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## C12T (Solid State Physics)

### Topic – Crystal Structure (Part – 1)

#### Introduction:

The solidification of elements or their compounds from gaseous or liquid state leads to the formation of an *ordered* or *disordered* state (phase). The ordered state is commonly called the *crystalline state* whereas the disordered one is termed the *amorphous state*. The crystalline state (or simply, *crystal*) refers to an infinite array of atoms or a group of atoms. The regularity in the arrangement or the periodicity extends over the whole volume of a crystal. The whole volume of a crystal can be constructed by moving a building block of the smallest acceptable size along its edges. This block consisting of atoms or a group of atoms is known as a *unit cell*. Even with the complete available knowledge of the laws of atomic packing and geometrical considerations for a certain material, it is generally not possible to predict the material's crystal structure. Predictions turn out to be wrong as often as right. Various crystal structures existing in nature can be understood by systematically exploring all the possible ways of arranging atoms in periodic arrays. This process involves the visualization of motional operations performed on atoms within a unit cell such that the operations leave the unit cell unchanged. These operations, called *Symmetry Operations*, form the most vital component of Geometrical Crystallography. Every crystal structure satisfies the requirements of a specific group (combination) of certain symmetry operations. Different combinations of symmetry operations result in different crystal structures. Thus the knowledge of the symmetry operations helps us in making a complete list of possible crystal structures and in classifying crystals.

#### Lattice, Basis and Crystal Structure:

An infinite periodic array of points in space is called a *lattice*. In more general terms, it is known as the *space lattice*. The arrangement of points defines the lattice symmetry. When an atom or an identical group of atoms is attached to every lattice point, we obtain a crystal structure. The attached atom or the group

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of atoms, called *basis*, is identical for every lattice point in terms of composition, relative orientation and separation. Therefore, in short we can write, lattice + basis = crystal structure. These features are explained in Fig. 1. The number of atoms in the basis of an inorganic crystal can be around 100, whereas it is known to be as large as a few thousands in organic crystals.

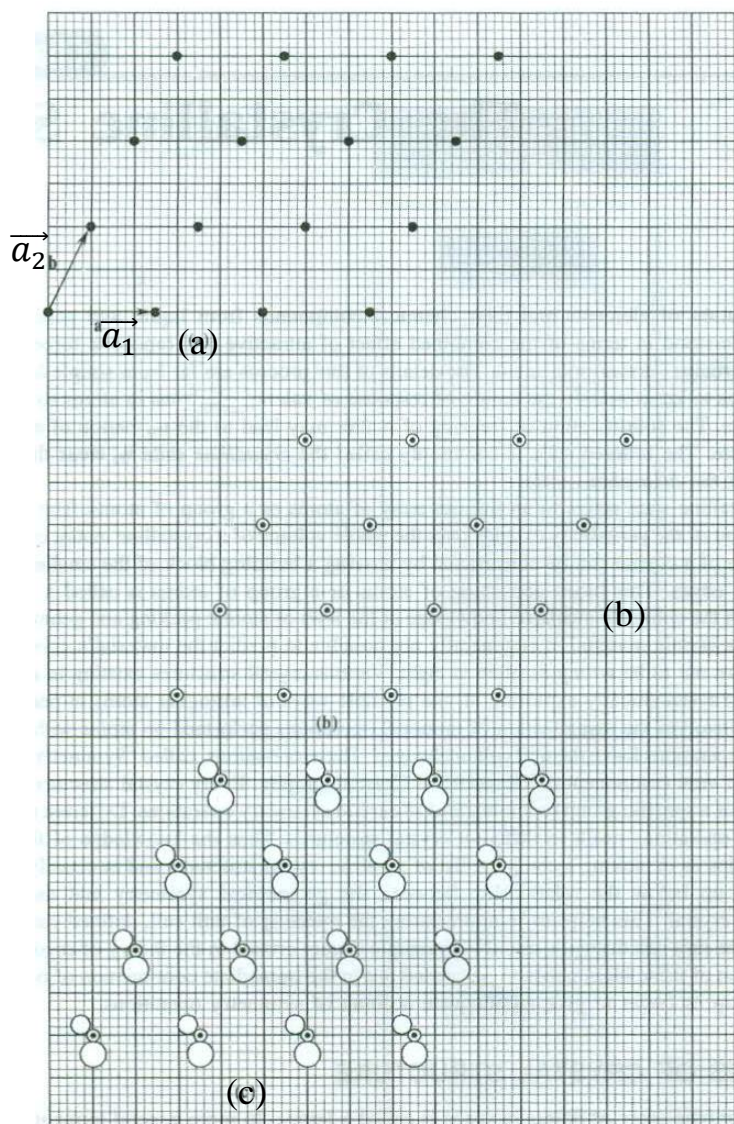


Fig. 1

Fig. 1(a) demonstrates a regular arrangement of points on a plane forming a two-dimensional space lattice. The points are the lattice points. Vectors  $\vec{a}_1$  and  $\vec{a}_2$  define the symmetry and size of the lattice, whereas in Fig. 1(b), a two-

dimensional crystal formed when an atom is placed at each lattice point of the space lattice. All atoms are identical (of the same element). The single atom forms the basis of the crystal structure. Here the basis of the crystal structure is one, although it can be more than one. In Fig. 1(c) a crystal structure with the same space lattice and the basis of three atoms, all of different elements has now been considered. The relative positions and orientations of atoms in the basis are identical for all lattice points which may now be taken as imaginary points.

### **Unit Cell: Primitive Cell and Non-Primitive Cell:**

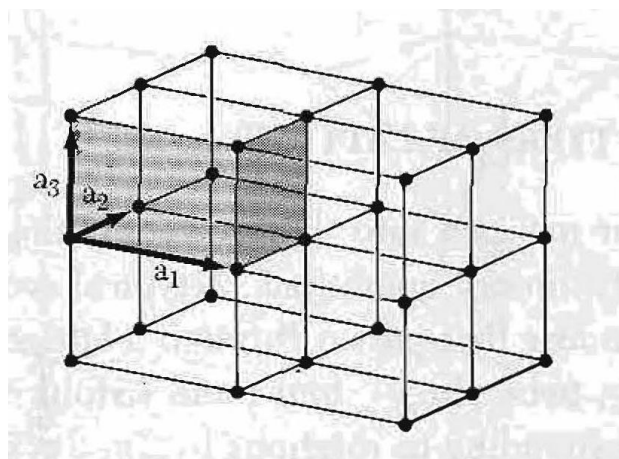


Fig. 2

We already have seen that by translating the unit cell in some specific manner, the whole crystal can be constructed. The translations along the crystal axes  $a_1$ ,  $a_2$  and  $a_3$  are the simplest of many translations that may map the crystal lattice completely (Fig. 2). These translations are actually the various combinations of  $a_1$ ,  $a_2$  and  $a_3$ , naturally, with certain restrictions. These restrictions are closely linked with the structural aspects of a unit cell which are discussed now. A proper description of the subject may be carried out by referring to the three-dimensional space lattices. A vector  $\vec{T}$  is drawn connecting two lattice points  $P_1$  and  $P_2$  (Fig. 3) represented by the position vectors  $\vec{r}_1$  and  $\vec{r}_2$ , respectively. Then, the vector  $\vec{T}$ , known as the *lattice translation vector*, is given by the relation  $\vec{r}_2 = \vec{r}_1 + \vec{T}$ , such that

$$\vec{T} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$$

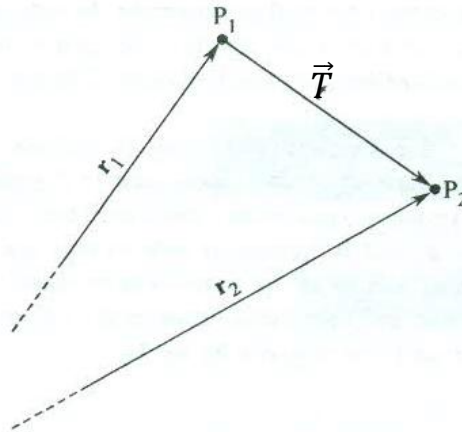


Fig. 3

When all the lattice points can be located for the arbitrary choice of only *integral values* of  $n_1$ ,  $n_2$  and  $n_3$ , the crystal axes or the fundamental vectors  $\vec{a}_1$ ,  $\vec{a}_2$  and  $\vec{a}_3$  are called as *primitive axes* and the resulting unit cell is known as a *primitive cell*. Fig. 4 shows a primitive and a non-primitive cell belonging to two different materials. The primitive cell is also defined as the minimum volume unit cell having *only one lattice point*. In Fig. 4(a) there is only one lattice point since one point at each of the 8 corners contributes 1/8th of a point to the cell. The other cell shown in Fig. 4(b) has two lattice points and, therefore, it is *non-primitive*. We can also say that in a primitive cell, lattice points are located only at the corners of the cell. All the lattice points are equivalent in a primitive cell, whereas it is not so in general.

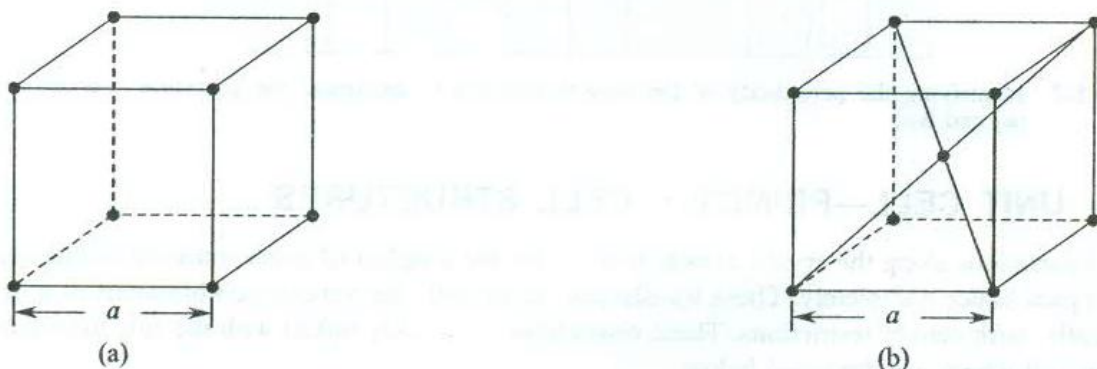


Fig. 4



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The use of a primitive cell or a non-primitive cell for the study of a crystalline material is purely a matter of convenience. There is no hard and fast rule in this context. It is also important to mention here that there can be more than one choice for the primitive cell for a given crystal. It clearly suggests that the shape of the primitive cell is not a unique one. All the different types of primitive cells are equally acceptable as long as they have the same volume given by

$$V = |\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)|$$

### **Wigner-Seitz Cell:**

An alternative primitive cell, known as *Wigner-Seitz Cell*, is of historic importance in the theory of Solid State Physics. The first proper electron energy bands calculation was made by Wigner and Seitz using this design of the primitive cell. The method of construction is as follows.

A lattice point is joined to all the nearby lattice points with the help of lattice vectors. Then, a plane perpendicular to each of these vectors, connecting the central lattice point, is drawn at the mid-point of the vector. The planes form a completely closed polyhedron which contains only one lattice point at its centre. The polyhedron serves as an ideal primitive cell and is named after Wigner and Seitz who are credited with having given the philosophy of its construction. Fig. 5 shows the pictures of Wigner-Seitz Cell of a two-dimensional lattice.

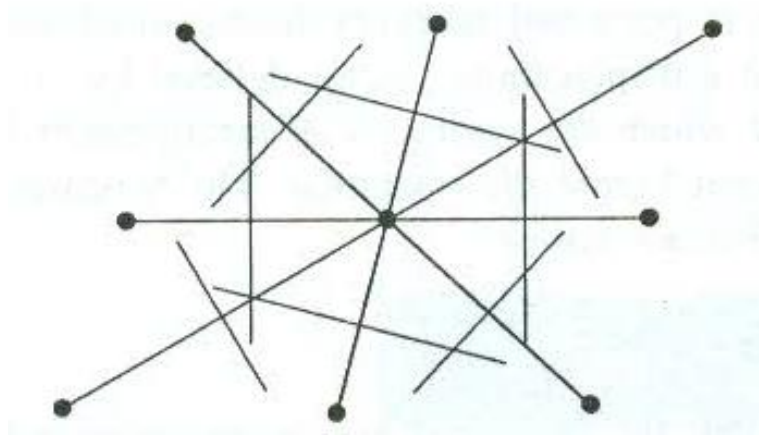


Fig. 5



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## **Bravais Lattice:**

In crystallography and geometry, the *Bravais Lattice* concept of an infinite array of discrete points is expanded using the concept of a unit cell which includes the space in between the discrete lattice points as well as any atoms in that space. A fundamental aspect of any Bravais Lattice is that, for any choice of direction, the lattice will appear exactly the same from each of the discrete lattice points when looking in that chosen direction. Therefore, in order to become a Bravais Lattice, every lattice point must be equivalent for a given arbitrary lattice.

**2D Bravais Lattice Types.** The discussion on lattices in two-dimensional (2D) space may look at first sight as a matter of theoretical concern. But its utility is appreciated on noticing how the involved ideas when extended make the relatively complex situation in three-dimensions easy for understanding. Moreover, two-dimensional lattices become most relevant in layered crystals (e.g. graphene) in which crystalline layers along one crystal edge are largely separated. In such a situation, the corresponding crystal edge (or lattice parameter) becomes almost insignificant whenever inter-atomic interactions are considered.

There are in all five Bravais lattices in two-dimensions. Out of the five Bravais lattices, one is general and the other four are obtained by exhausting the feasible axial relationships between  $\vec{a}_1$  and  $\vec{a}_2$  and the relative orientations of the two. The general lattice is termed as *oblique*. The lattice is invariant only under the rotations of  $\pi$  and  $2\pi$  about the axes passing through a lattice point. But special lattices of the oblique type can be invariant under rotation of  $2\pi/3$ ,  $2\pi/4$  or  $2\pi/6$ , or under mirror reflection. In principle we can have an infinite number of this type of lattice as there are no restrictions on  $a_1$ ,  $a_2$  and the angle  $\gamma$  between them. When all possible restrictions are imposed on  $a_1$ ,  $a_2$  and  $\gamma$ , we get four other special types of two-dimensional Bravais lattice (Fig. 6). All these lattices are primitive except the second of the two derived from the same centred rectangular arrangement of lattice points.

In the following table (Table 1), all the five 2D Bravais Lattices and their axial relationship have been listed.

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System	No of Lattices	Axial relationship
Oblique	1	$a_1 \neq a_2, \gamma$ arbitrary
Square	1	$a_1 = a_2, \gamma = 90^\circ$
Hexagonal	1	$a_1 = a_2, \gamma = 120^\circ$
Rectangular	1	$a_1 \neq a_2, \gamma = 90^\circ$
Centred rectangular	1	$a_1 \neq a_2, \gamma = 90^\circ$

Table 1

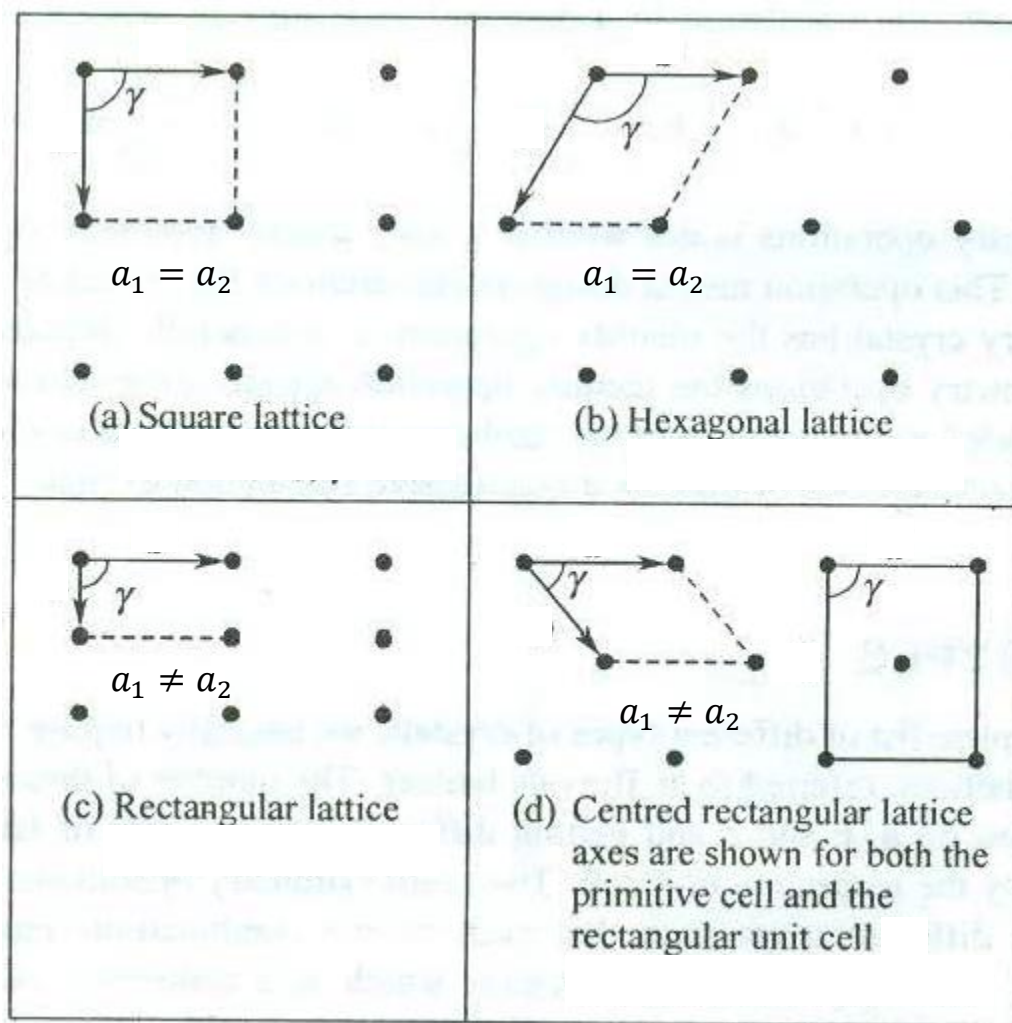


Fig. 6

**3D Bravais Lattice Types.** The point symmetry groups in three dimensions require the 14 different Bravais lattice types listed later. The general lattice is known as *triclinic*, and there are 13 special lattices. These are grouped for convenience into systems classified according to seven types of cells, which are

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triclinic, monoclinic, orthorhombic, tetragonal, cubic, trigonal, and hexagonal. The division into systems is expressed in the following table (Table 2) in terms of the axial relations ( $a_1, a_2, a_3$  and angles  $\alpha, \beta, \gamma$  between them) that describe the cells.

System	No of Lattices	Axial relationship
Triclinic	1	$a_1 \neq a_2 \neq a_3$ $\alpha \neq \beta \neq \gamma$
Monoclinic	2	$a_1 \neq a_2 \neq a_3$ $\alpha = \gamma = 90^\circ \neq \beta$
Orthorhombic	4	$a_1 \neq a_2 \neq a_3$ $\alpha = \beta = \gamma = 90^\circ$
Tetragonal	2	$a_1 = a_2 \neq a_3$ $\alpha = \beta = \gamma = 90^\circ$
Cubic	3	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 90^\circ$
Trigonal	1	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma < 120^\circ \neq 90^\circ$
Hexagonal	1	$a_1 = a_2 \neq a_3$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$

Table 2

The number of Bravais Lattices is obtained by imposing restrictions on  $a_1, a_2$  and  $a_3$  and getting different arrangements of lattice points each of which is represented by the respective unit cell. The point symmetry operations of a Bravais Lattice may be combined in different ways such that each of the combinations represents a different structure in terms of symmetry. Each combination which is a collection of certain symmetry operations is called a *Point Group*. A symmetry operation in this reference is given another name as *Symmetry Element*. It may be remarked that the symmetry of a crystal structure is completely specified only when its *Space Group* is known.

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This concludes part 1 of this e-report.

The discussion will be continuing in the part 2 of this e-report.

**Reference:**

**Introduction to Solid State Physics, Charles Kittel, Wiley**

**Elements of Solid State Physics, J.P. Srivastava, PHI Learning**

(All the figures have been collected from the above mentioned reference)

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