



## **UNIT III**

### **SOLID STATE PHYSICS**





# Elements of Crystallography

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## 6.1 INTRODUCTION

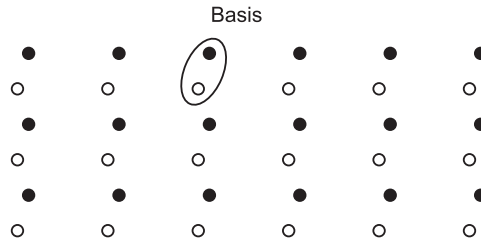
Usually all the elements and their chemical derivatives are found in three states viz, solid, liquid, and gaseous. At some specific conditions, sometimes they may lie in the fourth state of matter known as *plasma*, but it is rare. It is observed that nature loves symmetry due to which, starting from tiny particles like atoms and molecules to the giant particles like planet and stars, all are arranged in a regular fashion and obey their universal laws. The word *crystallography* is the combination of two words: *crystal* and *graphein*, where crystal has its usual meaning while the Greek word graphein means *to write*. Hence, crystallography means writing about the complete crystal. If the atoms and molecules in a solid are arranged in some regular fashion, then it is known as *crystalline solid*. The basic building blocks of a crystalline solid are stacked in a regular manner, just like the soldiers do on the parade ground, and thus form a three-dimensional pattern. Thus, the presence of long-range order and periodicity are the important properties of a crystal. In some crystals, there is a lack of long-range order in the arrangement of their constituent particles like atoms and molecules, and they are known as supercooled liquids or *amorphous solids*. The stiffness of such solids is due to their exceptionally high viscosity. The common examples of amorphous solids are glass, pitch, and plastics. The amorphous solids have no sharp melting point, whereas for crystalline solid, melting occurs at a definite temperature.

During his study on the properties of cathode rays in 1885, Professor Wilhelm Conrad Roentgen found that some highly penetrating radiations were coming from the discharge tube. Since the properties of these radiations were unknown at that time, he named these rays as X-rays. Later, X-rays were thoroughly investigated and it was established that they are electromagnetic waves. They have short wavelength, lying in the range of 0.01 Å to 10 Å. These X-rays are most commonly used to investigate crystal structure.

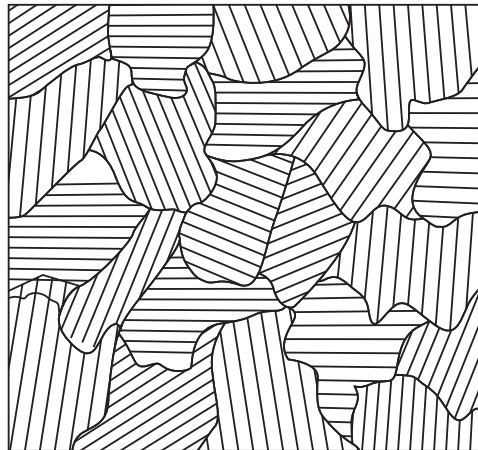
In this chapter, we will study about the basics of different crystal lattices, plane and directions of cubic system, and related parameters of crystal structures.

## 6.2 CRYSTAL STRUCTURE

In a crystalline solid, each basic building block (atoms or molecules) has a fixed position in space. It is at a definite distance and a definite angular orientation to the other atoms or molecules lying in its surroundings. In a perfect crystal, there is an infinite regular repetition of such identical structural units. In a single crystal, the position and orientation of atoms or molecules are uniform and continuous throughout the entire crystal (Fig. 6.1). The examples of single crystal are diamond, ruby, etc.

**Fig. 6.1** Structure of single crystal

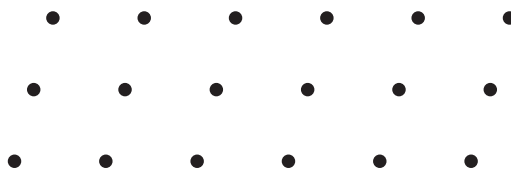
There is another class of material known as *polycrystalline* in which the whole crystal is made up of smaller crystallites, as shown in Fig. 6.2. Each constituent of the small crystallite is called *grain*. These grains are situated side by side to form the whole crystal, like in quartz. Within the boundary of a grain, there is same lattice pattern but grains are generally oriented randomly, and thus, form the *grain boundaries* in the polycrystalline solid. Since many properties of the solids are best studied with single crystals, so these are preferable than the polycrystalline solids. There are two types of single crystals known as *elemental* and *ionic*. The examples of elemental single crystals are Al, Fe, Cu, etc., while the examples of ionic single crystals are AgCl, CuSO<sub>4</sub>, etc.

**Fig. 6.2** Grain boundaries of different grains in a polycrystalline solid

In order to describe a crystal structure, it is must that the learner should know what are lattice, lattice translation vector, and basis. Without the knowledge of these important facts, it is very difficult to describe the crystal structure. For the better understanding of these fundamentals of the crystal structure, we have discussed them in the following sections.

### 6.3 SPACE LATTICE

In order to describe the arrangement of atoms in a crystal, it is always convenient to describe the arrangement of imaginary points in space which have a definite relationship with the atoms of the crystals. Actually, these set of points provide a base for the crystal structure. Such three-dimensional arrangement of imaginary points in space that have identical points in its surroundings is known as *space lattice*. A two-dimensional space lattice is shown in Fig. 6.3.

**Fig. 6.3** Space lattice

In the above discussion, it is mentioned that a point is surrounded by identical points which means that the lattice has same appearance when viewed from a point  $r'$  in the lattice as when viewed from any other point  $r'$  with respect to some arbitrary origin. It is possible on the cost of repetition of pattern unit in all directions by means of translation operation of vector  $T$ . Pattern unit may be considered as basic building block of lattice, containing a small group of points. Translation operation vector  $T$  is given as:

$$\vec{T} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c} \quad (6.1)$$

where  $n_1$ ,  $n_2$ , and  $n_3$  are arbitrary integers and vectors  $\vec{a}$ ,  $\vec{b}$ ,  $\vec{c}$  are known as *fundamental translation vectors*. With respect to the other point  $\vec{r}'$ , Eq. (6.1) can be given as

$$\vec{r}' = \vec{r} + \vec{T} = \vec{r} + n_1\vec{a} + n_2\vec{b} + n_3\vec{c} \quad (6.2)$$

The translation vectors are also known as *crystal axis*, or *basis vectors*.

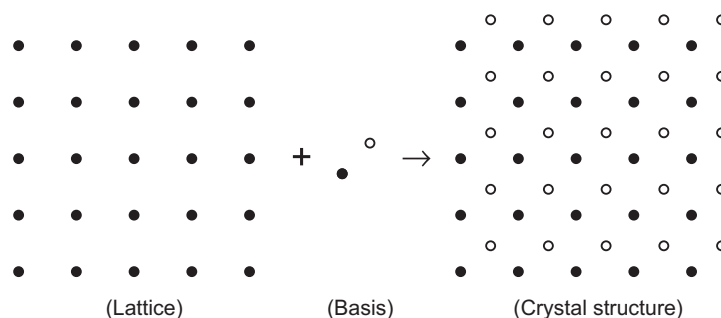
## 6.4 BASIS

A crystal structure is always described in terms of the atoms arranged in the lattice. A *space lattice* is defined as an infinite three-dimensional array of imaginary points in space which have identical surroundings. Thus, in order to obtain a crystal structure, an atom or a group of atoms must be placed on each lattice point in a regular fashion. Such an atom or a group of atoms placed on each lattice point is called the *basis*, and it acts as a building unit, or a structural unit, for the complete crystal structure. Thus, the crystal structure is generated by the combination of lattice with a basis. Thus, we can express a crystal structure as

$$\text{Space lattice} + \text{Basis} = \text{Crystal structure}$$

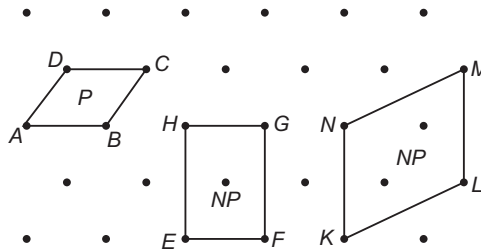
From the above discussion, it is clear that a lattice is a mathematical concept, whereas the crystal structure is a physical concept.

The generation of a crystal structure from a two-dimensional lattice and a basis is shown in Fig. 6.4. The basis consists of two atoms, represented by  $\circ$  and  $\bullet$ . The crystal structure is obtained by placing the basis on each lattice point such that the centre of the basis coincides with the lattice point.

**Fig. 6.4** Crystal structure generated from lattice and basis

## 6.5 UNIT CELL

A *unit cell* may be defined as the smallest unit of the lattice which, on continuous repetition, generates the complete lattice. Both primitive and non-primitive translation vectors may be used to construct a unit cell. Accordingly a unit cell is named as a primitive unit cell or a non-primitive unit cell. Some unit cells are shown in Fig. 6.5, out of which the parallelogram  $ABCD$  represents a two-dimensional primitive cell, whereas the parallelograms  $EFGH$  and  $KLMN$  represent non-primitive cells. The smallest volume is known as *primitive unit cell*.

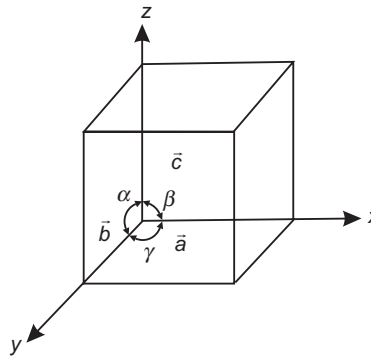


**Fig. 6.5** Primitive (P) and nonprimitive (NP) unit cells of 2-D lattice

In a primitive cell, all the lattice points belonging to it lie at its corners. Thus, the effective number of lattice points in a primitive cell is one. In a non-primitive cell, lattice points lie at the corner as well as at other locations, both inside and on the surface of the cell. Thus, the effective number of lattice points in a non-primitive cell is greater than one. The distance between two atoms or ions of same type is known as the length of the unit cell.

## 6.6 LATTICE PARAMETER

In a three-dimensional structure, a unit cell is usually represented by a parallelepiped as shown in Fig. 6.6. As mentioned in Fig. 6.6, vectors  $\vec{a}$ ,  $\vec{b}$ , and  $\vec{c}$  along  $x$ -,  $y$ -, and  $z$ -axes, respectively, are called *crystallographic axes*. The angles between these axes are called *interfacial angles*, which are measured as  $\alpha$ ,  $\beta$ , and  $\gamma$ . Primitive vectors  $\vec{a}$ ,  $\vec{b}$ , and  $\vec{c}$  and the interfacial angles  $\alpha$ ,  $\beta$ , and  $\gamma$  together are known as *lattice parameter* of a crystal. The actual size of the unit cell can be determined with the help of vectors  $\vec{a}$ ,  $\vec{b}$ , and  $\vec{c}$  and interfacial angles  $\alpha$ ,  $\beta$ , and  $\gamma$  (i.e., lattice parameter).



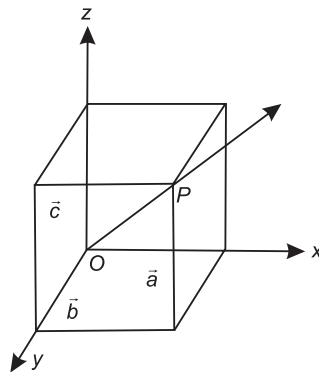
**Fig. 6.6** Three-dimensional structure of unit cell

## 6.7 LATTICE VECTOR AND DIRECTION

Any particular point or specific direction in a unit cell can be determined with the help of basic vectors  $\vec{a}$ ,  $\vec{b}$ , and  $\vec{c}$ . For example, if anyone wants to determine the position and the direction of point  $P$  in the unit cell shown in Fig. 6.7, then it can be expressed in terms of the basic vectors  $\vec{a}$ ,  $\vec{b}$ , and  $\vec{c}$  as

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

where  $n_1$ ,  $n_2$ , and  $n_3$  are three integers.



**Fig. 6.7** Position and direction of a point with the help of vectors  $\vec{a}$ ,  $\vec{b}$ ,  $\vec{c}$

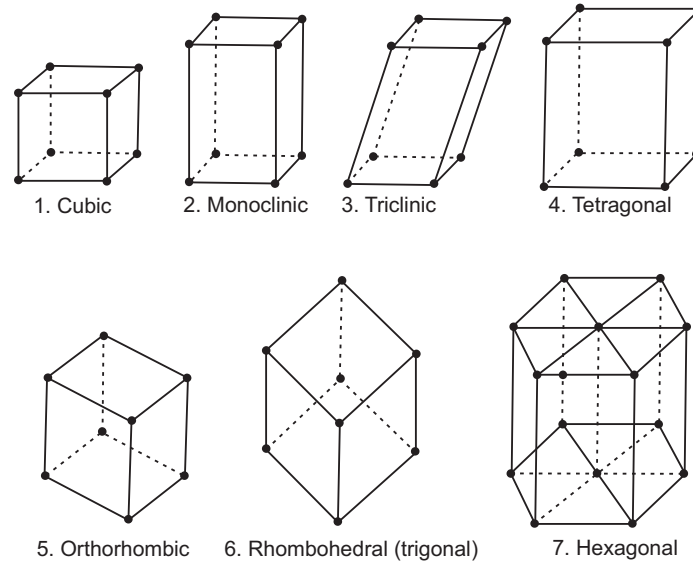
## 6.8 SEVEN CRYSTAL SYSTEMS

Corresponding to the different values of the lattice parameters, the crystal systems can be classified into seven types. Important information corresponding to these crystal systems is given in Table 6.1.

**Table 6.1** Seven crystal systems and their lattice parameters

S. No.	Crystal System	Lattice parameters	Examples
1.	Cubic	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$	Cu, Ag, Fe, Na, NaCl
2.	Tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	$\beta$ -Sn, $\text{TiO}_2$
3.	Orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	Ga, $\text{Fe}_3\text{C}$ (cementite)
4.	Rhombohedral or Trigonal	$a = b = c$ $\alpha = \beta = \gamma \neq 90^\circ$	As, Sb, Bi
5.	Hexagonal	$a = b \neq c$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$	Mg, Zn, Cd, NiAs
6.	Monoclinic	$a \neq b \neq c$ $\alpha = \gamma = 90^\circ \neq \beta$	$\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$ (gypsum)
7.	Triclinic	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90^\circ$	$\text{K}_2\text{Cr}_2\text{O}_7$

Simple sketch of all the seven crystal systems are given in Fig. 6.8.

**Fig. 6.8** Seven crystal systems

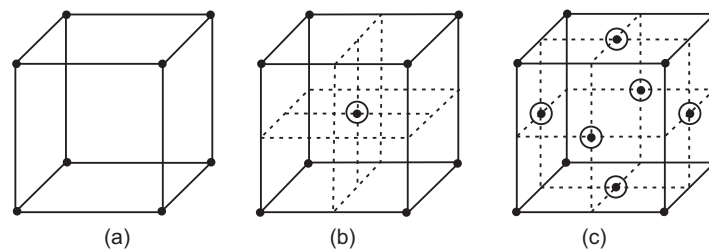
## 6.9 BRAVAIS SPACE LATTICE

During 1945, Bravais suggested that there are only 14 ways of arranging points in space. In such a situation, the system appears the same from each point. These arrangements give 14 lattices, which are called *Bravais space lattices*, each of which has the same collection of symmetry elements at the lattice points.

In the case of cubic system, there are three types of possible Bravais lattices which are as follows:

- (i) Simple cubic (SC)
- (ii) Body-centred cubic (BCC)
- (iii) Face-centred cubic (FCC)

The above mentioned Bravais lattices for cubic system are shown in Fig. 6.9.

**Fig. 6.9** (a) Simple cubic structure (SC), (b) body-centred cubic structure (BCC), and (c) face-centred cubic structure (FCC)

In the case of tetragonal system, there are following two types of Bravais lattices:

- (i) Simple tetragonal (ST)
- (ii) Body-centred tetragonal (BCT)



In the case of orthorhombic system, there are following four types of possible Bravais lattices:

- (i) Simple orthorhombic (SO)
- (ii) Body-centred orthorhombic (BCO)
- (iii) End-centred orthorhombic (ECO)
- (iv) Face-centred orthorhombic (FCO)

In the case of rhombohedral or trigonal system, there is only one possible Bravais lattice known as simple rhombohedral (SO).

In the case of hexagonal system, there is only one possible Bravais lattice known as simple hexagonal (SH).

Monoclinic system has two possible Bravais lattices known as simple monoclinic (SM) and end-centred monoclinic (ECM). Triclinic crystal system has only one possible lattice known as simple triclinic (ST). Thus, the total number of possible Bravais lattices corresponding to all the systems are 14.

## 6.10 SYMMETRY ELEMENT OF A CRYSTALLINE SOLID

There are three main symmetry elements used to describe a crystalline solid.

- (i) Axis of symmetry
- (ii) Plane of symmetry
- (iii) Centre of symmetry

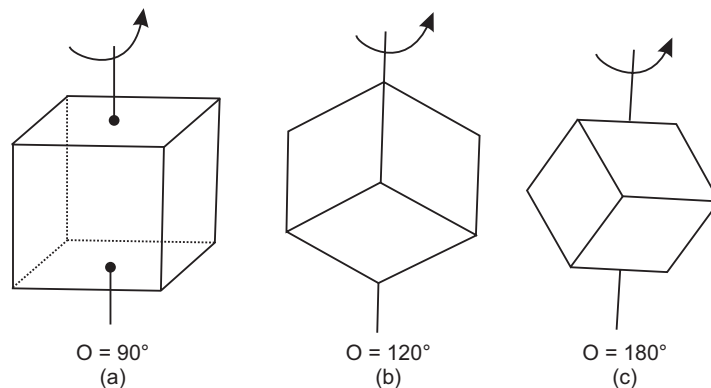
### 6.10.1 Axis of Symmetry

During the rotation of a crystal around an axis, if it occupies two or more identical positions in a complete rotation (i.e.,  $360^\circ$ ), then that axis is called the *axis of symmetry*.

When a cube is rotated around the axis passing through the opposite faces, then each rotation of  $90^\circ$  repeats the identical or congruent position, i.e., four congruent positions in one complete rotation. It is known as *four-fold axis of symmetry*. In general, if in a crystal  $n$ , the identical positions are repeated around an axis in one complete rotation, then that axis is called an  $n$ -fold axis of symmetry.

There are 13 axes of symmetry for a cube, which are as follows:

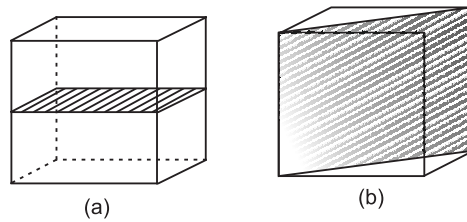
- (i) 3 axes have four-fold symmetry known as *tetrad*. These axes pass through opposite face centres as shown in Fig. 6.10 (a).
- (ii) 4 axes have three-fold symmetry known as *triad*. These axes pass through diagonally opposite corners as shown in Fig. 6.10 (b).
- (iii) 6 axes have two-fold symmetry known as *diad*. These axes pass through the centres of opposite edges as shown in Fig. 6.10 (c).



**Fig. 6.10** (a) 4-fold axes of symmetry, (b) 3-fold axes of symmetry, and (c) 2-fold axes of symmetry

### 6.10.2 Planes of Symmetry

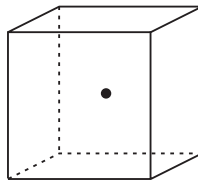
If a plane is able to cut a crystal into two halves in such a way that one half becomes the mirror image of the other half, then that plane is known as the *plane of symmetry*. There are 9 planes—3 are parallel to the face of the cube [Fig. 6.11(a)] and 6 are diagonal planes passing through diagonally opposite parallel edges [Fig. 6.11(b)].



**Fig. 6.11** (a) Parallel plane of symmetry and (b) diagonal plane of symmetry

### 6.10.3 Centre of Symmetry

It is defined as a point in a crystal such that if a line is drawn from any point on the crystal through this point and an equal distance is produced on the other side of this central point, then it meets an identical point. There is only one centre of symmetry for cubic system (Fig. 6.12).



**Fig. 6.12** Centre of symmetry in cubic system

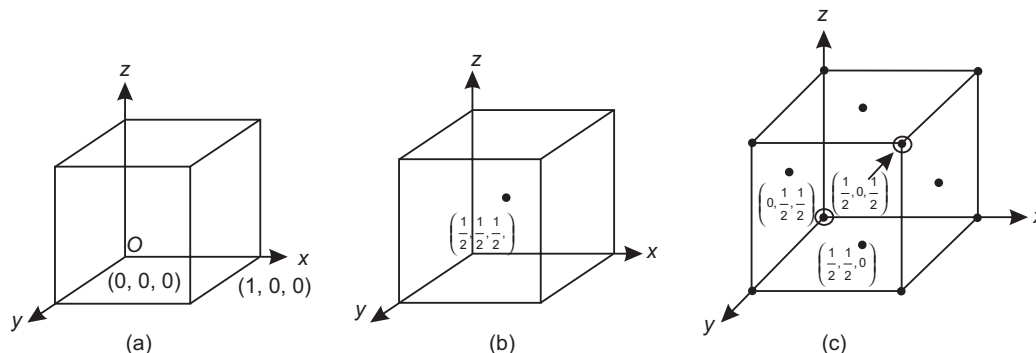
## 6.11 COORDINATES OF LATTICE POINT

The coordinates of the corner lattice points for simple cube, body-centred cube, and face-centred cube systems may be considered as (0,0,0). The coordinates of any one of such points can be considered as the origin. Considering the origin, the coordinates of the other lattice points can be determined [Fig. 6.13(a)]. The coordinates of the body-centred lattice point in BCC system are  $(1/2, 1/2, 1/2)$  [Fig. 6.13(b)]. Similarly, the coordinates of the face-centred lattice points in FCC system are  $(1/2, 1/2, 0)$ ,  $(0, 1/2, 1/2)$ , and  $(1/2, 0, 1/2)$  [Fig. 6.13 (c)].

## 6.12 NUMBER OF ATOMS PER UNIT CELL

The number of atoms per unit cell gives the idea of how the atoms are packed in the solid.

In the simple cubic crystal, there are 8 atoms—one at each corner, and each corner atom is shared by 8 unit cells. Thus, the total number of atoms per unit cell is given as  $N_C/8 = 8/8 = 1$  as shown in Fig. 6.14 (a), where  $N_C$  is the number of corner atoms.



**Fig. 6.13** (a) Coordinates of corner lattice points, (b) coordinates of body-centred lattice points, and (c) coordinates of face-centred lattice points

In the body-centred cubic crystal, there is one atom at the centre of the cell and 8 atoms are at the corner. Similar to SC crystals, each corner atom is shared by 8 unit cells. Therefore, the total number of atoms per unit cell is given as

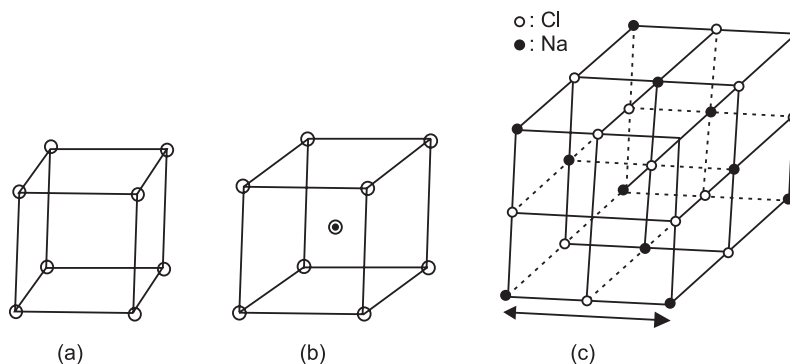
$$N_B + \frac{N_C}{8} = 1 + 1 = 2$$

where  $N_B$  is the number of body-centred atoms. The arrangement of the atoms per unit cell in a body-centred crystal is shown in Fig. 6.14 (b).

In the face-centred cubic crystal, there are 6 atoms at the centre of faces (one face has one atom) and 8 atoms at the 8 corners. Each corner atom is shared by 8 unit cells and each of the 6 face-centred atoms are shared by 2 unit cells. Thus, the total number of atoms can be given as

$$\frac{N_C}{8} + \frac{N_F}{2} = \frac{8}{8} + \frac{6}{2} = 1 + 3 = 4$$

where  $N_F$  is the number of face-centred atoms. The arrangement of the atoms in the face-centred cubic crystal is shown in Fig. 6.14 (c).



**Fig. 6.14** (a) Number of atoms per unit cell in simple cubic system, (b) number of atoms per unit cell in body-centred cubic system, and (c) number of atoms per unit cell in face-centred cubic system

### 6.13 PACKING DENSITY OR ATOMIC PACKING FACTOR

The packing efficiency of atoms or ions in a crystal gives an important concept in the study of crystal structure. Higher packing density provides efficient packing of atoms in solids. How the atoms or ions are packed in a crystal can be defined by a parameter known as *atomic packing factor* of the crystal. *Packing density*, or *atomic packing factor*, is defined as the ratio of the volume occupied by the atoms in the unit cell to the total volume of the unit cell.

$$\text{Atomic packing factor} = \frac{\text{Volume occupied by the atoms in the unit cell}}{\text{Volume of the unit cell}}$$

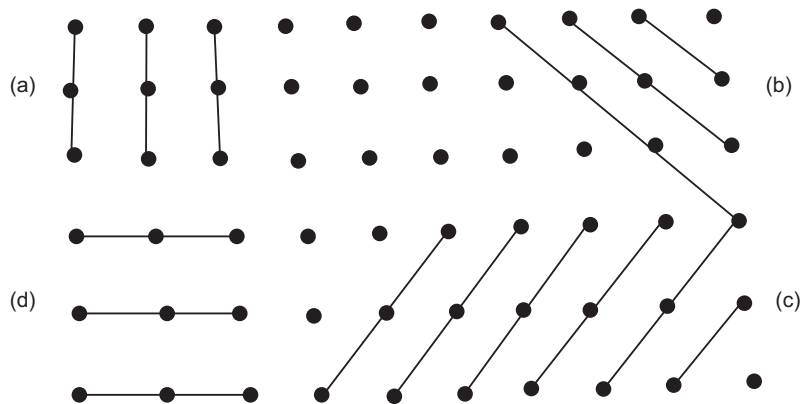
In the case of ionic crystal, the ionic packing factor is expressed as

$$\text{Ionic packing factor} = \frac{\text{Volume occupied by the ions in the unit cell}}{\text{Volume of the unit cell}}$$

Atomic packing factors for SC crystal, BCC crystal, and FCC crystal are given as  $\pi/6$ ,  $\sqrt{3}\pi/8$ , and  $\sqrt{2}\pi/6$ , respectively.

### 6.14 MILLER INDICES

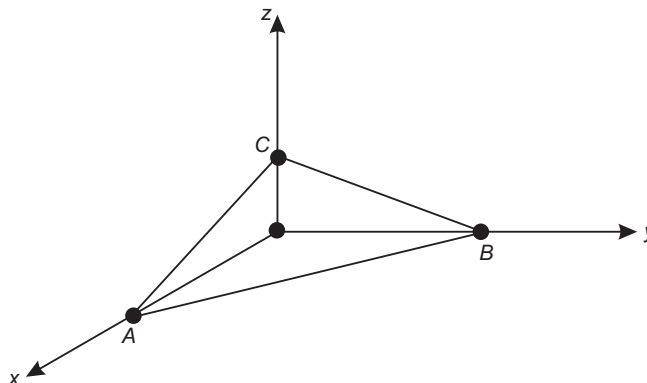
A crystal lattice consists of a large number of parallel equidistant planes passing through the lattice points. These planes are known as *lattice planes*. For a given crystal, the lattice planes can be chosen in different ways as shown in Figs. 6.15 (a), (b), (c), (d), and (e).



**Fig. 6.15** Different lattice planes

Miller introduced a system to designate a plane in a crystal. He suggested that it is more useful to describe the orientation of a plane by the reciprocal of its numerical parameters rather than by its linear parameters. The reciprocals when appropriately converted to whole numbers are called *Miller indices*. In other words, *Miller indices* are defined as three smallest possible integers which have the same ratios as the reciprocal of intercepts of the plane concerned on the three axes.

For example, in the plane  $ABC$  of Fig. 6.16, the  $x$ -axis has an intercept of 2 axial unit, the  $y$ -axis has an intercept of 2 axial unit, and the  $z$ -axis has an intercept of 1 axial unit. Thus, the orientation of the plane is  $(2, 2, 1)$ . The orientation of a plane is described by the reciprocal of the numerical parameters, i.e.,  $(1/2 : 1/2 : 1)$ . Now, reduce the reciprocal into whole numbers, i.e.,  $(1, 1, 2)$ . The Miller indices of a plane are always shown in parenthesis. The general form for indices of a plane is  $(hkl)$ .



**Fig. 6.16** Orientation of a plane with different axial intercepts

#### 6.14.1 Procedure for Finding Miller Indices

The Miller indices for a crystal plane can be determined with the following steps:

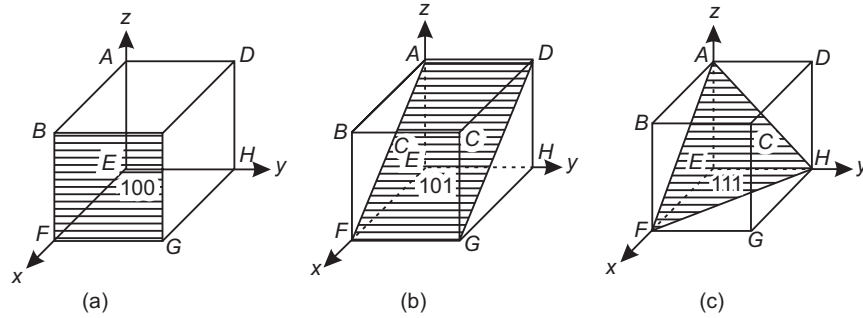
1. Choose a system of three coordinate axes, preferably along the crystallographic axis.
2. Find the intercepts of the plane along the coordinate axes  $x, y, z$ .
3. Express these intercepts in the terms of axial unit.
4. Take the reciprocal of these intercepts.
5. Taking LCM of numerical values of the above reciprocals, reduce them to the smallest three integers which have the same ratio.
6. Enclose the result obtained in step 5 in parentheses as  $(hkl)$ , which are known as Miller indices of the crystal plane.

#### 6.15 DIFFERENT CRYSTAL PLANES WITH MILLER INDICES

The Miller indices  $(hkl)$  are used to denote a single plane or a set of parallel planes. If a plane has negative intercept along a particular axis, then the corresponding index will be negative, which is usually denoted by placing a bar above that index. For example, if a plane has negative intercept along the  $y$ -axis, then the corresponding Miller indices can be given as  $(h\bar{k}l)$ . Miller indices for the six faces of a cubic crystal are given as

$BCGF$ (100)	$ADHE$ ( $\bar{1}00$ )
$CDHG$ (010)	$ABFE$ ( $0\bar{1}0$ )
$ABCD$ (001)	$EHGF$ ( $00\bar{1}$ )

Three planes  $BCGF$ ,  $ADGF$ , and  $AHF$  of a cubic crystal having Miller indices  $(100)$ ,  $(101)$ , and  $(111)$ , respectively, have been shown in Figs. 6.17 (a), (b), and (c).



**Fig. 6.17** (a)  $BCGF$  plane with Miller indices  $(100)$ , (b)  $ADGF$  plane with Miller indices  $(101)$ , and (c)  $AHF$  plane with Miller indices  $(111)$

## 6.16 IMPORTANT FEATURES OF MILLER INDICES

Some important features of Miller indices are given below:

- (i) Equally spaced parallel planes will have the same index numbers.
- (ii) If a plane is parallel to any one of the three coordinate axes, its intercept on that axis is infinity. Hence, the Miller index for that direction is zero.
- (iii) For negative intercept of a plane, a negative bar is put on the corresponding Miller index, e.g.,  $(\bar{1}00)$ .
- (iv) The Miller indices are used to define a set of parallel planes and not a particular plane.
- (v) A plane passing through the origin is defined in terms of a parallel plane having nonzero intercepts.
- (vi) For a cubic crystal system,
  - (a) the distance  $d$  between the adjacent planes of a set of parallel planes of the indices  $(hkl)$  is given as

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \quad (6.3)$$

where  $a$  is the edge of the cube.

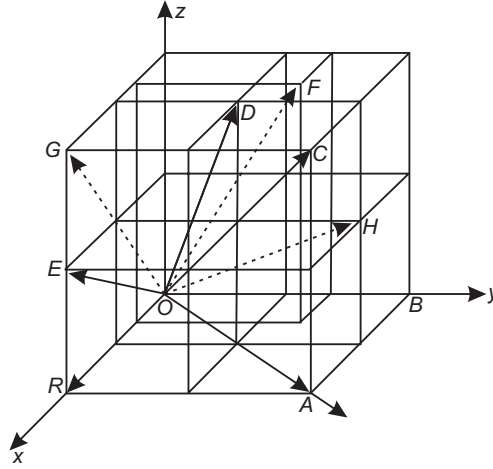
- (b) the angle  $\theta$  between two crystallographic directions  $[hkl]$  and  $[h', k', l']$  can be calculated as

$$\cos \theta = \frac{hh' + kk' + ll'}{(h^2 + l^2 + k^2)^{1/2} (h'^2 + k'^2 + l'^2)^{1/2}} \quad (6.4)$$

## 6.17 DIRECTION OF A LINE

The direction of a line in space can be defined with the coordinates through which it is passing. In order to indicate the direction, usually the square brackets are used. For a cubic system, the *direction of a line*  $(hkl)$  is defined as a normal to the plane whose Miller indices are  $(hkl)$ . The direction of different lines given below are shown in Fig. 6.18.

$$\begin{array}{lll}
OA = [110]; & OR = [100]; & OF = [1/3, 2/3, 1] \text{ or } [1, 2, 3] \\
OB = [010]; & OD = [1/2, 1/2, 1] \text{ or } [1, 1, 2]; & OG = [101] \\
OC = [111]; & OE = [1, 0, 1/2] \text{ or } [2, 0, 1]; & OH = [1/2, 1, 1/2] \text{ or } [1, 2, 1]
\end{array}$$



**Fig. 6.18** Direction of a line

## 6.18 INTERPLANAR SPACING

The perpendicular distance between the corresponding parallel planes of a family having Miller indices  $(hkl)$  is known as *interplanar spacing*, which is usually denoted by  $d_{hkl}$ .

In order to calculate the interplanar spacing, let us consider the case of plane  $ABC$  of a cubic crystal as shown in Fig. 6.19. This plane belongs to a family of planes whose Miller indices are  $hkl$ . As shown in Fig. 6.19,  $ON$  is the perpendicular drawn from the origin to this plane. Perpendicular  $ON$  is the interplanar spacing  $d_{hkl}$  of the family of planes. Let us consider that the normal  $ON$  makes angles  $\alpha'$ ,  $\beta'$ , and  $\gamma'$  with the coordinate axes  $x$ ,  $y$ , and  $z$ , respectively (Fig. 6.20). The intercepts of the plane  $ABC$  along the three axes can be given as

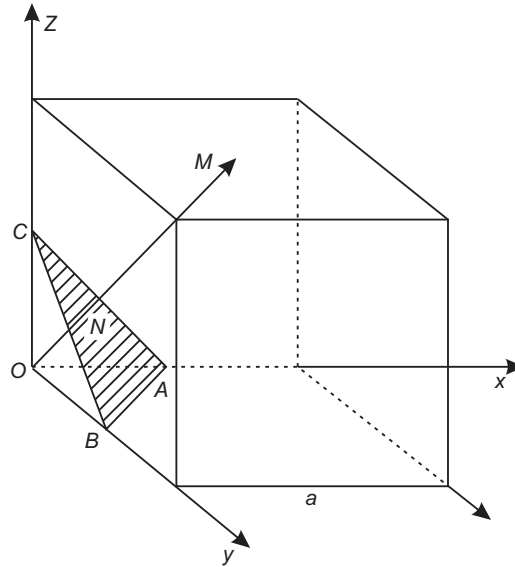
$$OA = \frac{a}{h}, OB = \frac{a}{k}, OC = \frac{a}{l} \quad (6.5)$$

where  $(hkl)$  are Miller indices of plane  $ABC$  and  $a$  is the lattice constant.

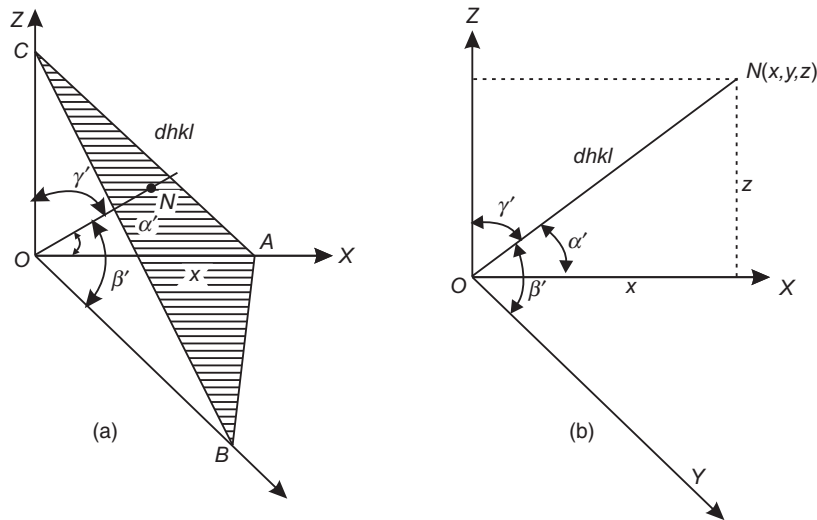
Now, from Figs. 6.19 and 6.20. (b),

$$\cos \alpha' = \frac{ON}{OA}, \cos \beta' = \frac{ON}{OB}, \cos \gamma' = \frac{ON}{OC} \quad (6.6)$$

The distance  $ON$  represents interplanar distance  $d_{hkl}$  of the family of parallel planes having Miller indices  $(hkl)$ .



**Fig. 6.19** Interplanar spacing



**Fig. 6.20** Angles made by normal with respective axes

Now, from Eqs. (6.5) and (6.6), we have

$$\cos \alpha' = \frac{d_{hkl}}{a/h}, \cos \beta' = \frac{d_{hkl}}{a/k}, \cos \gamma' = \frac{d_{hkl}}{a/l} \quad (6.7)$$

From Fig. 6.20 (b), the distance between the origin and the foot of the perpendicular at plane ABC can be given as

$$(ON)^2 = (d_{hkl})^2 = (x^2 + y^2 + z^2) \quad (6.8)$$



where  $x = d \cos \alpha', y = d \cos \beta', z = d \cos \gamma'$  (6.9)

i.e.,  $d_{hkl} = \sqrt{d_{hkl}^2 \cos^2 \alpha' + d_{hkl}^2 \cos^2 \beta' + d_{hkl}^2 \cos^2 \gamma'}$   
 or  $\cos^2 \alpha' + \cos^2 \beta' + \cos^2 \gamma' = 1$  (6.10)

By putting the value of  $\cos \alpha'$ ,  $\cos \beta'$ , and  $\cos \gamma'$  from Eq. (6.7) in Eq. (6.10), we get

$$\frac{d_{hkl}^2 h^2}{a^2} + \frac{d_{hkl}^2 k^2}{a^2} + \frac{d_{hkl}^2 l^2}{a^2} = 1$$

or  $\frac{d_{hkl}^2}{a^2} (h^2 + k^2 + l^2) = 1$

or  $d_{hkl}^2 = \frac{a^2}{(h^2 + k^2 + l^2)}$

or  $d_{hkl} = \frac{a}{\sqrt{(h^2 + k^2 + l^2)}}$  (6.11)

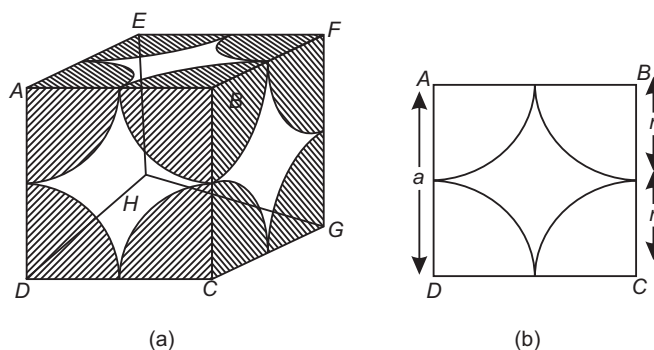
With the help of above expression we can calculate the interplanar spacing in terms of lattice constant  $a$  and Miller indices  $h$ ,  $k$ , and  $l$ .

## 6.19 ATOMIC RADIUS IN A CUBIC SYSTEM

Atoms in a cubic system are arranged such that any two adjacent atoms touch each other. The radius of such atoms may be found in the terms of length of the side of the cubic system and is denoted as  $a$ . The radius of the atoms is known as *atomic radius* and is equal to half of the distance between the centres of two adjacent atoms placed symmetrically in the cube.

### 6.19.1 Atomic Radius of Simple Cubic Structure

Consider an SC structure that contains atoms as shown in Figs. 6.21 (a) and (b).



**Fig. 6.21** Simple cubic structure

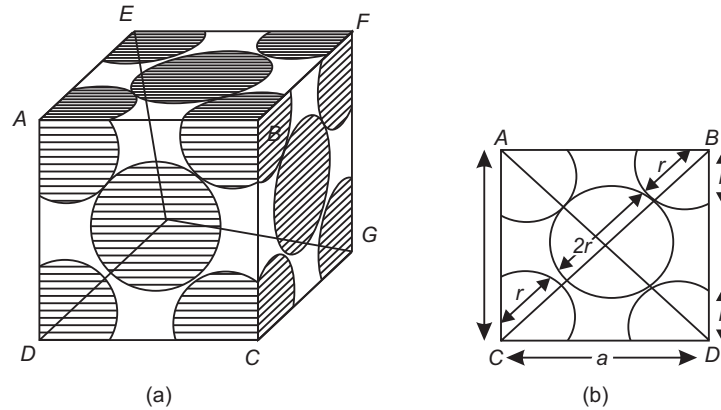
We know that each simple cubic structure consists of 8 atoms, one at each of its corner.

From Fig. 6.21 (b), it is clear that  $r = a/2$ .

Thus, the atomic radius of SC structure,  $r = a/2$ .

### 6.19.2 Atomic Radius of Face-Centred Cubic Structure

Consider an FCC structure as shown in the Figs. 6.22 (a) and (b).



**Fig. 6.22** Face-centred cubic structure

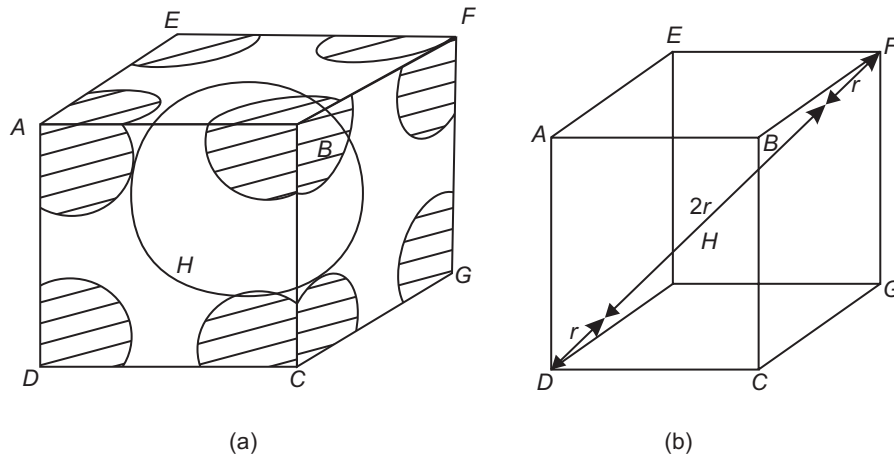
From the geometry of Fig. 6.22 (b), the diagonal

$$BC = 2r + r + r = 4r = \sqrt{a^2 + a^2} = a\sqrt{2}$$

$$\therefore r = \frac{a\sqrt{2}}{4}$$

### 6.19.3 Atomic Radius of Body-Centred Cubic Structure

Consider a BCC structure as shown in Figs. 6.23 (a) and (b).



**Fig. 6.23** Body-centred cubic structure

From the geometry of Fig. 6.23 (b),

$$DF = 4r = \sqrt{DG^2 + GF^2} = \sqrt{DC^2 + CG^2 + GF^2}$$

or 
$$4r = \sqrt{a^2 + a^2 + a^2}$$

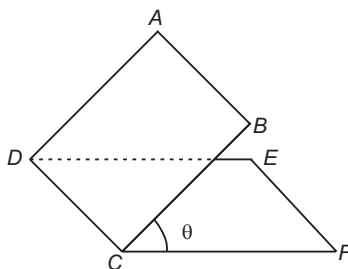
$$= \sqrt{3}a$$

or 
$$r = \frac{\sqrt{3}a}{4}$$

## 6.20 ANGLE BETWEEN TWO PLANES

Consider a cube having two planes  $ABCD$  and  $EFCD$  inclined at an angle  $\theta$  with each other as shown in Fig. 6.24. If  $(h_1 k_1 l_1)$  be Miller indices of the plane  $ABCD$  and  $(h_2 k_2 l_2)$  of the plane  $EFCD$ , then the angle between these planes is given by the relation

$$\cos \theta = \frac{h_1 h_2 + k_1 k_2 + l_1 l_2}{\sqrt{h_1^2 + k_1^2 + l_1^2} \times \sqrt{h_2^2 + k_2^2 + l_2^2}} \quad (6.12)$$



**Fig. 6.24** Angle between two planes

## 6.21 DIMENSIONS OF UNIT CELL

The dimensions of a unit cell, or (we can call) the interatomic distance in a crystal, may be obtained mathematically. Let us consider a unit cell of lattice constant  $a$  having  $n$  number of atoms per unit cell. Now, if  $A$  is the atomic weight of the crystalline substance or compound and  $N$  the Avogadro's number, then according to the basic definitions,

$$\text{mass of } N \text{ molecules} = A \text{ gram}$$

$\therefore$  mass of  $n$  molecules =  $\frac{An}{N}$  gram

$\therefore$  Density of a unit cell is

$$\begin{aligned} \rho &= \frac{\text{Mass of a unit cell}}{\text{Volume of unit cell}} = \frac{An / N}{a^3} \\ &= \frac{An}{Na^3} \end{aligned}$$

$$\text{or} \quad a = \frac{An}{N\rho} \quad (6.13)$$

This expression gives the dimension of a unit cell.

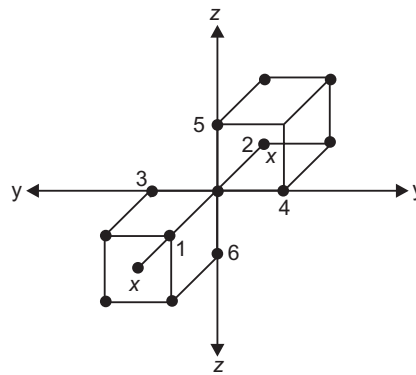
## 6.22 COORDINATION NUMBER

It is defined as the number of atoms directly surrounding a given atom. In a given SC structure, each corner atom is directly surrounded by six other atoms of the adjacent unit cell as shown in Fig. 6.25.

It may be clear from Fig. 6.25 that two atoms (1 and 2) surround the corner atom of the unit cell along the  $x$ - $x$  axis. Similarly, two atoms (3 and 4) surround the corner atom along the  $y$ - $y$  axis, and two atoms (5 and 6) along the  $z$ - $z$  axis, respectively. Thus, the coordination number of an SC structure is six.

In a BCC structure, each corner atom is surrounded by eight other body-centred unit cells. Thus, the coordinate number of BCC structure is eight.

Similarly, an FCC structure has coordination number twelve.



**Fig. 6.25** Coordination number

## 6.23 INTERPLANAR SPACING IN CUBIC SYSTEM

There are three types of cubic crystals, namely, SC crystal, FCC crystals, and BCC crystals. The interplanar spacing for different families of planes is discussed under the following sub sections.

### 6.23.1 Simple Cubic Crystal

- (i) The interplanar spacing for the family of parallel planes having Miller indices (100) and lattice constant  $a$  can be given as

$$d_{100} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} = \frac{a}{\sqrt{1^2 + 0^2 + 0^2}} = a$$

- (ii) For the family of parallel planes having Miller indices (110) and lattice constant  $a$ , the interplanar spacing can be given as

$$d_{110} = \frac{a}{\sqrt{1^2 + 1^2 + 0^2}} = \frac{a}{\sqrt{2}}$$

- (iii) Similar to the above calculations, the interplanar spacing for the family of planes having Miller indices (111) can be given as

$$d_{111} = \frac{a}{\sqrt{1^2 + 1^2 + 1^2}} = \frac{a}{\sqrt{3}}$$

Now,  $(d_{100} : d_{110} : d_{111}) = 1 : \frac{a}{\sqrt{2}} : \frac{a}{\sqrt{3}} = 1 : 0.71 : 0.53$

or  $\left[ \frac{1}{d_{100}} : \frac{1}{d_{110}} : \frac{1}{d_{111}} \right] = 1 : \sqrt{2} : \sqrt{3}$  (6.14)

### 6.23.2 Face-Centred Cubic Crystal

The planes of the FCC lattice corresponding to the Miller indices (100), (110), and (111), respectively, are shown in Figs. 6.26 (a), (b), and (c). It is observed that there are some additional planes, in addition to the original planes in an SC crystal. These additional planes are due to the presence of an extra lattice point on each face of FCC crystal.

- (i) (100) plane: The family of parallel planes in an FCC crystal is shown in Fig. 6.26 (a). It is clear from Fig. 6.26 (a) that there is an additional plane (100) arising halfway between two (100) planes. The interplanar spacing of the new (100) plane for the FCC crystal is given as

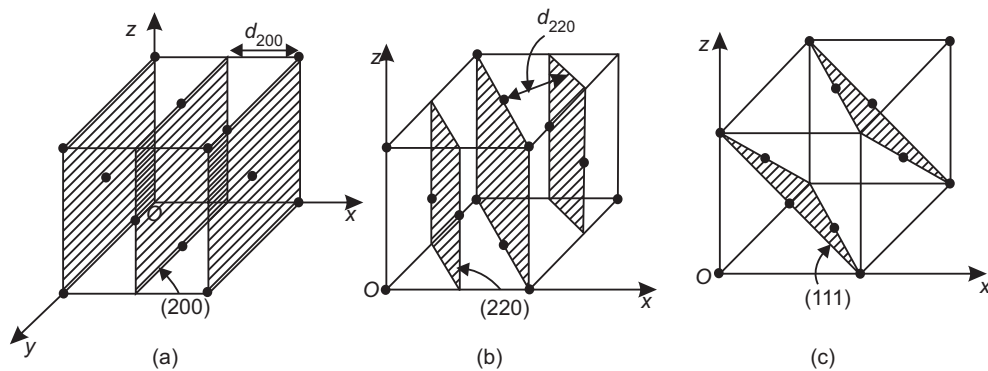
$$\text{new } d_{100} = (d_{200})_{FCC} = \frac{1}{2} (d_{100})_{SC} = \frac{a}{2} \quad (6.15)$$

Actually, the new (100) plane is known as (200) plane with respect to the origin  $O$ .

- (ii) (110) plane: As shown in Fig. 6.26 (b), an additional set of planes (110) arises which is parallel to the first set. These additional planes lie between two (110) planes. Thus, the interplanar spacing for the new (110) plane for FCC crystal is given as

$$\text{new } d_{110} = (d_{220})_{FCC} = \frac{1}{2} (d_{110})_{SC} = \frac{a}{2\sqrt{2}} \quad (6.16)$$

The new (110) plane is known as (220) plane with respect to the origin  $O$ .



**Fig. 6.26** (a) Family of parallel planes for FCC crystal with an additional plane (100), (b) family of parallel planes for FCC crystal with an additional plane (110), and (c) Original (111) plane for FCC crystal

- (iii) (111) plane: It is clear from Fig. 6.26 (c) that in case of (111) plane, no new plane arises due to face-centred point, so

$$(d_{111})_{FCC} = (d_{111})_{SC} = \frac{a}{\sqrt{3}} \quad (6.17)$$

Now, from Eqs. (6.15), (6.16), and (6.17), we can write

$$\left[ \frac{1}{d_{200}} : \frac{1}{d_{220}} : \frac{1}{d_{111}} \right]_{FCC} = 1 : \sqrt{2} : \frac{\sqrt{3}}{2} \quad (6.18)$$

### 6.23.3 Body-Centred Cubic Crystal

For the BCC crystal, (100), (110), and (111) planes are shown in Figs. 6.27 (a), (b), and (c), respectively. Due to an extra lattice point at the body centre of the BCC crystal, some additional planes also arise in the case of these crystals.

- (i) (100) plane: As shown in Fig. 6.27 (a), there is an additional (100) plane which arises midway between two (100) planes in BCC. Thus,

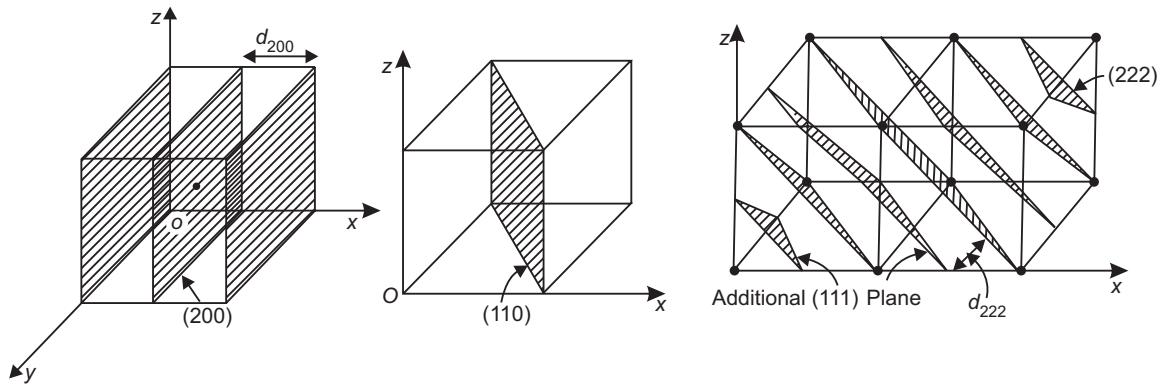
$$\text{new } (d_{100}) = (d_{200})_{BCC} = \frac{1}{2} (d_{100})_{SC} = \frac{1}{2} a \quad (6.14)$$

The new plane (100) is also known as (200) plane with respect to the origin  $O$ .

- (ii)  $(d_{110})$  plane: It is clear from Fig. 6.27 (b) that no extra (110) plane is possible for a BCC. Thus, we can write

$$(d_{110})_{BCC} = (d_{110})_{SC} = \frac{a}{\sqrt{2}} \quad (6.20)$$

- (iii) (111) plane: It is clear from Fig. 6.27 (c) that for a BCC crystal, an additional (111) plane arises midway between two (111) planes. This new plane is known as (222) plane with respect to the origin  $O$ .



**Fig. 6.27** (a) Additional plane (100) for BCC, (b) original plane (110) for BCC, and (c) additional plane (111) for BCC

Thus, we can write

$$\text{new } (d_{111}) = (d_{222})_{BCC} = \frac{1}{2} (d_{111})_{SC} = \frac{a}{2\sqrt{3}} \quad (6.21)$$

Using Eqs. (6.19), (6.20), and (6.21), we can write

$$\left( \frac{1}{d_{200}} : \frac{1}{d_{110}} : \frac{1}{d_{222}} \right) = BCC = 1 : \frac{1}{\sqrt{2}} : \sqrt{3} \quad (6.22)$$

## Solved Examples

### Example 6.1

A substance with the FCC lattice has density  $6200 \text{ kg/m}^3$  and molecular weight  $60.2$ . Calculate the lattice constant  $a$ . [Given that the Avogadro number is  $6.02 \times 10^{26} / \text{kg mol}$ ]

#### **Solution**

The lattice constant  $a$  is given as

$$a = \left( \frac{nm}{N\rho} \right)^{\frac{1}{3}}$$

Here  $n$ , the number of molecules per unit cell in the FCC lattice =  $4$ ,  $M = 60.2$ ,  $N = 6.02 \times 10^{26}$ , and  $\rho = 6200 \text{ kg/m}^3$ .

$$\begin{aligned} \text{Now, } a &= \left( \frac{4 \times 60.2}{6200 \times 6.02 \times 10^{26}} \right)^{1/3} \\ &= 4.01 \times 10^{-10} \text{ m} \\ &= 4.01 \text{ \AA} \end{aligned}$$

### Example: 6.2

Copper has FCC structure and the atomic radius is  $1.278 \text{ \AA}$ . Calculate its density.

#### **Solution**

Density can be given as

$$\rho = \frac{nM}{Na^3}$$

where  $n = 4$  atoms,  $M = 63.54$ ,  $N = 6.023 \times 10^{23}$ , and  $r = 1.278 \text{ \AA} = 1.278 \times 10^{-8} \text{ cm}$ .

We can calculate  $a$  as

$$a = \frac{4r}{\sqrt{2}} \text{ for FCC lattice}$$

$$\text{Now, } a = \frac{4 \times 1.278 \times 10^{-8}}{\sqrt{2}}$$

$$\begin{aligned}\text{Now, } \rho &= \frac{4 \times 63.54}{6.023 \times 10^{23} \times (4 \times 1.278 \times 10^{-8} / \sqrt{2})^3} \\ &= 8.94 \text{ gm/cm}^3\end{aligned}$$

**Example 6.3**

Find the Miller indices of a set of parallel planes which makes intercepts in the ratio  $4a : 3b$  on the  $X$ - and  $Y$ -axes and is parallel to the  $Z$ -axis;  $a$ ,  $b$ ,  $c$  being primitive vectors of the lattice.

**Solution**

According to the problem, the planes are parallel to the  $Z$ -axis. Therefore, their intercepts on the  $Z$ -axis are infinite. If  $pa$ ,  $qb$ , and  $rc$  are the intercepts of the given set of planes on the  $X$ -,  $Y$ -, and  $Z$ -axes, respectively, then

$$\begin{aligned}pa : qb : rc &= 4a : 3b : \infty c \\ p : q : r &= 4 : 3 : \infty \\ \frac{1}{p} : \frac{1}{q} : \frac{1}{r} &= \frac{1}{4} : \frac{1}{3} : \frac{1}{\infty} = \frac{1}{4} : \frac{1}{3} : 0 \\ &= 3 : 4 : 0\end{aligned}$$

$\left\{ \begin{array}{l} \text{Since the set of parallel planes are} \\ \text{parallel to the } Z\text{-axis, therefore, their} \\ \text{intercepts on the } Z\text{-axis are infinite} \end{array} \right.$

Thus, the Miller indices for the given set of planes are  $(3 \ 4 \ 0)$ .

**Example 6.4**

Calculate the interplanar spacing for  $(221)$  plane in an SC lattice, where lattice constant is  $4.2 \times 10^{-10} \text{ m}$ .

**Solution**

For the SC lattice, the interplanar spacing is given as

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

Given that  $a = 4.2 \times 10^{-10} \text{ m}$ ,  $h = 2$ ,  $k = 2$ , and  $l = 1$ .

$$\begin{aligned}\text{Now, } d_{221} &= \frac{4.2 \times 10^{-10}}{\sqrt{(2^2) + (2^2) + (1^2)}} \\ &= \frac{4.2 \times 10^{-10}}{\sqrt{9}} = \frac{4.2}{3} \times 10^{-10} = 1.4 \times 10^{-10} \text{ m} \\ &= 1.4 \text{ \AA}\end{aligned}$$

**Example 6.5**

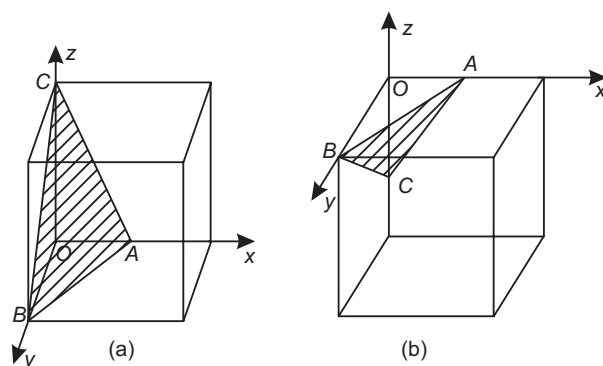
Draw the following Miller planes:

- (i)  $(211)$  and (ii)  $(212)$



### **Solution**

- (i) Corresponding to the Miller planes (211),  
intercepts are  $(1/2, 1, 1)$ .  
Thus, the plane  $ABC$  shown in Fig. 1 (a) is the (211) plane.
- (ii) Corresponding to the Miller indices  $(2\bar{1}2)$ ,  
intercepts are  $(1/2, 1, -1/2)$ .  
Now, the plane  $ABC$  shown in Fig. 1 (b) is the  $(2\bar{1}2)$  plane.



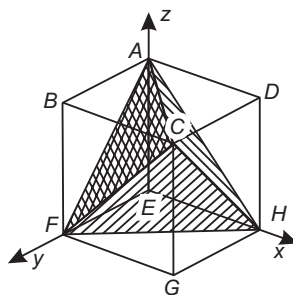
**Fig. 1** (a) Miller plane (211) and (b) Miller plane  $(2\bar{1}2)$

### **Example 6.6**

Draw the different planes of Miller indices (111) in the unit cell of an SC system.

### **Solution**

Four planes  $AFH$ ,  $CFH$ ,  $ACH$ , and  $ACF$  of a unit cell of a cubic system are shown in Fig. 1.



**Fig. 1**  $AFH$ ,  $CFH$ ,  $ACH$ , and  $ACF$  are four planes of a unit cell of a cubic system

### **Example 6.7**

Show in a diagram the (111) plane of a cubic lattice. Calculate their interplanar distance.

**Solution**

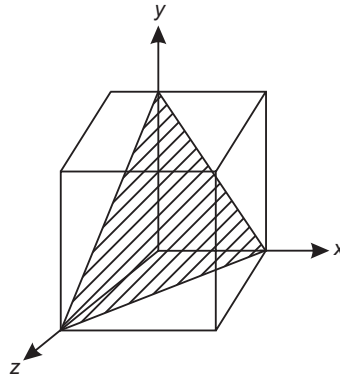
Given Miller indices: (111) ( $a, b, c$ )

Intercepts on axes:  $\left(\frac{1}{1}, \frac{1}{1}, \frac{1}{1}\right) = (1, 1, 1)$

Hence, the plane is as shown in Fig. 1

If  $l$  is the edge of the cube, then the interplanar distance is

$$d = \frac{l}{\sqrt{a^2 + b^2 + c^2}} = \frac{l}{\sqrt{1+1+1}} = \frac{l}{\sqrt{3}} \text{ Å}$$



**Fig. 1** (1, 1, 1) plane

**Example 6.8**

Find the perpendicular distance between the two planes having Miller indices (1, 1, 1) and (2, 2, 2) in a unit cell of a cubic lattice with lattice constant parameter  $a$ .

**Solution**

We know that the perpendicular distance between the origin and the plane is given by

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

Hence, for the plane (1, 1, 1),  $d_1$  is the perpendicular distance from the origin and is given by

$$d_1 = \frac{a}{\sqrt{1^2 + 1^2 + 1^2}} = \frac{a}{\sqrt{3}}$$

Similarly, for the plane (2, 2, 2),

$$d_2 = \frac{a}{\sqrt{2^2 + 2^2 + 2^2}} = \frac{a}{\sqrt{12}} = \frac{a}{2\sqrt{3}}$$

Thus, the perpendicular distance between the given planes is

$$d = d_1 - d_2 = \frac{a}{\sqrt{3}} - \frac{a}{2\sqrt{3}} = \frac{a}{2\sqrt{3}}$$

### Example 6.9

Find the packing efficiency of the Ge (DC) crystal. If the radius of the Ge atom is 1.22 Å, find its lattice parameter.

### Solution

Given  $r = 1.22 \text{ Å}$

Since the Ge crystal has a BCC structure, its packing efficiency can be given as  $\sqrt{3}\pi/8 = 0.68$ .

The lattice parameter for the Ge crystal is

$$a = \frac{4r}{\sqrt{3}} = \frac{4 \times 1.22}{\sqrt{3}} = 2.82 \text{ Å}$$

## 6.24 FORMULAE AND HIGHLIGHTS

1. In a single crystal, the position and orientation of atoms or molecules are uniform and continuous throughout the crystal.
2. The distinction between the crystalline and amorphous solids does not depend on the external appearance but depends only on the arrangement of the fundamental particles.
3. Space lattice + Basis  $\rightarrow$  Crystal structure.
4. Unit cell is the fundamental unit of the complete lattice.
5. The primitive vectors  $\vec{a}$ ,  $\vec{b}$ ,  $\vec{c}$  and the interfacial angles  $\alpha$ ,  $\beta$ ,  $\gamma$  together are known as lattice parameters.
6. Corresponding to the different values of the lattice parameter the crystal systems can be classified into seven types.
7. There are three main symmetry elements that are used to describe a crystalline solid. These are axes, plane, and centre of symmetry.
8. Atomic packing factor = 
$$\frac{\text{Volume occupied by the atoms in the unit cell}}{\text{Volume of the unit cell}}$$
9. Miller indices are used to designate a plane in a crystal. They are expressed as  $(hkl)$ .
10. Interplanar spacing can be given as

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

11. X-rays are the electromagnetic radiations of short wavelength lying in the range of 0.01 Å to 10 Å.

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**Exercises**


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**Section A**  
**Theoretical Questions**

1. Define space lattice. How is it helpful to describe a crystal structure?
2. What is lattice plane? How are the lattice planes described in terms of Miller indices?
3. Show the planes (211) and (111) with a neat diagram in an SC unit cell.
4. What is meant by basis?
5. Define the unit cell and describe the lattice parameters.
6. Discuss the seven types of crystal systems? How are they different from each other?
7. What is Bravais lattice? Discuss with suitable example.
8. What are Miller indices? How can they be determined for a particular family of planes?
9. What is interplanar spacing? Derive the formula for calculating interplanar spacing.
10. For SC, FCC, and BCC, determine the following:
  - (i) Lattice points per unit cell
  - (ii) Nearest neighbour distance
  - (iii) Atomic packing factor
11. Show the planes (101) and  $\bar{1}10$  in SC crystal with neat diagrams. Calculate the interplanar spacing  $d$ .
12. Explain the term interplanar spacing in a crystal and show that the interplanar spacing of corresponding planes of SC of (100), (110), and (111) are in the ratio 1: 0.71: 0.53.
13. Draw (110) and (111) planes, and (110) and (111) directions in the SC crystal. What do you infer from these diagrams?

**Section B**  
**Numerical Problems**

1. NaCl crystals have FCC structure. The density of sodium chloride is  $2.18 \text{ gm/cm}^3$ . Calculate the distance between two adjacent atoms. Atomic weight of sodium = 23 and that of chlorine = 35.5. (Ans.  $2.18 \text{ \AA}$ )

[Hint:

$$a = \left( \frac{nM}{N\rho} \right)^{1/3}$$

where  $M = 23 + 35.5 = 58.5$ ,  $N = 6.02 \times 10^{23} \text{ g/mol.}$

2. For the diatomic crystal Si, calculate the atomic packing factor (APF). Lattice constant of Si is  $5.43 \times 10^{-8} \text{ cm}$ . (Ans. 0.34)

[Hint: Given diatomic crystal has diamond structure, so the number of atoms/unit cell = 8.

$$\text{Radius of Si atom} = r = \frac{\sqrt{3}a}{8}$$

$$\text{and APF for Si} = \frac{8 \cdot \frac{4}{3} \pi r^3}{a^3} = \frac{8 \times \frac{4}{3} \pi \left( \frac{\sqrt{3}}{8} \right)^3 a^3}{a^3} = 0.34]$$

3. Ni is having FCC structure. Calculate the atomic radius, APF, and mass density. Lattice constant  $a = 3.52$  a.u., atomic weight of Ni is 58.71, and Avogadro number =  $6.023 \times 10^{26}$ .

(Ans. Radius = 1.244 Å, APF = 0.74, mass density = 8930 kg/m<sup>3</sup>)

$$\left[ \text{Hint : Atomic radius (FCC)} = r = \frac{a\sqrt{2}}{4} \right]$$

$$\text{APF} = \frac{\sqrt{2}}{6} \pi = 0.74$$

$$\text{Mass density, } d = \frac{nM}{N} \cdot \frac{1}{a^3} \left] \right.$$

4. In a general lattice,  $a = b = 2.5$  Å and  $c = 1.8$  Å. Deduce the lattice spacing between (111) planes. (Ans. 3.96 Å)

$$\left[ \text{Hint : } d_{hkl} = \left( \frac{a^2}{h^2} + \frac{b^2}{k^2} + \frac{c^2}{l^2} \right)^{1/2} \right]$$

5. Calculate the lattice constant of rock salt (NaCl) crystal with the following given data:

(Ans. 5.643 Å)

Molecular weight of NaCl = 58.45.

Density of NaCl = 2170 kg/m<sup>3</sup>.

Avogadro No. =  $6 \times 10^{26}$ /kg mol.

6. Obtain the Miller indices of a plane which intercepts at  $(a, b/2, 3c)$  in an SC unit cell.

(Ans. (361))

7. For an SC lattice of lattice parameter 2.014 Å, calculate the spacing of the lattice plane (212).

(Ans. 0.68 Å)

8. A certain orthorhombic crystal has axial unit  $a : b : c$  or 0.424 : 1 : 0.367. Find the Miller indices of crystal faces whose intercepts are

[Ans. (i) (212), (ii) (103)]

(i) 0.212 : 1 : 0.183 and (ii) 0.424 : ∞ : 0.123

9. The Miller indices of a crystal plane in an SC crystal are (110). Find the ratio of intercepts of the three axes.

(Ans. 1 : 1 : ∞)

[Hint: Reciprocal of intercepts of the three axes are given as the Miller indices.]

10. Draw the Miller plane for Miller indices ( $\bar{1}\bar{1}0$ ).

[Hint: Miller plane is ( $\bar{1}\bar{1}0$ )

Intercepts are (1 ∞ 1)]

**Section C**  
**Multiple Choice Questions**

1. The relation between lengths of axes of a unit cell in a monoclinic crystal system is
  - (a)  $a = b = c$
  - (b)  $a = b \neq c$
  - (c)  $a \neq b \neq c$
  - (d)  $a \neq b = c$
2. The relation among angles between the axes of a triclinic crystal system is
  - (a)  $\alpha = \beta = \gamma = 90^\circ$
  - (b)  $\alpha \neq \beta = \gamma = 90^\circ$
  - (c)  $\alpha \neq \beta \neq \gamma \neq 90^\circ$
  - (d)  $\alpha = \beta = \gamma \neq 90^\circ$
3. According to the different values of the lattice parameter, the number of crystal systems are
  - (a) seven
  - (b) nine
  - (c) five
  - (d) eleven
4. The coordination number for FCC lattice is
  - (a) 12
  - (b) 8
  - (c) 6
  - (d) 26
5. The packing density of BCC is
  - (a)  $\frac{\pi}{6}$
  - (b)  $\frac{\sqrt{3}\pi}{8}$
  - (c)  $\frac{\sqrt{2}\pi}{6}$
  - (d)  $\frac{8}{\sqrt{3}\pi}$
6. The atomic radius for SC lattice is
  - (a)  $a/2$
  - (b)  $\frac{\sqrt{3}}{4}a$
  - (c)  $\frac{\sqrt{2}}{4}a$
  - (d)  $\frac{a}{4}$
7. The Miller indices of a plane which cuts the intercepts of 2, 3, and 4 units along the three axes, respectively, are
  - (a) (643)
  - (b) (234)
  - (c) (321)
  - (d) (232)
8. The basis relation  $a = b \neq c$  is true for
  - (a) tetragonal
  - (b) hexagonal
  - (c) both (a) and (b)
  - (d) none of these
9. The relation between interfacial angles, i.e.,  $\alpha = \beta = \gamma = 90^\circ$  is true for
  - (a) cubic crystals
  - (b) tetragonal crystals
  - (c) orthorhombic crystals
  - (d) all of the above
10. Number of Bravais lattices for a tetragonal crystal system is
  - (a) one
  - (b) two
  - (c) three
  - (d) four

11. The range of X-ray wavelength is  
 (a) 0.01 Å to 10 Å (b) 10 Å to 100 Å  
 (c) 0.01 pm to 10 pm (d) none of these

### Answers

- |        |        |        |         |         |        |
|--------|--------|--------|---------|---------|--------|
| 1. (c) | 2. (c) | 3. (a) | 4. (a)  | 5. (b)  | 6. (a) |
| 7. (a) | 8. (c) | 9. (d) | 10. (b) | 11. (a) |        |

### Section D

#### Fill in the Blanks

- In case of cubic crystal system, three types of ..... are possible.
- Primitive vectors  $\vec{a}$ ,  $\vec{b}$ ,  $\vec{c}$  and the interfacial angles  $\alpha$ ,  $\beta$ ,  $\gamma$  together are called ..... of the crystal.
- In a cube, each rotation of  $90^\circ$  brings it into a .....
- For cubic system, there are ..... of symmetry.
- The total number of atoms per unit cell of an SC system is .....
- In an FCC crystal, there are 8 atoms at .....
- Atomic packing factor for FCC crystal is .....
- All equally spaced parallel planes have the same ..... ( $hkl$ ).
- The ..... is the perpendicular distance  $d_{hkl}$  between the corresponding ( $hkl$ ) planes.
- For a cube, there are ..... axes of symmetry.

### Answers

- |                        |                       |
|------------------------|-----------------------|
| 1. Bravais lattices    | 2. lattice parameters |
| 3. congruent position  | 4. 9 planes           |
| 5. one                 | 6. 8 corners          |
| 7. $\sqrt{2}\pi/6$     | 8. index number       |
| 9. interplanar spacing | 10. 13                |