axis



4mm

In 2 dimension, rotation plus reflection symmetry at a point is called point group Symmetry. A total of point 10 groups in 2 dimensional space are allowed and they are,

1, 1m, 2, 2mm, 3, 3m, 4, 4mm, 6, 6mm

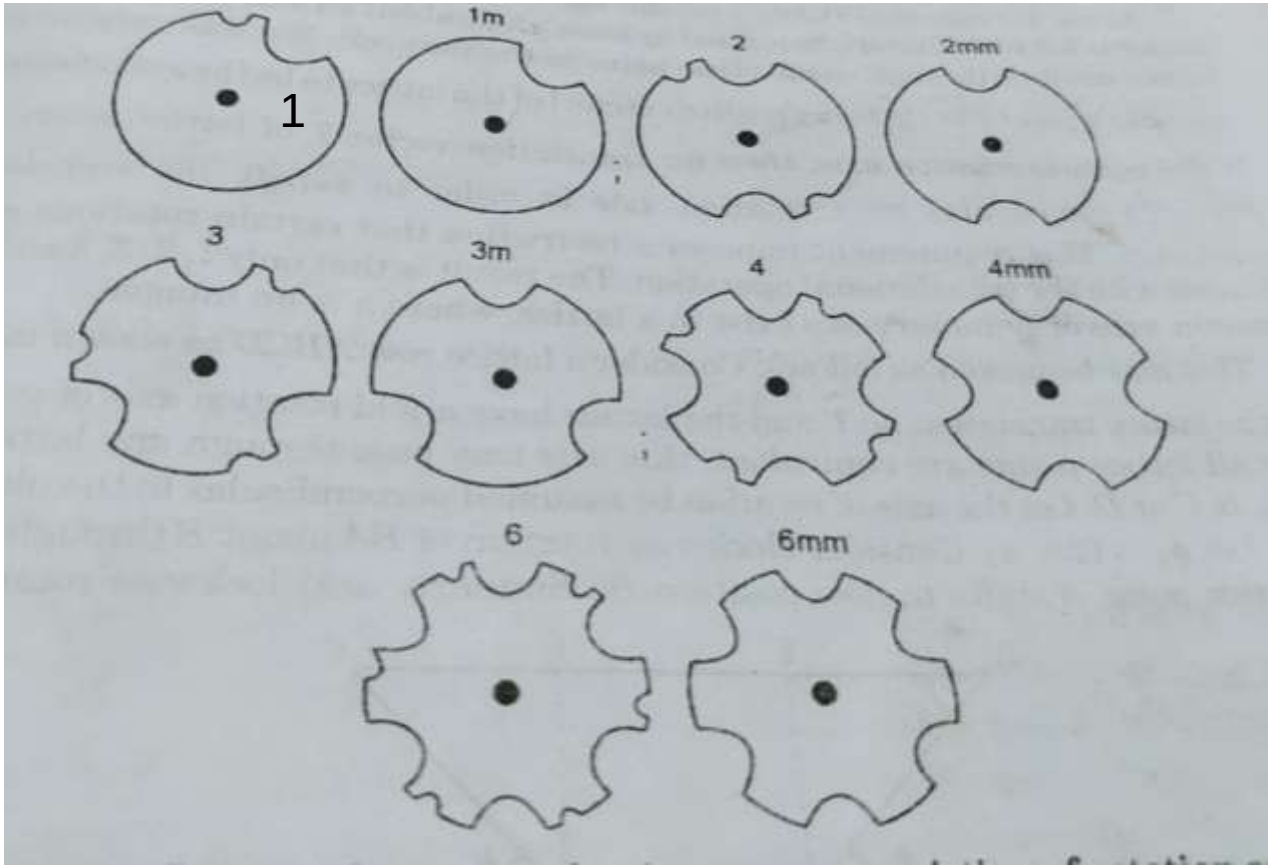
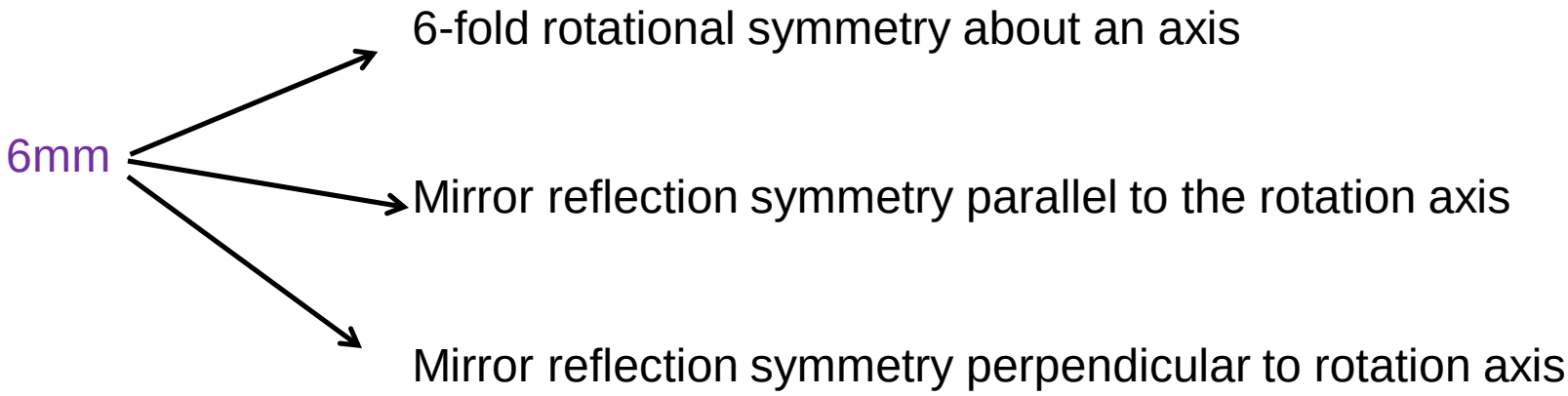


Figure taken from J. P. Agarwal Book

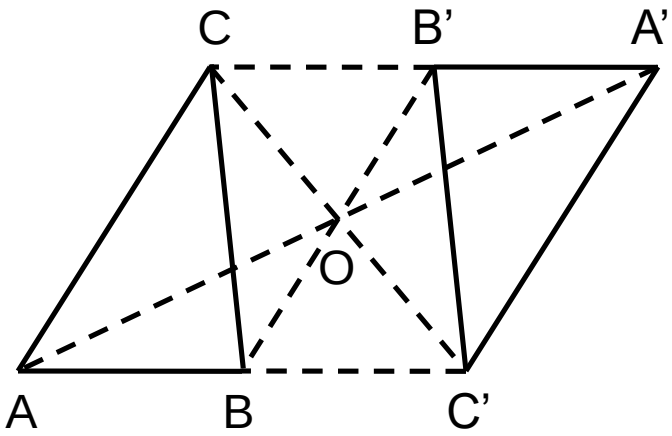
1. The first symbol means rotation about a point
2. The second symbol means reflection line/lines parallel to the rotation axis
3. The third symbol means reflection line/lines perpendicular to the rotation axis



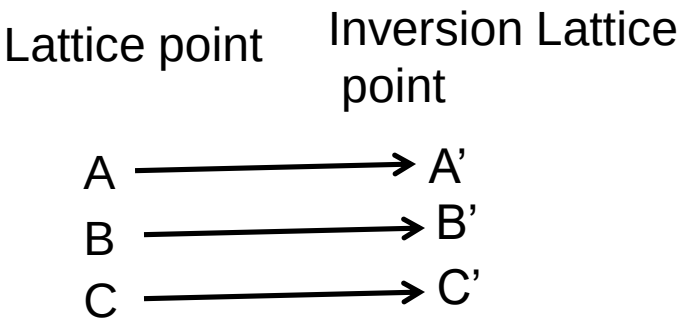
A crystal having any particular point group symmetry is said to belong to a particular crystal class

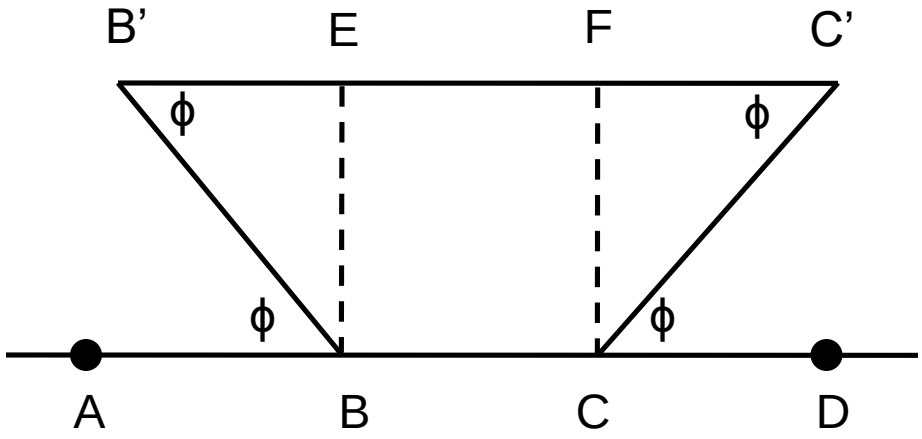
Inversion Symmetry

A crystal has an inversion symmetry if for every lattice point at **r** we have corresponding lattice points at (**-r**). The inversion centre is denoted by "I".



Reflection about a point





Since B' and C' are lattice points of the crystal obtained by the rotation of BA and CD, so B' and C' must be some lattice points in the crystal Lattice, therefore

B'C'=pT, where p is an integer and T is lattice translation

B'C'=B'E+EF+FC'

=T Cosϕ+T+TCosϕ

=T+2TCosϕ

pT=T+2TCosϕ

Cosϕ=(p-1)/2, p=0,1,2,-1,-2

Since p is integer so (p-1) is also integer

Cosϕ=N/2

For N=0, Cosϕ=0

→ ϕ=90°, 270°,

For N=1, Cosϕ=1/2

ϕ=60°

For N=2, ϕ=0, 2π

For N=-1, ϕ=120°

For N=-2, ϕ=180°

So multiplicity factor

n=2π/ϕ

For ϕ=2π, n=1

For ϕ=π, n=2

For ϕ=120°, n=3

For ϕ=90°, n=4

For ϕ=60°, n=6

For ϕ=0, n=infinite

So n≠5

Translational symmetry Elements(Identity of crystals):

A crystal is said to have translational symmetry if for every lattice point at r there exists a lattice point at (r+T) with identical environment.

Where

$$\vec{T} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c}$$

(a) Glide plane: Reflection+translation=Glide plane

Axial Glide plane(a, b, c) means translation along different axes by (a/2, b/2, c/2)

Diagonal Glide plane (n) means translation along the diagonal by {(a/2+b/2), (b/2+c/2), (c/2+a/2)}

Diamond Glide plane(d) means translation in diamond crystal by {(a/4+b/4), (b/4+c/4), (c/4+a/4)

(b) **Screw axis:** rotation+translation (parallel to rotation axis)=Screw axis

Space groups = point group symmetry+ trannslational symmetry

Total 230 space groups

Knowing space group we can specify crystal symmetry completely

It is collection of all the symmetry elements, determined by lattice and basis

It determines the positions of equivalent points within the unit cell through its symmetry elements