PT-203: BASIC ELEMENTS OF SOLID STATE PHYSICS

Unit-1 Crystal Structure

Space lattice

Imaginary array of distinct identical points organized periodically in space constitutes a **space lattice**. When actual atoms/group of atoms of a crystalline material is replaced by points in space, the resulting array of distinct points obtained is known as **space lattice**.

It is very important to know that the choice of selecting a lattice for a given crystalline material is not unique and is totally decided by the configuration of the atoms defining a lattice point. The atoms/group of atoms that define a lattice point is known as **basis.** Consider the following example:

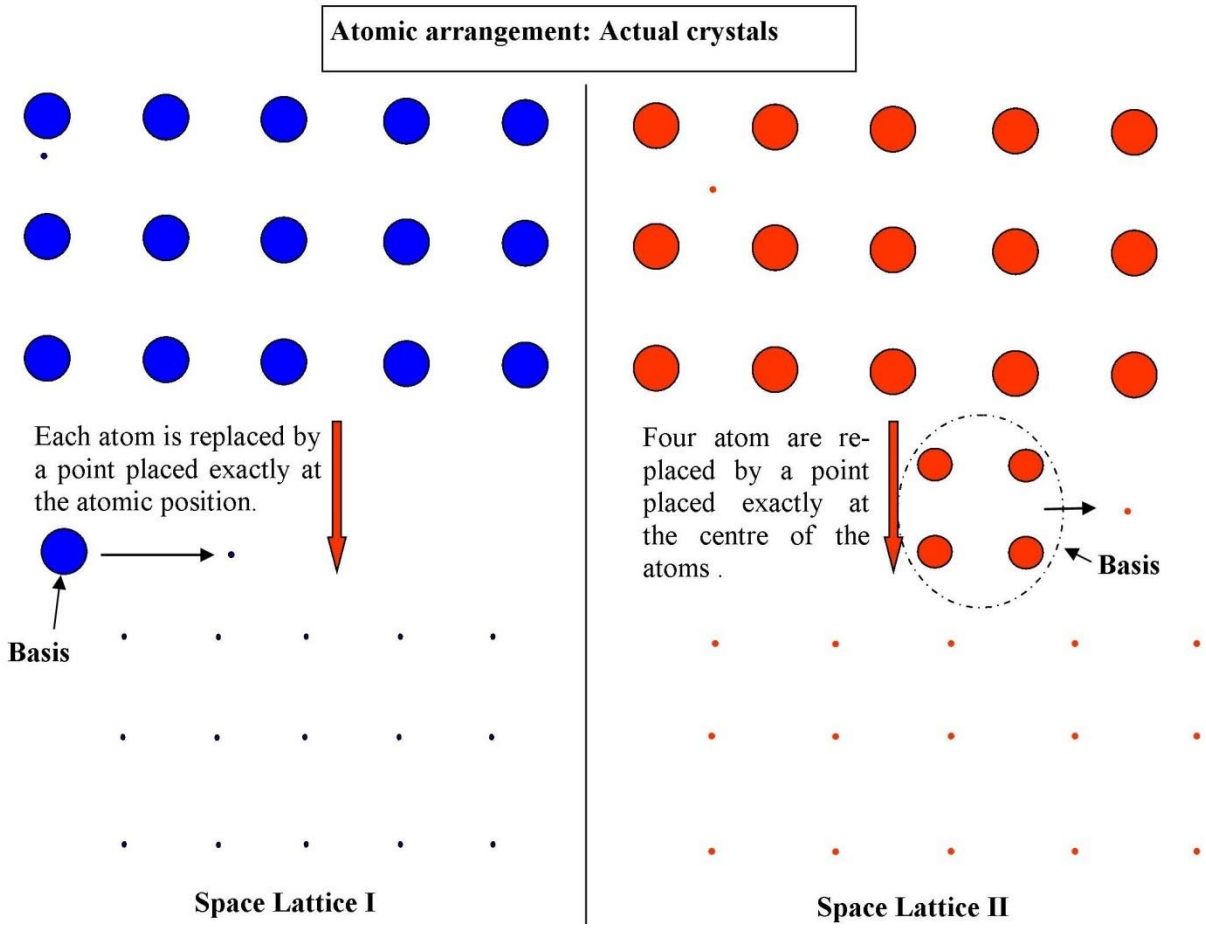


Fig.1: Construction of space lattice from a given arrangement of atoms in crystalline materials.

In the case of crystalline material I (left side), the lattice is constructed by replacing each atom of the crystal by a point in space whereas in the case of material II (right side) four atoms of the crystal are replaced by a single point. Thus in the case of material I one atom defines the lattice point and constitutes the basis of this system. However, in the case of material II, configuration of four atoms defines a single lattice point and defines the basis.

Bravais Lattice

A Bravais lattice is a geometrical collection of identical distinct points satisfying the following two conditions:

(1) The arrangement and orientation of the points in the lattice around any lattice point should look exactly the same.

To understand this, consider the following examples of two dimensional lattices:

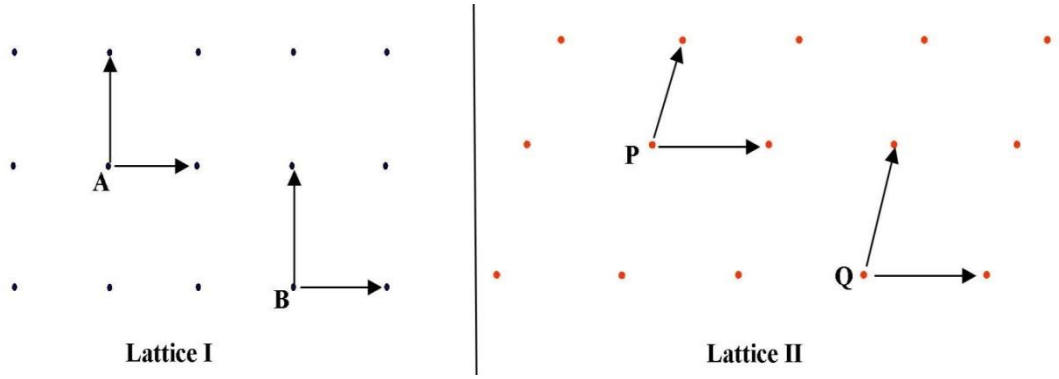


Fig. 2: Lattices having identical arrangement as well as orientation around every lattice point.

Both the lattices shown in Fig. 2 have identical environment for all the lattice points (arrangement as well as orientation) as can be checked for lattice points A and B in Lattice I and for P and Q in lattice II.

An important material in material science nowadays would give you the best way to understand the arrangement and orientation. The material is known as grapheme and it has a honey comb lattice as shown below in Fig.3:

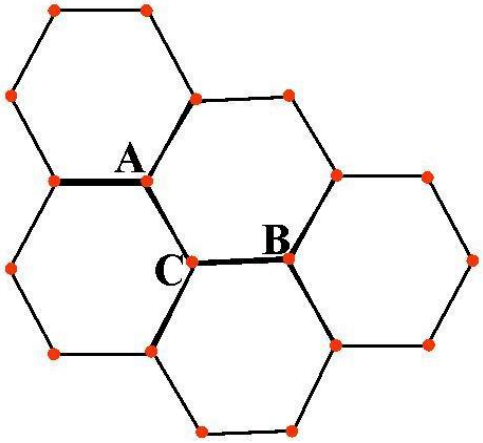


Fig. 3: Honey comb lattice of graphene.

On clearly observing this lattice, points A and B have the same arrangement and orientation. However, when the structure is viewed along point C, the structure seems to have been rotated through 60º. Thus, the lattice has an arrangement but lacks the identical orientation of the lattice points. Hence, the honey comb lattice of grapheme is a lattice but not a Bravais lattice.

(2) All The points of the lattice can be reached from any lattice point using the relation:

$$\bar{R} = n_1\bar{a}_1 + n_2\bar{a}_2 + n_3\bar{a}_3$$

Where, $\bar{a}_1$, $\bar{a}_2$ and $\bar{a}_3$ are called the primitive vectors. $\bar{R}$ is known as Translation vector and n_1, n_2 and n_3 are integers.

In order to understand this, consider an example of a 2D lattice as shown in Fig.4:

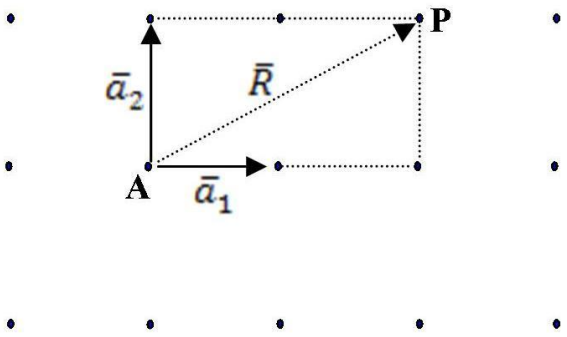


Fig.4: Two dimensional Bravais lattice.

In this case, in order to travel from point A to the point P the translation vector $\bar{R}$ is given by:

$$\bar{R} = 2\bar{a}_1 + \bar{a}_2$$

having n_1 = 2, n_2 = 1 and n_3 = 0 satisfying the second criteria for Bravais lattice. Moreover, it is important here to know that choosing $\bar{a}_1$ and $\bar{a}_2$ is not a unique choice.

It is now clear that each Bravais lattice has a preferred identical arrangement as well as orientation about every lattice point. These arrangements are however defined by several symmetry elements underlying a point lattice and hence the bravais lattices are classified based on the symmetry exhibited.

Symmetry

An object is said to be symmetric with respect to a geometric operation if it can brought into self coincidence by that operator. For example a square lattice has a translational symmetry when shifted through by a lattice translational vector. A lattice may also possess other non-translational symmetry also known as point symmetry. There are two basic point symmetries exhibited by the Bravais lattices:

(1) Rotation:

An object is said to possess an n-fold axis of rotation if it is brought into self coincidence by a rotation through a minimum angle $\theta_{min} = 360^o/n$

When n = 1, $\theta_{min} = 360^o$ (one fold rotation symmetry or no symmetry)

For n =2, $\theta_{min} = 180^o$ (two fold rotation symmetry)

In this case, consider capital letter **N** and rotate it with an angle of 180º, the letter gets back to self coincidence. Hence letter **N** is having two-fold rotation symmetry. Consider few two dimensional examples as shown in Fig.5:

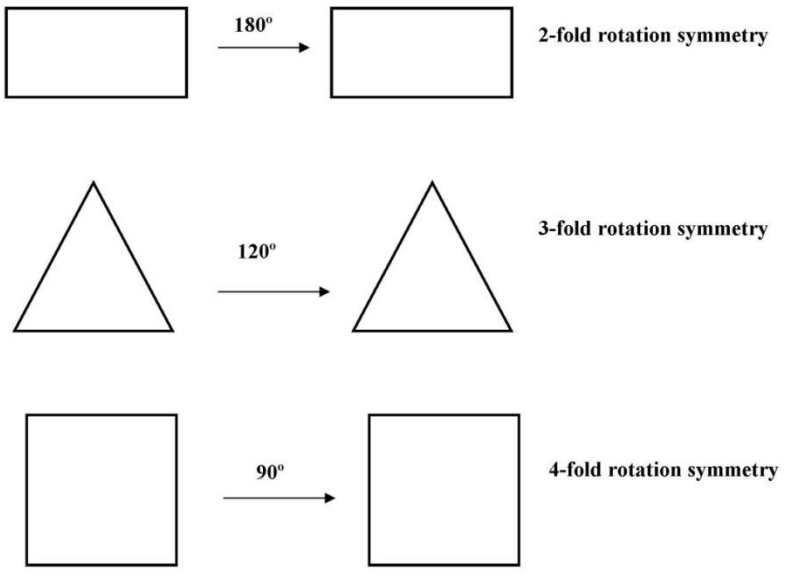
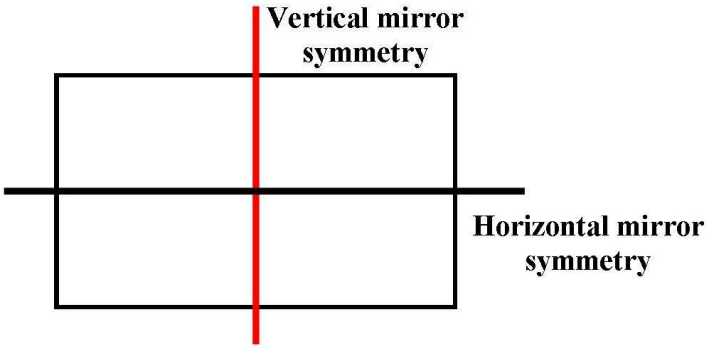


Fig.5: Rotation symmetry of some regular two dimensional polygons.

From Fig.5 rectangle exhibits two-fold rotation symmetry, equilateral triangle three-fold where as square possesses four-fold symmetry. In general regular polygons of n sides have n-fold rotation symmetry. Besides this there is a crystallographic restriction theorem which states that " crystal or lattice (by virtue of their translational symmetry) can possess rotation axes of n-fold only for n = 1, 2, 3, 4 and 6."

(2) Reflection or mirror symmetry:

If an object can be divided into two halves by an imaginary plane such that each half appears to be the image of the other by reflection in the plane we say that the object possess a reflection symmetry. Consider the example of a rectangle as shown below:



Red line and black bold lines are two way mirrors splitting each one the rectangle into exactly two halves which are mirror images of each other. Thus rectangle exhibits the mirror or reflection symmetry.

Classification of 3D Bravais lattices on the basis of symmetry

On the basis of symmetry (point symmetry) there are seven crystal systems summarized in table 1and pictorized in Fig. 6:

Table 1: Classification of 3D lattices on the basis of point symmetry.

S.No.	Defining Symmetry	Crystal System
1	1-fold symmetry	Triclinic
2	A single 2-fold symmetry	Monoclinic
3	A single 3-fold symmetry	Trigonal or Rhombohedral
4	A 6-fold symmetry	Hexagonal
5	Three 2-fold symmetry	Orthorhombic
6	A single 4-fold symmetry	Tetragonal
7	Four 3-fold symmetry (along body diagonals)	Cubic

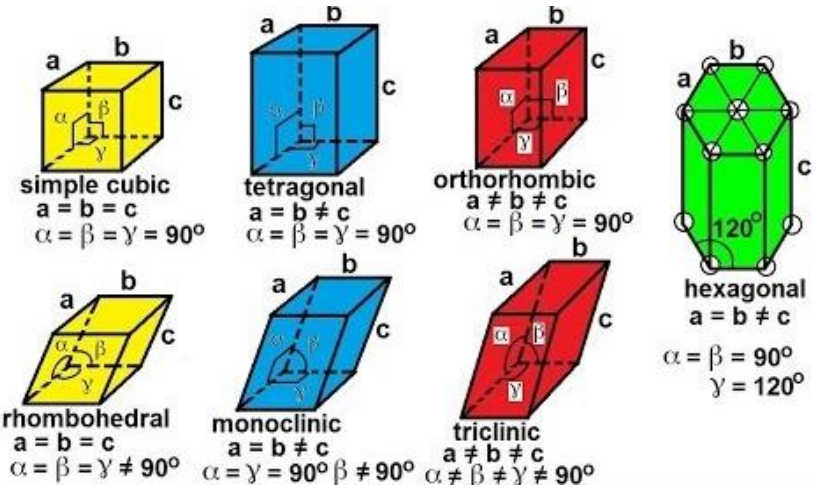


Fig.6: Pictorial representation of seven crystal systems.

Unit cell and Primitive cell

A unit cell is defined as a connected region of space which can generate the entire lattice by repetition through lattice translation. However, primitive cell is the minimum volume unit cell. There is only one lattice point per primitive cell that too only at the corners. Commonly the cells are **parallelograms (in 2D)** or **parallelepiped (in 3D)** with corners at the lattice points. For illustration consider an example of following 2D square lattice:

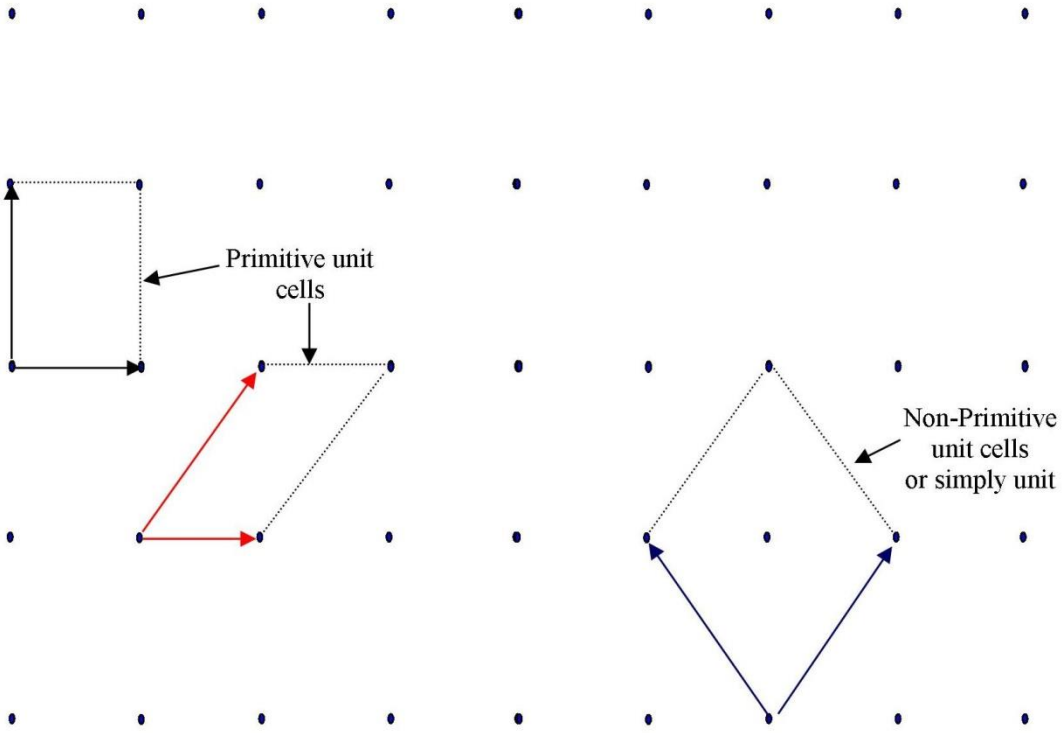


Fig.7: 2D lattice depicting different types of unit cells.

From Fig.7 it is illustrated that for a particular lattice, we can have many (infinitely many) unit cells that might be primitive as well as non-primitive.

Construction of Primitive cell for general Bravais lattice (Wigner-Seitz Cell)

Wigner Seitz cell is a primitive cell which is by far the common way of constructing a primitive cell out of a given Bravais lattice. The Wigner Seitz cell around a lattice point is the region of the space that is closer to that point than to any other lattice point. Fig. 8 illustrates the Wigner Seitz cell for a 2D lattice.

For constructing a Wigner-Seitz cell simply complete the following steps.

1. Choose any lattice site as the origin.
2. Starting at the origin **draw** vectors to all neighbouring lattice points.
3. **Construct** a plane perpendicular to and passing through the midpoint of each vector.
4. The area enclosed by these planes is the **Wigner-Seitz cell**.

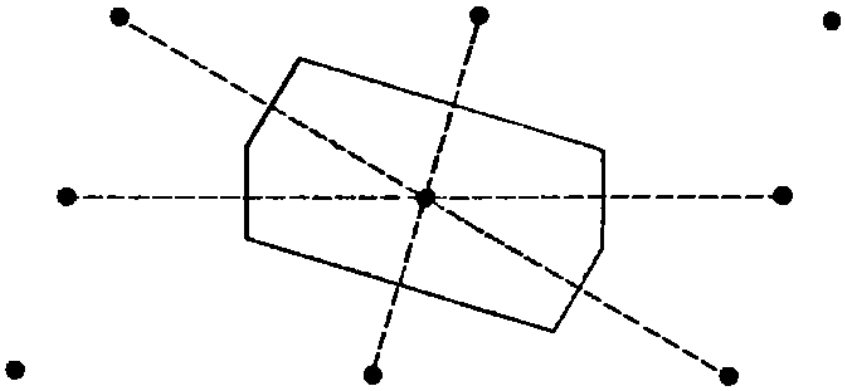


Fig.8: Wigner-Seitz cell for a 2D lattice.

Miller indices for directions and planes

Miller indexing is a tool or standard method to specify directions and planes in the crystalline materials. There are certain steps to be considered while indexing the directions and planes.

In the case of directions the steps are:

1. Choose a point **on the direction** as the origin.
2. Choose a coordinate system with axes parallel to the unit cell edges.
3. Find the coordinates of another point on the direction in terms of the lattice parameters a, b and c.
4. Reduce the coordinates to smallest integers.
5. Put the reduced coordinates in square brackets.

The square bracket thus achieved will represent the direction. It has to be keep in mind that the directions are always represented by the square brackets [] and the components are not separated by any commas.

Miller indices of a direction represent only the orientation of the line corresponding to the direction and not its position or sense. Moreover, all parallel directions have same Miller indices. (Note: For examples please visit the link: https://youtu.be/mc-VocwArHY).

In the case of planes, the steps involved are:

1. Select a crystallographic coordinate system with **origin not on the plane**.
2. Find the intercepts along the axes in terms of respective lattice parameters.
3. Take reciprocals of the intercepts.
4. Reduce to smallest integers in the same ratios.
5. Enclose in parenthesis.

Miller indices of a plane specifies only its orientation in space not its position. Moreover, all parallel planes have the same Miller indices. (Note: For examples please visit the link: https://youtu.be/1vsNxkdlcXw).