

## **Elements of Crystallography**

#### 61 INTRODUCTION

Usually all the elements and their chemical derivatives are found in three states viz, solid, liquid, and gascous. 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.

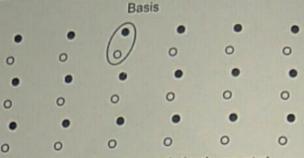
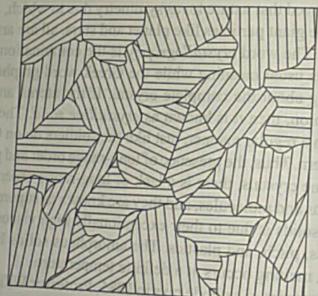


Fig. 6.1 Structure of single crystal

There is another class of material known as polycrystalline in which the whole crystal is made a smaller crystallites, as shown in Fig. 6.2. Each constituent of the small crystallite is called grain be grains are situated side by side to form the whole crystal, like in quartz. Within the boundary of a state is same lattice pattern but grains are generally oriented randomly, and thus, form the grain boundary of a state is same lattice pattern but grains are generally oriented randomly, and thus, form the grain boundary of a state is same lattice pattern but grains are generally oriented randomly, and thus, form the grain boundary of a state is same lattice pattern but grains are generally oriented randomly, and thus, form the grain boundary of a state is same lattice pattern but grains are generally oriented randomly, and thus, form the grain boundary of a state is same lattice pattern but grains are generally oriented randomly, and thus, form the grain boundary of a state is same lattice pattern but grains are generally oriented randomly, and thus, form the grain boundary of a state is same lattice pattern but grains are generally oriented randomly, and thus, form the grain boundary of a state is same lattice pattern but grains are generally oriented randomly, and thus, form the grain boundary of a state is same lattice pattern but grains are generally oriented randomly, and thus, form the grain boundary of a state is same lattice pattern but grains are generally oriented randomly, and thus, form the grain boundary of a state is same lattice pattern but grains are generally oriented randomly, and thus, form the grain boundary of a state is same lattice pattern but grains are generally oriented randomly, and thus, form the grain boundary of a state is same lattice pattern but grains are generally oriented randomly, and thus, form the grain but grains are generally oriented randomly, and thus, form the grain but grains are generally oriented randomly.



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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, it is 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

### 6.3 SPACE LATTICE

In order to describe the arrangement of atoms in a crystal, it is always convenient to describe arrangement of imaginary points in space which have a definite relationship with the atoms of the crystal of imaginary points in space that have identical points in its surroundings is known as space lattice is shown in Fig. 6.3.

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:

$$\vec{T} = n_1 \vec{a} + n_2 \vec{b} + n_3 \vec{c} \tag{6.1}$$

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

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

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

Space lattice + Basis = Crystal structure

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

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 o and •. 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.

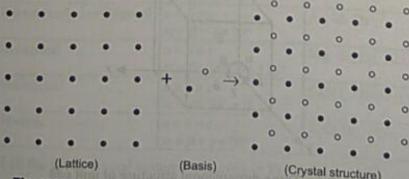


Fig. 6.4 Crystal structure generated from lattice and basis

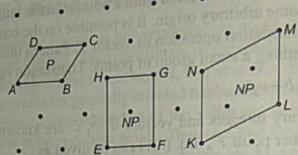
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6.5 UNIT CELL

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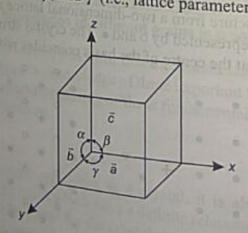


Primitive (P) and nonprimitive (NP) unit cells of 2-D lattice

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

#### LATTICE PARAMETER 6.6

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



Three-dimensional structure of unit cell

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## 67 LATTICE VECTOR AND DIRECTION

In particular point or specific direction in a unit cell can be determined with the help of basic vectors  $\tilde{c}$ . For example, if anyone wants to determine the position and the direction of point P in the and 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

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

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

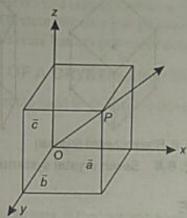


Fig. 6.7 Position and direction of a point with the help of vectors  $\vec{a}$ ,  $\vec{b}$ ,  $\vec{c}$ 

#### 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 para

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

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

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Fig. 6.8 Seven crystal systems

6. Rhombohedral (trigonal)

7. Hexagonal

#### **BRAVAIS SPACE LATTICE**

5. Orthorhombic

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

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.

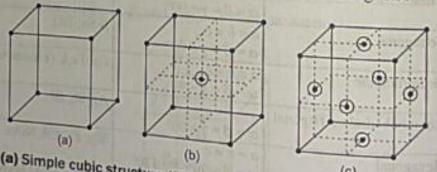


Fig. 6.9 (a) Simple cubic structure (SC), (b) body-centred cubic structure (BCC), and (c) face-centred cubic structure (FCC) In the case of tetragonal system, there are following two types of Bravais lattices:

- (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°), 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° 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).

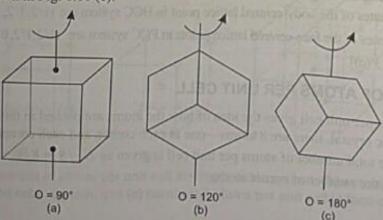


Fig. 6.10 (a) 4-fold axes of symmetry, (b) 3-fold axes of symmetry, and (c) 2-fold axes of symmetry

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## 6.10.2 Planes 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 in the plane of symmetry. There are 9 planes—3 are a street of the plane of symmetry. If a plane is able to cut a crystal into two naives in sacratic matter. There are 9 planes—3 are pane the other half, then that plane is known as the plane of symmetry. There are 9 planes—3 are pane the other half, then that plane is known as the planes passing through diagonally opposite per the face of the cube [Fig. 6.11(a)] and 6 are diagonal planes passing through diagonally opposite per edges [Fig. 6.11(b)].

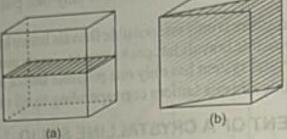


Fig. 6.11 (a) Parallel plane of symmetry and (b) diagonal plane of symmetry

### 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 point and an equal distance is produced on the other side of this central point, then it meets an idpoint. There is only one centre of symmetry for cubic system (Fig. 6.12).

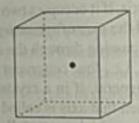


Fig. 6.12 Centre of symmetry in cubic system

### 6.11 COORDINATES OF LATTICE POINT

The coordinates of the comer lattice points for simple cube, body-centred cube, and face-centred systems may be considered as (0,0,0). The coordinates of any one of such points can be considered the origin. the origin. Considering the origin, the coordinates of the other lattice points can be determined to 6.13(a)]. The coordinates of the body-centred lattice point in BCC system are (1/2, 1/2, 1/2) [Fig 613] Similarly, the coordinates of the face-centred lattice points in FCC system are (1/2, 1/2, 0), (0, 1/2, 1/2). (1/2,0,1/2) [Fig. 6.13 (c)].

## 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 shall init cells. Thus, the total number of atoms—one at each corner, and each corner atom is shall init cells. 8 unit cells. Thus, the total number of atoms per unit cell is given as  $N_C/8 = 8/8 = 1$  as shown 6.14 (a), where  $N_c$  is the number of corner atoms.

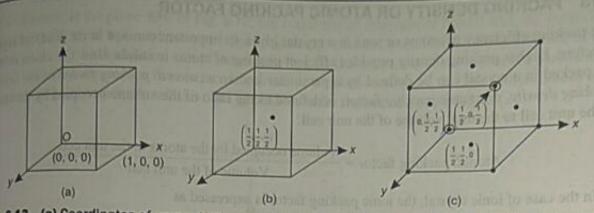


Fig. 6.13 (a) Coordinates of corner lattice points, (b) coordinates of body-centred lattice points, and (c) coordinates of face-centred lattice points

In the body-centred cubic crystal, there is one atom at the centre of the cell and 8 atoms are at the comer. 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, is the number of body-centred atoms. The arrangement of the atoms per unit cell in a bodycentred 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  $N_p$  is the number of face-centred atoms. The arrangement of the atoms in the face-centred cubic

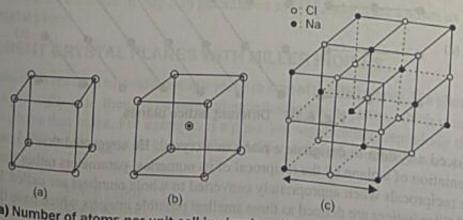


Fig. 6.14 (a) Number of atoms per unit cell in simple cubic system, (b) number of atoms per unit cell in face-centred cubic system. cell in body-centred cubic system, and (c) number of atoms per unit cell in face-centred cubic system

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# 6.13 PACKING DENSITY OR ATOMIC PACKING FACTOR

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

Volume occupied by the atoms in the unit cell Volume of the unit cell Atomic packing factor =

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

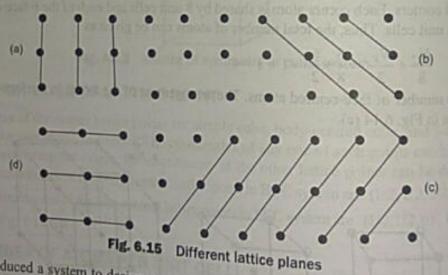
Volume occupied by the ions in the unit cell Ionic packing factor = Volume of the unit cell

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

#### MILLER INDICES

A crystal lattice consists of a large number of parallel equidistant planes passing through the lattice pin 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).

Th



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

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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, plane is described by the reciprocal of the numbers of the numbers of a plane are always shown in parenthesis. The general form for indices of a plane is (hkl).

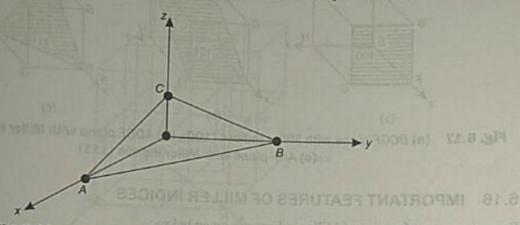


Fig. 6.16 Orientation of a plane with different axial intercepts

## 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 extremely 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 decorresponding Miller indices can be given as (hkl). Miller indices for the six faces of a cubic crystal DIRECTION OF A LINE

BCGF (100)	ADHE (100
CDHG (010)	ABFE (010)
ABCD (001)	EHGF (001)
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Three planes BCGF, ADGF, and AHF of a cubic crystal having Miller indices (100), (101), and (c). 188

respectively, have been shown in Figs. 6.17 (a), (b), and (c).

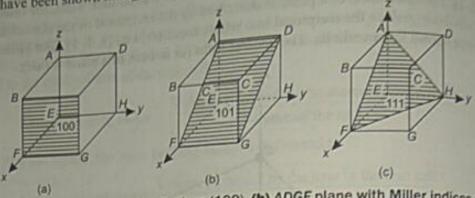


Fig. 6.17 (a) BCGF plane with Miller Indices (100), (b) ADGF plane with Miller Indices (101) by (c) AHF plane with Miller indices (111)

## 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 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 to
- (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 interest.
- (vi) For a cubic crystal system,
  - (a) the distance d between the adjacent planes of a set of parallel planes of the indices (b) given as

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

where a is the edge of the cube. (b) the angle  $\theta$  between two crystallographic directions [hkl] and [h', k', l'] can be calculated

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$$\theta$$
 between two crystallographic directions  $[hkl]$  and  $[h', k', l']$  can be calculated  $\cos \theta = \frac{hh' + kk' + ll'}{\left(h^2 + l^2 + k^2\right)^{1/2} \left(h'^2 + k'^2 + l'^2\right)^{1/2}}$ 
TION OF A LINE

## 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 our indicate the direction, usually the square brackets. to indicate the direction, usually the square brackets are used. For a cubic system, the direction of a cubic system, the direction of a cubic system, the direction of a cubic system. (hkl) is defined as a normal to the plane whose Miller indices are (hkl). The direction of different given below are shown in Fig. 6.18.

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> (hkl) In show

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OA = [110]; OR = [100]; OF = [1/3, 2/3, 1] or [1, 2, 3]

OB = [010]; OD = [1/2, 1/2, 1] or [1, 1, 2]; OG = [101]

OC = [111]; OE = [1, 0, 1/2] or [2, 0, 1]; OH = [1/2, 1, 1/2] or [1, 2, 1]

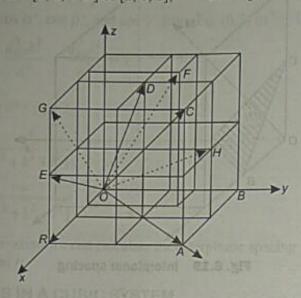


Fig. 6.18 Direction of a line

#### 6.18 INTERPLANAR SPACING

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

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  $d_{kkl}$  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

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

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

The distance ON represents interplanar distance  $d_{kkl}$  of the family of parallel planes having Miller

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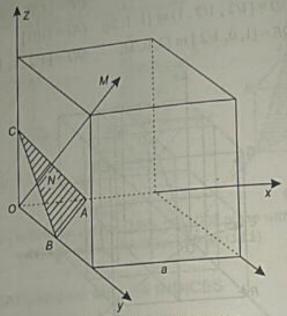
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Interplanar spacing Fig. 6.19

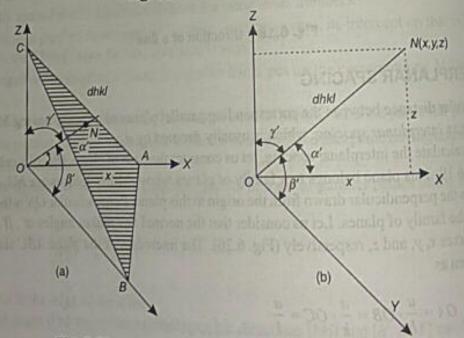


Fig. 6.20 Angles made by normal with respective axes

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

$$\cos \alpha' = \frac{d_{hkl}}{a_h'}, \cos \beta' = \frac{d_{hkl}}{a_k'}, \cos \gamma' = \frac{d_{hkl}}{a_l'}$$

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

$$(ON)^2 = (d_{hij})^2 = (x^2 + y^2 + z^2)$$

where

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Consider

$$x = d \cos \alpha', y = d \cos \beta', z = d \cos \gamma' \text{ and } \Omega \text{ and$$

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

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$$d_{hkl} = \sqrt{d_{hkl}^2 \cos^2 \alpha' + d_{hkl}^2 \cos^2 \beta' + d_{hkl}^2 \cos^2 \gamma'}$$

$$\cos^2 \alpha' + \cos^2 \beta' + \cos^2 \gamma' = 1$$
(6.10)

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

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

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

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

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

With the help of above expression we can calculate the interplanar spacing in terms of lattice constant From the ecometry of Fig. 6 02 (b), the diagonal, a and Miller indices h, k, and l.

### 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).

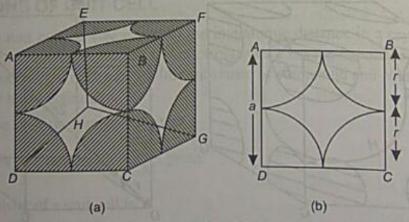


Fig. 6.21 Simple cubic structure

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).

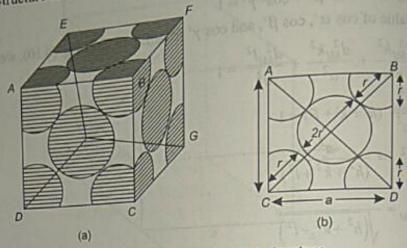


Fig. 6.22 Face-centred cubic structure

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

$$BC = 2r + r + r = 4r = \sqrt{a^2 + a^2} = a\sqrt{2}$$
 DIBUO A 111 SUIGAR DIMON

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

## 6.19.3 Atomic Radius of Body-Centred Cubic Structure

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

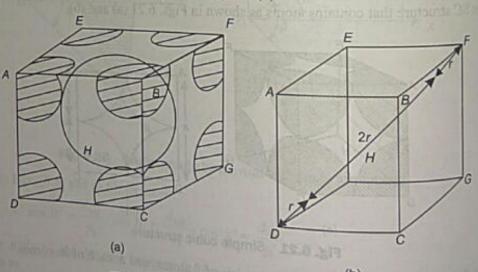


Fig. 6.23 Body-centred cubic structure

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Fig. 6.24. I between th

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From the geometry of Fig. 6.23 (b),
$$DF = 4r = \sqrt{DG^2 + GF^2} = \sqrt{DC^2 + CG^2 + GF^2}$$

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

$$= \sqrt{3}a$$

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

## 820 ANGLE BETWEEN TWO PLANES

tesder a cube having two planes ABCD and EFCD inclined at an angle  $\theta$  with each other as shown in february  $a_1 = a_2 + a_3 + a_4 + a_4 + a_4 + a_5 + a_4 + a_5 +$ 

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

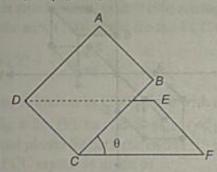


Fig. 6.24 Angle between two planes

### 121 DIMENSIONS OF UNIT CELL

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

mass of N molecules = A gram

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

Density of a unit cell is

$$\rho = \frac{\text{Mass of a unit cell}}{\text{Volume of unit cell}} = \frac{An/N}{a^3}$$

$$= \frac{An}{N^3}$$

$$a = \frac{An}{N\rho}$$

This expression gives the dimension of a unit cell.

## COORDINATION NUMBER

It is defined as the number of atoms directly surrounding a given atom. In a given SC structure, at the structure of the adjacent unit cell as shown in the structure of the structure of the adjacent unit cell as shown in the structure of th It is defined as the number of atoms directly surrounded by six other atoms of the adjacent unit cell as shown in Fig. 61 mer atom is directly surrounded by six other atoms (1 and 2) surround the corner atom of the unit cells.

It may be clear from Fig. 6.25 that two atoms (1 and 2) surround the corner atom along the v-v axis and

It may be clear from Fig. 6.25 that two atoms (4 and 4) surround the corner atom along the y-y axis, and two atoms (3 and 4) surround the corner atom along the y-y axis, and two atoms (3 and 4) surround the corner atom along the y-y axis, and two atoms (3 and 4) surround the corner atom along the y-y axis, and two atoms (3 and 4) surround the corner atom along the y-y axis, and two atoms (5 and 5 an the x-x axis. Similarly, two atoms (5 and 7) and two z (5 and 6) along the z-z axis, respectively. Thus, the coordination number of an SC structure is z (5 and 6) along the z-z axis, respectively. and 6) along the z-z axis, respectively. Thus, and a BCC structure, each corner atom is surrounded by eight other body-centred unit cells. Thus

coordinate number of BCC structure is eight.

Similarly, an FCC structure has coordination number twelve.

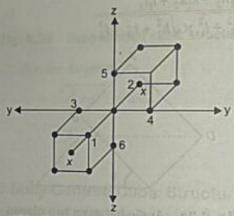


Fig. 6.25 Coordination number

## INTERPLANAR SPACING IN CUBIC SYSTEM

There are three types of cubic crystals, namely, SC crystal, FCC crystals, and BCC crystals. The interpretable of the complete 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 constant a can be given as

a can be given as
$$d_{100} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} = \frac{a}{\sqrt{1^2 + 0^2 + 0^2}} = a$$
amily of parallel planes having Miller in the

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

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

(iii) Sim indi

Now,

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6.23.2 The planes are shown i to the origin point on each

(i) (100 from The

Actu (ii) (110

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The

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(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, 
$$(d_{100}; d_{110}; d_{111}) = 1; \frac{a}{\sqrt{2}} : \frac{a}{\sqrt{3}} = 1; 0.71; 053$$
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

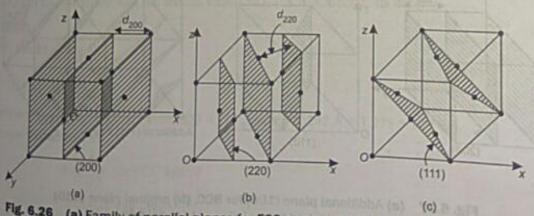
new 
$$d_{100} = (d_{200}) FCC = \frac{1}{2} (d_{100}) SC = \frac{a}{2}$$
 (6.15)

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

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

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



(c) 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

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structure

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

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

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

m Eqs. (6.15), (6.16), and (6.17)
$$\left[\frac{1}{d_{200}}; \frac{1}{d_{220}}; \frac{1}{d_{111}}\right] FCC = 1; \sqrt{2}; \frac{\sqrt{3}}{2}$$
(6)

#### **Body-Centred Cubic Crystal** 6.23.3

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 any the case of these crystals.

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

reen two (100) planes in BCC. Thus,  

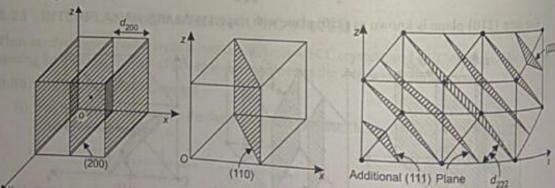
$$new(d_{100}) = (d_{200}) BCC = \frac{1}{2} (d_{100}) SC = \frac{1}{2} a$$
(614)

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. The

$$(d_{110})BCC = (d_{110})SC = \frac{a}{\sqrt{2}}$$
(62)

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



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

Thus, we can

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Example 6.

Asubstance wit constant a. [Giv

Solution The lattice con:

Here n, the r  $\rho = 6200 \text{ kg/m}$ 

Now,

Example: 6.

Copper has FC

Solution

Density can be

where n=4 ato We can calcu

Now,

Thus, we can write

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

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

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

### Solved Examples

### Example 6.1

A substance with the FCC lattice has density 6200 kg/m<sup>3</sup> and molecular weight 60.2. Calculate the lattice constant a. [Given that the Avogadro number is 6.02 × 10<sup>26</sup>/kg mol]

#### Solution

urises to

a BCC The

) plane ma respect to to 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  $\rho = 6200 \text{ kg/m}^3$ .

Now, 
$$a = \left(\frac{4 \times 60.2}{6200 \times 6.02 \times 10^{26}}\right)^{1/3}$$

$$= 4.01 \times 10^{-10} \,\text{m}$$

$$= 4.01 \,\text{Å}$$

### Example: 6.2

Copper has FCC structure and the atomic radius is 1.278 Å. 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 Å = 1.278 × 10<sup>-8</sup> cm. We can calculate n as

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

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

Now, 
$$\rho = \frac{4 \times 63.54}{6.023 \times 10^{23} \times \left(4 \times 1.278 \times 10^{-8} / \sqrt{2}\right)^3}$$

#### Example 6.3

Find the Miller indices of a set of parallel planes which makes intercepts in the ratio 4a:3b on the primitive vectors of the lattice. 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  $Z_{-}$   $V_{-}$ According to the problem, the planes are planes of the given set of planes on the X-, Y-, and Z-, are infinite. If pa, qb, and rc are the intercepts of the given set of planes on the X-, Y-, and Z-, Yrespectively, then

$$pa:qb:rc = 4a:3b: \infty c$$

$$p:q:r = 4:3:\infty$$

$$\frac{1}{p}:\frac{1}{q}:\frac{1}{r}=\frac{1}{4}:\frac{1}{3}:\frac{1}{\infty}=\frac{1}{4}:\frac{1}{3}:0$$

Since the set of parallel planes at parallel to the Z-axis, therefore, to intercepts on the Z-axis are infine

Do

For

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 × 10th

#### Solution

For the SC lattice, the interplanar spacing is given as

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

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

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

#### Example 6.5

Draw the following Miller planes: (i) (211) and (ii) (212)

Solution

10 X-24

C Z-20 Z-auc

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10-HE

(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 (212),

intercepts are (1/2, 1, -1/2).

Now, the plane ABC shown in Fig. 1 (b) is the (212) plane.

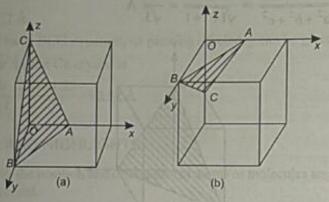


Fig. 1 (a) Miller plane (211) and (b) Miller plane (212)

Example 6.6

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

Solution

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

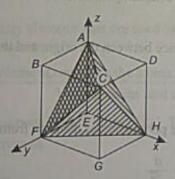


Fig. 1 AFH, CFH, ACH, and ACF are four planes of a unit cell of a cubic system

Example 6.7

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

## Solution

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

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

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

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 I is the edge of the cube, then the interplanar distance is  $d = \frac{1}{\sqrt{a^2 + b^2 + c^2}} = \frac{1}{\sqrt{1 + 1 + 1}} = \frac{1}{\sqrt{3}} \text{ A}$ 

$$A = \frac{1}{\sqrt{a^2 + b^2 + c^2}} = \sqrt{1 + 1 + 1}$$

Fig. 1 (1, 1, 1) plane planes of Miller induces ([11]) [n.t]

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

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

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

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

$$r = 1.22 \text{ Å}$$

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

- 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 → 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.
- Corresponding to the different values of the lattice parameter the crystal systems can be classified into seven types.
- 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 = Volume occupied by the atoms in the unit cell

  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

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

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

, 1) and (2,22)

by

is given by

## Exercises =

## 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 Bravias 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 (110) in SC crystal with neat diagrams. Calculate the interplanar on ing d.
  - 12. Explain the term interplanar spacing in a crystal and show that the interplanar spacing of a responding 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 from these diagrams?

### Section B **Numerical Problems**

1. NaCl crystals have FCC structure. The density of sodium chloride is 2.18 gm/cm<sup>2</sup>. Calculate the distance between two editors of the density of sodium chloride is 2.18 gm/cm<sup>2</sup>. the distance between two adjacent atoms. Atomic weight of sodium = 23 and that of charges = 35.5.

[Hint:

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

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

2. For the diatomic crystal Si, calculate the atomic packing factor (APF). Lattice constant of Single Circum.

[Hint: Given 1]

[Hint: Given diatomic crystal has diamond structure, so the number of atoms/unit cell = 8 Radius of Si atom =  $r = \frac{\sqrt{3}a}{2}$ 

and API

3. Ni is ha

Hint

Mass (

4. In a g planes

Hint

5. Calcu

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6. Obtai

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8. A cer of cr

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Inter

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

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>)

Hint: Atomic radius (FCC) = 
$$r = \frac{a\sqrt{2}}{4}$$

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

Mass density, 
$$d = \frac{nM}{N} \cdot \frac{1}{a^3}$$

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

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

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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>2</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).

8. A certain orthorhombic crystal has axial unit a: b: c or 0.424: 1: 0.367. Find the Miller indices [Ans. (i) (212), (ii) (103)] of crystal faces whose intercepts are

(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.

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

10. Draw the Miller plane for Miller indices (110).

[Hint: Miller plane is (110)

Intercepts are (1 oo 1)]

## Section C

11.

2. P

3. I

9. T 10. F

## ultiple Choice Questions

	AV.	Luxur	allala ametal
		aves	of a unit cell in a monoclinic crystal system is
1.	The relation between lengths of (a) $a = b = c$	(h)	of a unit cell in a monoclinic crystal system is $a = b \neq c$
	(a) $a - b = c$	100000	11-0
	(c) $a \neq b \neq c$	(u)	the axes of a triclinic crystal system is $\alpha \neq \beta = \gamma = 90^{\circ}$
2.	The relation among angles bety	veen t	$\alpha \neq \beta = \gamma = 90^{\circ}$
	(a) $\alpha = \beta = \gamma = 90$	(0)	$\alpha = \beta = \gamma \neq 90^{\circ}$ $\alpha = \beta = \gamma \neq 90^{\circ}$
	(c) $\alpha \neq \beta \neq \gamma \neq 90^{\circ}$	(a)	a p p prameter the number of crystal system
3.	According to the different value	es of	the lattice parameter, the number of crystal systems
	(a) seven	(0)	mine and the second sec
	(c) five		eleven
4.	The coordination number for F	CC la	ttice is
	(a) 12	(b)	8
	(c) 6	(d)	26
5.	The packing density of BCC is		second lattice, a = b = 2.5 A and a = 1.5 A
	Maria de la company de la comp	(b)	$\frac{\sqrt{3}\pi}{8}$
	(a) $\frac{\pi}{6}$	(0)	O .
	5-		8
	(c) $\frac{\sqrt{2}\pi}{6}$	(d)	$\frac{8}{\sqrt{3}\pi}$
	0		V3%
6.	The atomic radius for SC lattic		
	(a) a/2	(1)	$\frac{\sqrt{3}}{4}a$
	(a) u/2	(b)	$\frac{1}{4}a$
	J2		
	(c) $\frac{\sqrt{2}}{4}a$	(d)	$\frac{a}{\Lambda}$ of NaCl = 2170 kg/m <sup>2</sup> .
			lorge to the lorge to the first of the lorge to the lorge
7.	The Miller indices of a plane w	hich	cuts the intercepts of 2, 3, and 4 units along the three
	respectively, are		and 4 units along me and
	(a) (643)	(b)	(234)
	(c) (321)	(4)	(Occidental and American Action of the Control of t
8.	The basis relation $a = b \neq c$ is t	rue fo	or .
	(w) icuagonai		hexagonal have and interest ordered by the second
0	(c) both (a) and (b)		
110	(a) cubic services interfacia	langl	es i.e. e
	(c) orthorhombi-	(b)	none of these les, i.e., $\alpha = \beta = \gamma = 90^{\circ}$ is true for tetragonal crustale
10	(c) orthorhombic crystals	(d)	tetragonal crystals all of the above
	(a) one Bravais lattices for	a tetra	all of the above agonal crystal system is two
	(c) three	(b)	two
		(d)	two four
		321	- Marian

11. The range of (a) 0.01 Å to (c) 0.01 pm	X-ray waveleng o 10 Å to 10 pm	th is (b) 10 Å to (d) none o	o 100 Å f these		
	BA WIT	Ansv	wers		6. (a)
1. (c) 7. (a)	2. (c) 8. (c)	3. (a) 9. (d) Secti Fill in th	4. (a) 10. (b) on D e Blanks	5. (b) 11. (a)	6. (a)
In case of cu     Primitive vectorstal.	bic crystal system ctors $\vec{a}$ , $\vec{b}$ , $\vec{c}$ and	m, three types o	of are p all angles $\alpha$ , $\beta$ , $\gamma$	ossible. together are called.	of the
<ul><li>3. In a cube, ea</li><li>4. For cubic sy</li><li>5. The total num</li><li>6. In an FCC cu</li></ul>	stem, there are mber of atoms pe	er unit cell of ar atoms at	nmetry.  a SC system is	Withelm Centred  Life Stace the pro  Life X stays a	
9. The	AND THE RESERVE OF THE PERSON NAMED IN COLUMN TWO IN COLUMN TO SERVE OF THE PERSON NAMED IN COLUMN TWO IN COLUMN TO SERVE OF THE PERSON NAMED IN COLUMN TWO	icular distance	21000	orresponding (hkl)	planes.
	THE CALL PARTY	Ans	wers	to del of outline	
3. congrue 5. one 7. $\sqrt{2}\pi/$	is lattices lent position  6 anar spacing	4. 9 pl 6. 8 cc			

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