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Paper I- PHY 361 Solid State Physics

Unit-1 The crystalline structures

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CH.1 THE CRYSTALLINE STRUCTURES

Crystalline state:

A solid shows definite volume, definite shape and definite mass. The atoms in solids are arranged closely. This leads to higher densities in solids. With a little change in temperature or pressure, a solid maintains its shape. In some solids such as glasses and amorphous materials, there is no orderly arrangement of atoms or molecules. Solids are classified in to two groups as crystalline solids and amorphous solids. Crystalline solids are either polycrystalline or single crystal type. Crystalline solids show a regular orderly arrangement. Amorphous solids do not show a regular orderly arrangement. These solids do not have sharp melting points.

Lattice:

Lattice is defined as an infinite, regular, periodic arrangement of points in space. Every lattice point has identical surrounding. The periodicity of lattice points can be different in different directions. To understand the pattern of atomic arrangement in a crystal, atoms or molecules can be located at these points in space.

Basis:

A crystal structure is formed by associating with every lattice point, a unit assembly of atoms or molecules identical in composition. It is the structural unit of a crystal consisting of an atom, an ion or a molecule.

Lattice and basis together form a crystal structure as shown in fig.1.

Where, Lattice + Basis = Crystal structure

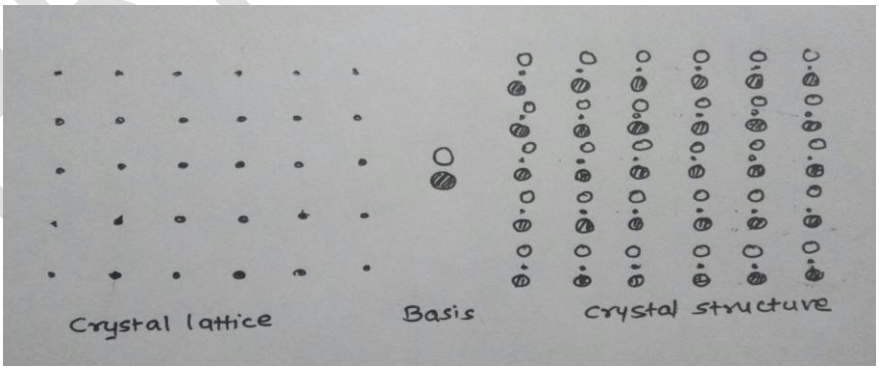


Fig. 1

Translational vectors:

The translation vector is the distance through which an atom must be moved (translated) in order to be in the next unit cell.

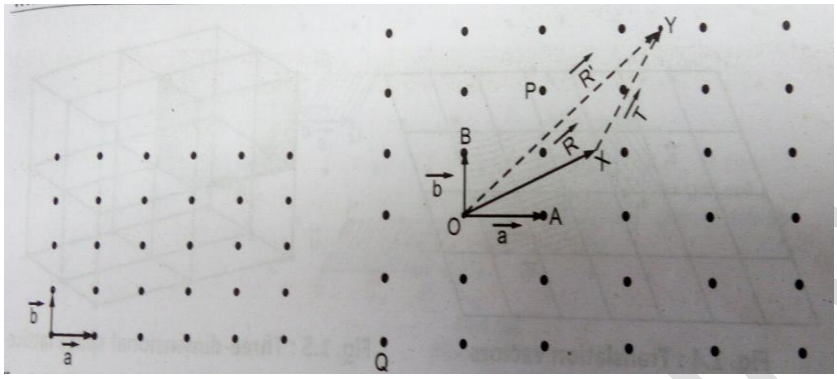


Fig.2

a, b are distances between two neighboring points along x and y directions.
Repeated translations of two vectors $\bar{a}$ and $\bar{b}$ can generate an array.
These vectors are called fundamental translational vectors.

Primitive unit cell:

A cell is considered to be a primitive cell, if primitive translation vectors are used to construct it. In two dimensions, a primitive cell has minimum area and the lattice points lie at its corner only. So effective number of lattice points in a primitive cell is one. In a non-primitive cell, lattice points are present at the corners of the cell as well as at other position(s) within the cell. Hence effective number of lattice points in a primitive cell is greater than one.

The small identical building units, repeating again in three dimensional space to form a crystalline structure are called unit cells. The unit cell may be a primitive or non-primitive cell.

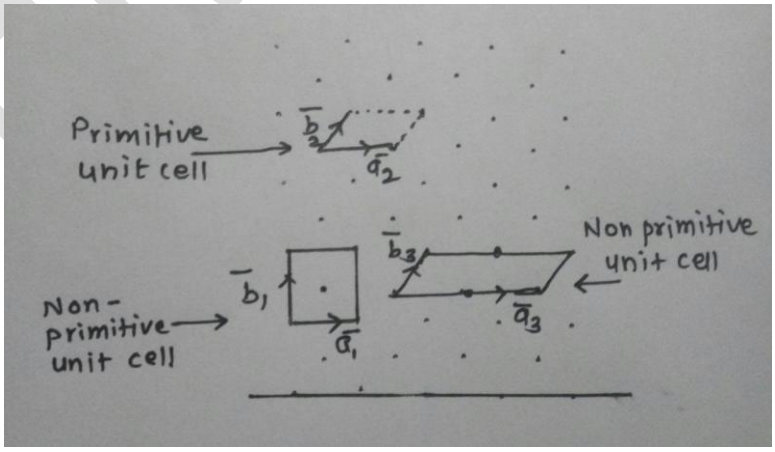


Fig.3

Symmetry operations:

There are certain operations which when performed on a structure, show no change in the appearance of the structure. Such operations are called symmetry operations. The structure here is said to possess symmetry under that operation.

The symmetry operations carried about a point or a line are called point group symmetry operations. The symmetry operations carried out by translation as well as rotation are called space group symmetry operations.

The commonly occurring symmetry operations are as enlisted here.

1. Translational symmetry
2. Rotational symmetry
3. Symmetry under mirror reflection
4. Symmetry under inversion
5. Screw symmetry
6. Glide Plane symmetry

The discussion regarding these operations is as follows.

1. Translational symmetry:

The translational symmetry is observed when a structure undergoes a movement or a shift in a specified direction through a specified distance without any rotation or reflection. The distances between points and angles within the figure do not change. The size and shape of the figure does not change. Only location of it changes through some distance.

2. Rotational symmetry:

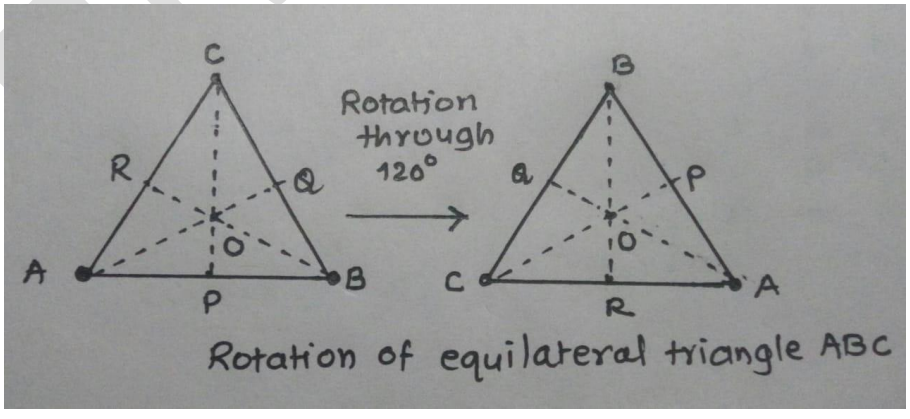


Fig.4

An equilateral triangle ABC rotated around point O through angles 120°, 240°, 360° show the same structure. The symmetry of this kind is known as rotational symmetry.

The fold number is given by the formula…..

Fold number = 2 π / (Minimum angle of rotation to show the same structure)

Hence an equilateral triangle possesses a 3 fold rotational axis of symmetry around the rotational axis. This symmetry can be observed in case of a cube with different fold numbers. The crystalline solids show 1,2,3,4 and 6 fold symmetry.

3. Symmetry under mirror reflection:

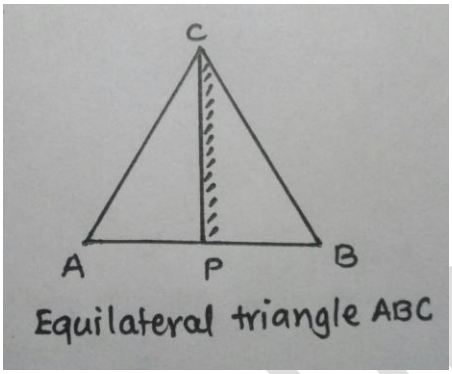


Fig.5

A structure is said to have reflection symmetry, if it is invariant after reflected by a plane.

If a plane mirror perpendicular to plane of equilateral triangle ABC is placed along CP, the image reproduces the other half portion of triangle. Such a plane is called a plane of symmetry.

4. Symmetry under inversion:

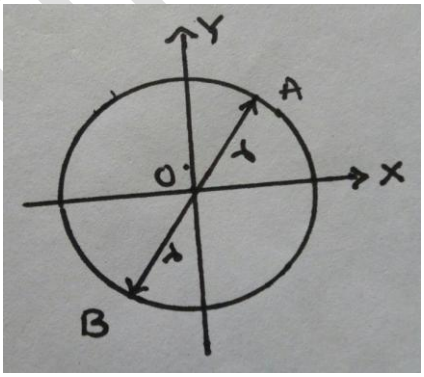


Fig.6

The centre of symmetry is also known as the centre of inversion (I). It is the point in the crystal such that if a line is drawn from any point on the crystal through this point and produces an equal distance on the other side of this centre, it meets an identical point.

In above figure AO = OB. The points A and B lie in opposite quadrants on the circumference of a circle. The point O is the centre of symmetry.

5. Screw symmetry:

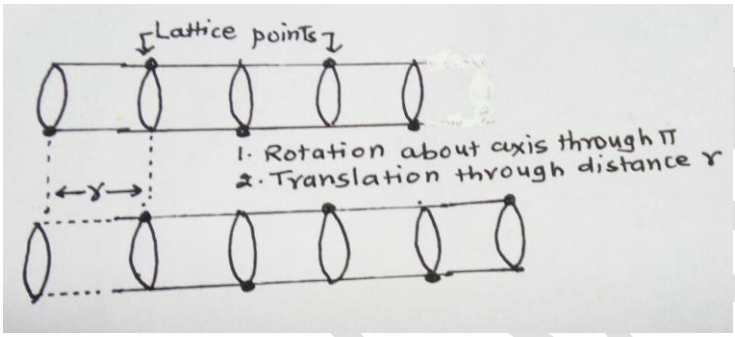


Fig.7

It is a compound symmetry operation with translation and rotation applied successively. If the cylinder shown in the figure is rotated through an angle of 180° and then translated through a distance r parallel to the axis of the cylinder, the same structure is observed. As the above operation is like screw, the structure is said to possess screw symmetry.

6. Glide Plane symmetry:

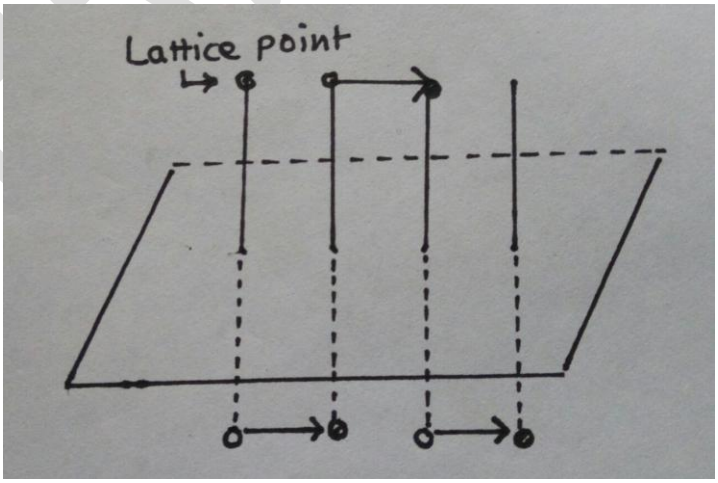


Fig.8

It is a compound symmetry operation with translation and mirror reflection applied successively leaving the structure invariant or unchanged. The glide plane in the crystal is always parallel to the mirror plane. The structure possessing this property is said to have glide plane symmetry.

Different types of lattices:

2D lattices:

In 2 dimensions, different lattices can be generated with different magnitudes of vectors a and b as well as different angles between them.

This gives us following five types of lattices.

1. Oblique lattice
2. Square lattice
3. Hexagonal lattice
4. Rectangular Lattice
5. Centred Rectangular lattice

1. Oblique Lattice:

In this kind of lattice, magnitudes of two vectors $\bar{a}$ and $\bar{b}$ are not equal.
The angle θ between them is not equal to π/2.

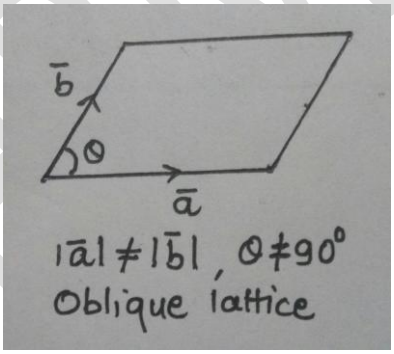


Fig.9

2. Square lattice

Magnitudes of two vectors $\bar{a}$ and $\bar{b}$ are equal.
The angle θ between them is equal to π/2.

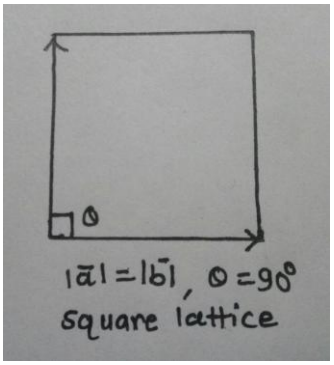


Fig.10

3. **Hexagonal lattice**
   Magnitudes of two vectors $\bar{a}$ and $\bar{b}$ are equal.
   The angle θ between them is equal to $2\pi/3$.

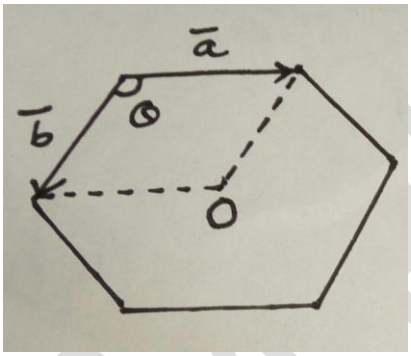


Fig.11

4. **Rectangular Lattice**
   Magnitudes of two vectors $\bar{a}$ and $\bar{b}$ are not equal.
   The angle θ between them is equal to $\pi/2$.

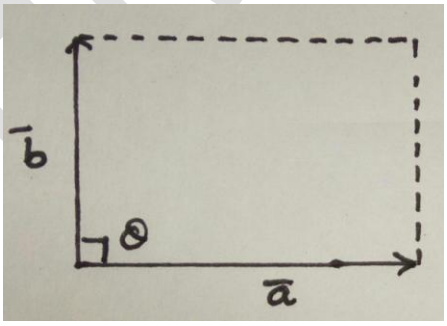


Fig.12

5. **Centred Rectangular lattice**
   Magnitudes of two vectors $\bar{a}$ and $\bar{b}$ are not equal.

The angle between them θ is equal to π/2,
There is an extra lattice point at the centre.

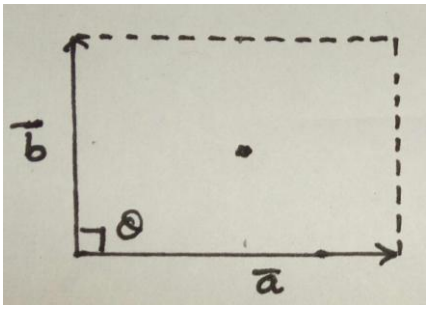


Fig.13

3D lattices (Bravais lattices)

In three dimensional case, fourteen different types of lattices can be generated with the three translational vectors $\bar{a}$, $\bar{b}$, $\bar{c}$ having different magnitudes and different angles between them α, β, γ as shown in the figure.

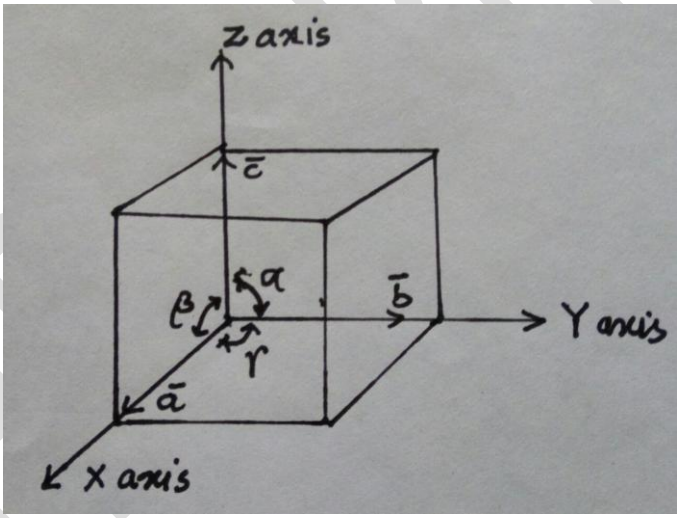


Fig.14

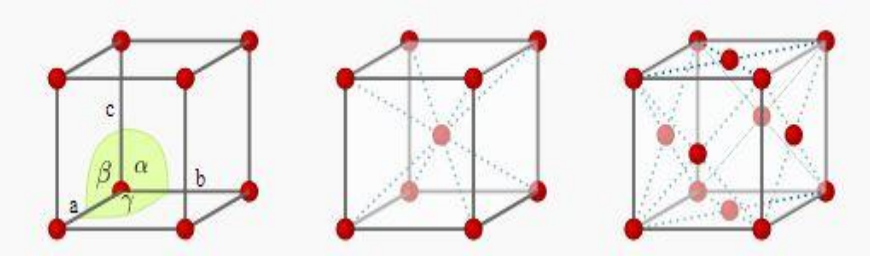
All crystals can be classified in to following seven systems.

1. Cubic
2. Tetragonal
3. Orthorhombic
4. Rhombohedral
5. Hexagonal
6. Monoclinic
7. Triclinic

The shapes of unit cells based on three unit vectors and three angles have been shown in figures.

1. **Cubic:**

In cubic structure, a = b = c and $\alpha = \beta = \gamma = 90°$.

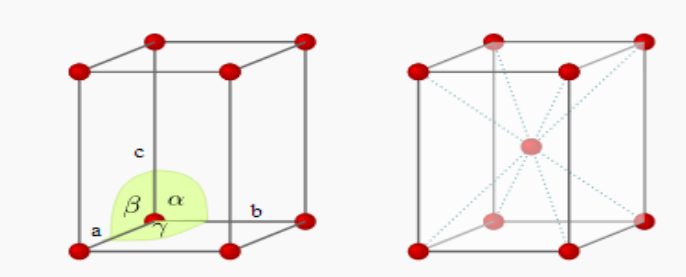


Simple Cubic **Body Centred Cubic** **Face Centred Cubic**

Fig.15

2. **Tetragonal:**

In tetragonal structure, a = b ≠ c and $\alpha = \beta = \gamma = 90°$.

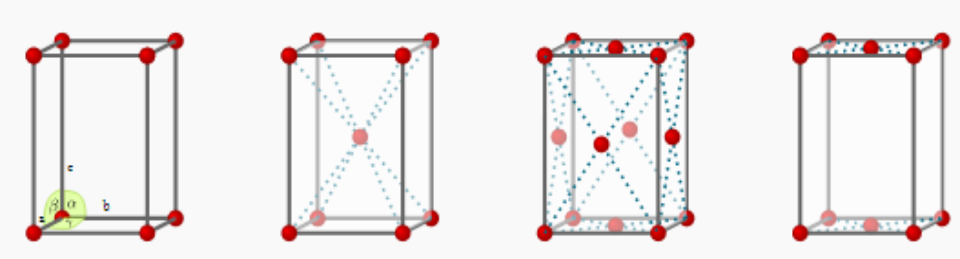


Simple Tetragonal **Body Centred Tetragonal**

Fig.16

3. **Orthorhombic**

In Orthorhombic structure, a ≠ b ≠ c and $\alpha = \beta = \gamma = 90°$.



Simple **Body Centred** **Face Centred** **End Centred**

Fig.17

4. Rhombohedral (Trigonal)

In Rhombohedral structure, a = b = c and $\alpha = \beta = \gamma \neq 90°$.

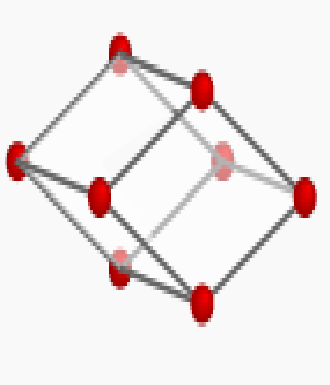


Fig.18

5. Hexagonal

In Hexagonal structure, a = b $\neq$ c and $\alpha = \beta = 90°$, $\gamma = 120°$.

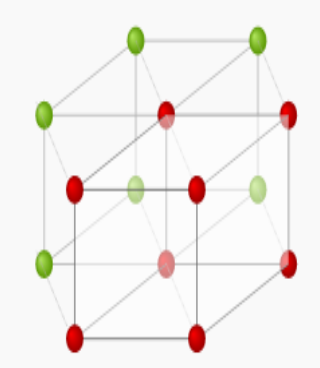
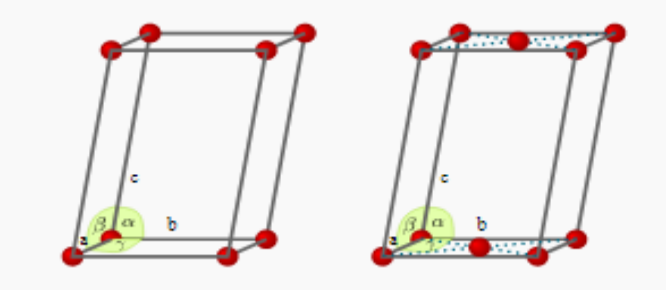


Fig.19

6. Monoclinic

In cubic structure, a $\neq$ b $\neq$ c and $\alpha = \gamma = 90° \neq \beta$.



Simple Monoclinic **Base Centred Monoclinic**

Fig.20

7. Triclinic

In Triclinic structure, $a \neq b \neq c$ and $\alpha \neq \beta \neq \gamma \neq 90°$.

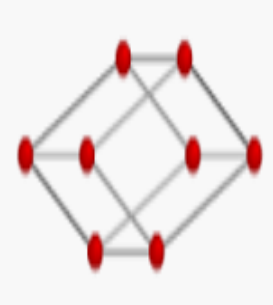


Fig.21

Sr. No	Crystal System	Lengths	Angles	Bravais Lattice	No. of lattices and symbols	Examples
1	Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90°$	SC, BCC, FCC	3 (P, I, F)	Cu, NaCl, CsCl etc.
2	Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90°$	Simple, Body Centred	2 (P, I)	TiO_2, SnO_2 etc.
3	Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90°$	Simple, Body Centred, Base/End Centred, Face Centred	4 (P,C,I,F)	Ga, KNO_3 etc.
4	Rhombohedral or Trigonal	$a = b = c$	$\alpha = \beta = \gamma \neq 90°$	Simple	1 (P)	As, $CaSO_4$ etc.
5	Hexagonal	$a = b \neq c$	$\alpha = \beta = 90°$, $\gamma = 120°$	Simple	1 (P)	Mg, Zn, SiO_2 etc.

6	Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90° \neq \beta$	Simple, Base Centred	2 (P,C)	Na_2SO_4
7	Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90°$	Simple	1 (P)	$K_2Cr_2O_7$