

Chapter I

CRYSTAL STRUCTURE AND CRYSTALLOGRAPHY

1.0 What is meant by Crystallography and why to study the structure of crystalline solids?

Crystallography is the experimental science of determining the arrangement of atoms in the crystalline solids. The properties of some materials are directly related to their crystal structures. For example, pure and undeformed magnesium and beryllium, having one crystal structure, are much more brittle (i.e., fracture at lower degrees of deformation) than pure and undeformed metals such as gold and silver that have yet another crystal structure. Furthermore, significant property differences exist between crystalline and non-crystalline materials having the same composition. For example, non-crystalline ceramics and polymers normally are optically transparent; the same materials in crystalline (or semi-crystalline) form tend to be opaque or, at best, translucent.

An important reason to have an understanding of interatomic bonding in solids is that, in some instances, the type of bond allows us to explain a material's properties. For example, consider carbon, which may exist as both graphite and diamond. Whereas graphite is relatively soft and has a “greasy” feel to it, diamond is the hardest known material. This dramatic disparity in properties is directly attributable to a type of interatomic bonding found in graphite that does not exist in diamond.

Thus by studying the crystal structure and bonding nature of different materials, we can investigate the reasons for the similar or dissimilar nature of the selected materials in terms of different properties or different parameters. The crystal structure and symmetry of a material play a vital role in determining many of its physical properties, such as cleavage, electronic band structure, and optical transparency, etc.

1.1 Introduction

Based on the atomic arrangement in a substance, solids can be broadly classified as either crystalline or non-crystalline. In a crystalline solid, all the atoms are arranged in a periodic manner in all three dimensions whereas in a non-crystalline solid the atomic arrangement is random or non-periodic in nature. A crystalline solid can either be a single crystalline or a polycrystalline. In the case of single crystal the entire solid consists of only one crystal and hence, periodic arrangement of atoms continues throughout the entire material. A polycrystalline material is an aggregate of many small crystals separated by well-defined grain boundaries and hence periodic arrangement of atoms is limited to small regions of the material called as grain boundaries as shown in Fig. 1.1. The non-crystalline substances are also called as amorphous substances materials. Single crystalline materials

exhibit long range as well as short range periodicities while long range periodicity is absent in case of polycrystalline materials and non-crystalline materials.

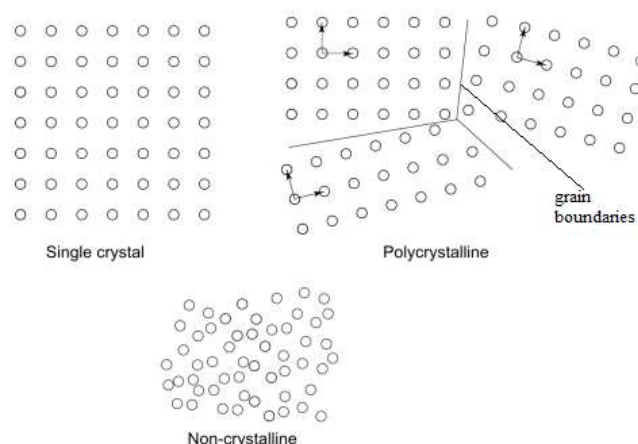


Fig. 1.1 Two dimensional representation of single crystal, polycrystalline and non-crystalline materials

Some more differences between crystalline solids and amorphous solids is listed in Table 1.1.

Table 1.1 Distinction between crystalline and amorphous solids

Crystalline Solids	Amorphous Solids
1. The atoms or molecules of the crystalline solids are periodic in space.	1. The atoms or molecules of the amorphous solids are not periodic in space.
2. Some crystalline solids are anisotropic i.e., the magnitude of physical properties [such as refractive index, electrical conductivity, thermal conductivity, etc.,] are different along different directions of the crystal.	2. Amorphous solids are isotropic i.e., the magnitude of the physical properties are same along all directions of the solid.
3. Crystalline solids have sharp melting points.	3. Amorphous solids do not possess sharp melting points.
4. Breaks are observed in the cooling curve of a crystalline solid.	4. Breaks are not observed in the cooling curve.
5. A crystal breaks along certain crystallographic planes.	5. When an amorphous solid breaks, the broken surface is irregular because it has no crystal planes.

The majority of materials like minerals, alloys, metals, organic and inorganic salts, etc. in their natural forms normally exist as polycrystalline solids. However some organic materials made up of large sized molecules (polymers) mostly exist in non-crystalline form. Among inorganic materials, ordinary glass (soda lime glass) is a typical example of a non-crystalline solid. It requires great effort and skill to make single crystal specimens of these polycrystalline or non-crystalline materials.

Table 1.2 lists examples of some common single crystals, polycrystalline and non-crystalline materials.

Table 1.2 Examples for different categories of solid materials

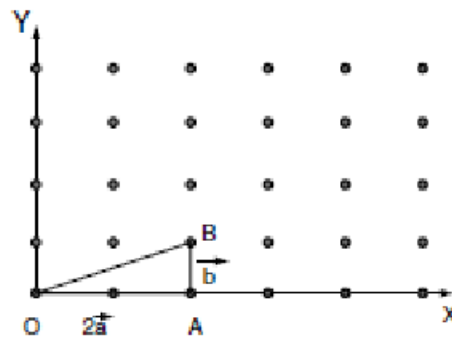
<i>Type of Material</i>	<i>Examples</i>
Single Crystals	Silicon chips used in integrated circuits, quartz crystals used in watches, ruby rods used in ruby lasers, gallium arsenide crystals used in light-emitting diodes, etc.
Polycrystalline Materials	Metals like copper, steel, aluminium, brass etc., used in ordinary engineering and household appliances. Organic and inorganic materials used in powder form like sugar, salts, etc.
Non-Crystalline Materials	Soda lime glass (ordinary window glass), polymers (plastics like polyethylene, polyvinylchloride, polytetrafluoroethylene (teflon), plexiglass, polyurethane foam, bakelite, etc.).

In this chapter, as we are studying about crystal structures of materials, we restrict our discussion to crystalline solids. As already mentioned in table 1.1, a crystal has regular shape and when it is broken all broken pieces have the same regular shape. A crystal has sharp melting point. Since the crystals may have different periodic arrangements in all three dimensions, the physical properties vary with direction and therefore they are called anisotropic substances. Crystalline solids may be made up of metallic crystals or non metallic crystals. Copper, Silver, aluminum, tungsten and magnesium are examples of metallic crystals while carbon, crystallized polymers and plastics are examples of nonmetallic crystals. Let us now discuss the elementary concepts of crystallography.

1.1.1 Space Lattice or Crystal Lattice:

In a solid crystalline material, the atoms or molecules are arranged regularly and periodically in all three dimensions. The atomic arrangement in a crystal is called crystal structure. To explain crystal symmetries easily, it is convenient to represent an atom or a group of atoms that repeats in three dimensions in the crystal as a unit. If each such atom or unit of atoms in a crystal is replaced by a point in space, then the resultant points in space are called space lattice. Each point in a space lattice is called a lattice point and each atom or unit of atoms is called basis or pattern. A space lattice represents the geometrical pattern of crystal in which the surroundings of each lattice point is the same. If the surroundings of each lattice point is same or if the atom or all the atoms at lattice points are identical, then such a lattice is called Bravais lattice. On the other hand, if the atom or the atoms at lattice points are not same, then it is said to be a non-Bravais lattice. Figure 1.2 shows a two- dimensional lattice.

Figure 1.2 Two-dimensional lattice



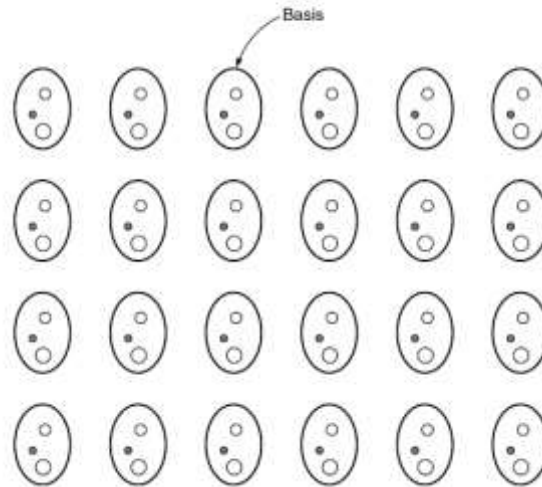
In the same manner, it is very convenient to imagine periodic arrangement of points in space in 3-dimensions about which these atoms are located. “A *space lattice or a crystal lattice is defined as a three dimensional infinite array of points in space in which every point has surroundings identical to that of every other point in the array*”.

To represent translational vectors or basis vectors, consider a co-ordinate system with its origin at the lattice point ‘O’. Let $\overrightarrow{OA} = 2\vec{a}$ and $\overrightarrow{AB} = \vec{b}$, such that $\overrightarrow{OB} = 2\vec{a} + \vec{b}$. where \vec{a} and \vec{b} are called translational or basis vectors along X and Y directions. The position vector \vec{R} of any lattice point can be represented as $\vec{R} = n_1\vec{a} + n_2\vec{b}$. where n_1 and n_2 are integers, their values depend on the position of the lattice point under consideration with respect to the origin. In three dimensions, the position vector of a point can be expressed as $\vec{R} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c}$, where \vec{a} , \vec{b} and \vec{c} are the translational or basis vectors along X, Y and Z directions, respectively. They are also called translational primitives.

1.1.2 Basis and Crystal Structure

The atomic arrangement in a crystal is called crystal structure. The crystal structure is formed by associating every lattice point with an atom or an assembly of atoms or molecules or ions, which are identical in composition, arrangement and orientation, called the basis. i.e. an atom, or a group of atoms or molecules identical in composition is called the basis or the pattern. The basis provides the number of atoms per lattice point, their types, mutual orientations and distances of separation between the atoms. If the basis is substituted for the lattice points, then the resulting structure is called crystal structure as shown in Fig. 1.3. Thus lattice + basis = crystal structure. The basis shown in Fig. 1.3 contains three different atoms. In copper and sodium crystals the basis is single atoms; in NaCl, the basis is diatomic and in CaF_2 the basis is triatomic. A lattice is an imaginary assumption while the crystal structure is a real concept.

Figure 1.3 Two-dimensional crystal structure

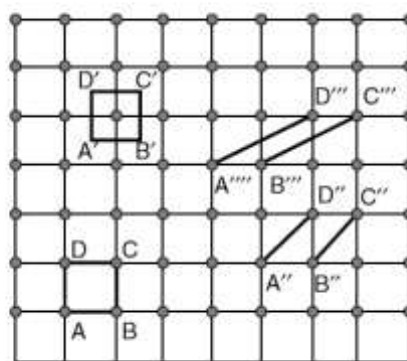


1.1.3 Unit Cell and

Lattice Parameters

Unit cells for most of the crystals are parallelopipeds or cubes having three sets of parallel faces. A unit cell is the basic structural unit or building block of the crystal. A unit cell is defined as the smallest paralleloiped volume in the crystal, which on repetition along the crystallographic axes gives the actual crystal structure or the smallest geometric figure, which on repetition in three-dimensional space, gives the actual crystal structure is called a unit cell. The choice of a unit cell is not unique but it can be constructed in a number of ways; Fig. 1.4 shows different ways of representing unit cells in a two-dimensional lattice. A unit cell can be represented as ABCD or A'B'C'D' or A''B''C''D'', etc.

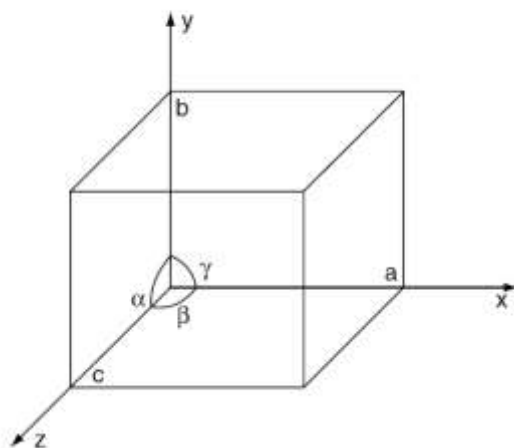
Figure 1.4 Unit cells in crystal lattice



To define the unit cell parameters or lattice parameters, first we define crystallographic axes. These axes are obtained by the intersection of the three non-coplanar faces of the unit cell. The angle between these faces or crystallographic axes are known as interfacial or interaxial angles. The angles between the axes Y and Z is α , between Z and X is β and between X and Y is γ . The translational vectors or primitives a, b, c of a unit cell along X, Y, Z axes and interaxial angles α , β , γ are called

cell parameters. These cell parameters are shown in Fig. 1.5. The cell parameters determine the actual size and shape of the unit cell.

Figure 1.5 Unit cell parameters



1.1.4 Primitive and non-primitive unit cells: The unit cell formed by primitives is called a simple or a primitive unit cell. A primitive unit cell contains only one lattice point. If a unit cell contains more than one lattice point, then it is called a non-primitive unit cell or a multiple unit cell. Most of the unit cells of various crystal lattices contain two or more lattice points and hence it is not necessary that unit cell should be a primitive unit cell. For example, BCC and FCC are non-primitive unit cells.

1.1.5 Bravais Lattice: If the surroundings of each lattice point is same or if the atom or all the atoms at lattice points are identical, then such a lattice is called Bravais lattice. Based on the number of lattice points present per unit cell and stacking sequence of base atoms in a crystal structure, the Bravais lattices are classified into Simple or Primitive (P), Body Centered (I), Face Centered (F) and Base Centered (C) lattices. In simple or primitive lattice, 8 lattice points or 8 atoms are present at the 8 corners of the unit cell, each contributing $1/8^{\text{th}}$ to the unit cell and hence there will be $8 \times 1/8 = 1$ lattice point per unit cell. In body-centered lattice, in addition to the 8 atoms at 8 corners each contributing $1/8^{\text{th}}$ to the unit cell, there will be one complete atom at the center of the unit cell. Therefore number of atoms or lattice points in a body centered unit cell becomes $8 \times 1/8 + 1 \times 1 = 2$. In case of face-centered lattice, in addition to the 8 atoms at 8 corners each contributing $1/8^{\text{th}}$ to the unit cell, six atoms will be present at the center of six faces of the cell each contributing $1/2^{\text{nd}}$ to the unit cell. Therefore number of atoms or lattice points in a face centered unit cell becomes $8 \times 1/8 + 6 \times 1/2 = 4$. Similarly, in case of base-centered lattice, in addition to the 8 atoms at 8 corners each contributing $1/8^{\text{th}}$ to the unit cell, two atoms will be present at the center of upper and lower faces of

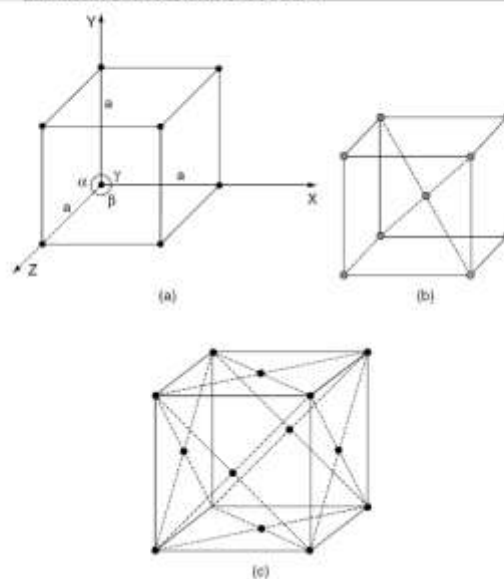
the unit cell each contributing $1/2^{\text{nd}}$ to the unit cell and hence the number of atoms or lattice points in a base centered unit cell becomes $8 \times 1/8 + 2 \times 1/2 = 2$.

1.2 Crystal Systems and Bravais Lattices:

For representing the type of distribution of lattice points in space, seven different co-ordinate systems are required. These co-ordinate systems are called crystal systems. The crystal systems are named on the basis of geometrical shape and symmetry. The seven crystal systems are: (1) Cubic (2) Tetragonal (3) Orthorhombic (4) Monoclinic (5) Triclinic (6) Trigonal (or Rhombohedral) and (7) Hexagonal. Space lattices are classified according to their symmetry. In 1948, Bravais showed that 14 lattices are sufficient to describe all crystals. These 14 lattices are known as Bravais lattices and are classified into 7 crystal systems based on cell parameters. The Bravais lattices are categorized as primitive lattice (P); body-centered lattice (I); face-centered lattice (F) and base-centered lattice (C). These seven crystal systems and Bravais lattices are described below.

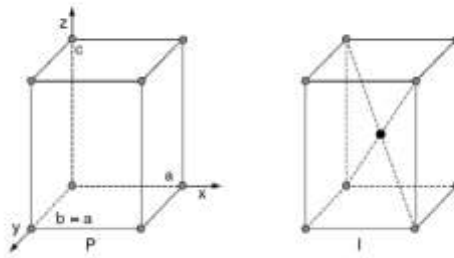
- 1. Cubic crystal system:** In this crystal system, all the unit cell edge lengths are equal and are at right angles to one another i.e., $a = b = c$ and $\alpha = \beta = \gamma = 90^\circ$. In cubic system, there are three Bravais lattices; they are simple (primitive); body-centered and face-centered. Examples for cubic system are Au, Cu, Ag, NaCl, diamond, etc. In simple cubic lattice, lattice points or atoms are present at the corners of the cube. In body-centered cube, atoms are present at the corners and one atom is completely present at the center of the cube. In the case of face-centered cube, atoms are present at corners and at the centers of all faces of cube.

Figure 1.6 Cubic crystal system: (a) Simple cubic (P); (b) Body-centred cube (I) and (c) Face-centred cube (F)



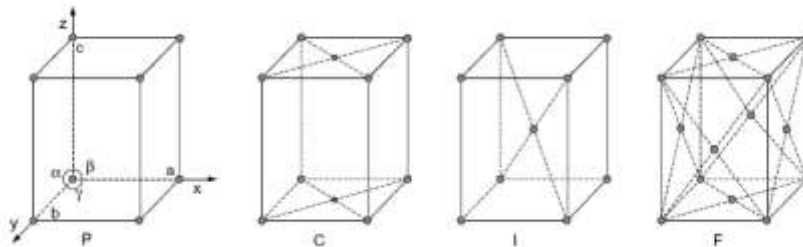
2. **Tetragonal crystal system:** In this crystal system, two lengths of the unit cell edges are equal whereas the third length is different. The three edges are perpendicular to one another i.e., $a = b \neq c$ and $\alpha = \beta = \gamma = 90^\circ$. In tetragonal system, there are two Bravais lattices; they are simple and body-centered. These are shown in Fig. 1.7. Examples for tetragonal crystal systems are TiO_2 , SnO_2 , etc.

Figure 1.7 Tetragonal crystal system



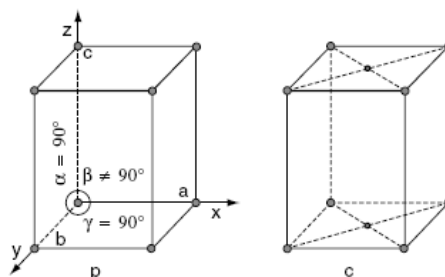
3. **Orthorhombic crystal system:** In this crystal system, unit cell edge lengths are different and they are perpendicular to one another i.e., $a \neq b \neq c$ and $\alpha = \beta = \gamma = 90^\circ$. There are four Bravais lattices in this system. They are simple, face centered, body centered and base centered. These are shown in Fig. 1.8. Examples for orthorhombic crystal system are BaSO_4 , K_2SO_4 , SnSO_4 , etc.

Figure 1.8 Orthorhombic crystal system



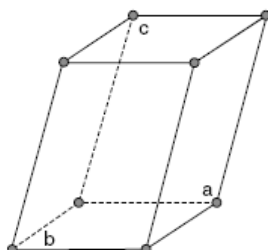
4. **Monoclinic crystal system:** In this crystal system, the unit cell edge lengths are different. Two unit cell edges are not perpendicular, but they are perpendicular to the third edge i.e., $a \neq b \neq c$; $\alpha = \gamma = 90^\circ \neq \beta$. This crystal system has two Bravais lattices; they are simple and base centered. These are shown in Fig. 1.9. Examples for Monoclinic crystal system are $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$ (gypsum), Na_3AlF_6 (cryolite), etc.

Figure 1.9 Monoclinic crystal system



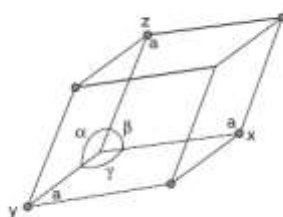
5. **Triclinic crystal system:** In this crystal system, the unit cell edge lengths are different and are not perpendicular i.e., $a \neq b \neq c$ and $\alpha \neq \beta \neq \gamma \neq 90^\circ$ and all the angles are different. This crystal exists in primitive cell only. This is shown in Fig. 1.10. Examples for triclinic crystal system are $\text{K}_2\text{Cr}_2\text{O}_7$, $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$, etc.

Figure 1.10 Triclinic crystal system



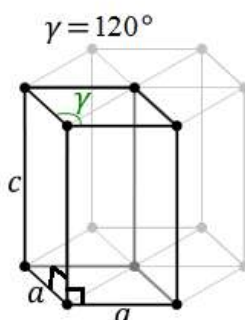
6. **Trigonal or Rhombohedral crystal system:** In this crystal system, all the lengths of unit cell edges are equal. The angles between the axes are equal but other than 90° i.e., $a = b = c$ and $\alpha = \beta = \gamma \neq 90^\circ$. The Bravais lattice is simple only as shown in Fig. 1.11. Examples for Rhombohedral crystal system are As, Bi, Sb, etc.

Figure 1.11 Rhombohedral crystal system



7. **Hexagonal crystal system:** In this crystal system, two sides of the unit cell edge lengths are equal and the angle between these edges is 120° . These two edges are perpendicular to the third edge, and not equal in length i.e., $a = b \neq c$ and $\alpha = \beta = 90^\circ$; $\gamma = 120^\circ$. The Bravais lattice is primitive only. This is shown in Fig. 1.12. The atoms in this crystal system are arranged in the form of a hexagonal close pack.

Figure 1.12 Hexagonal crystal system



The fourteen Bravais lattices of seven crystal systems are summarized in Table 1.3.

Table 1.3 Seven crystal systems and fourteen Bravais lattices

Sl. No	Crystal System	Types of Bravais Lattices	No. of Bravais Lattices	Relation between Lengths and Angles
1	Cubic	P, I, F	3	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$
2	Tetragonal	P, I	2	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$
3	Orthorhombic	P, I, F, C	4	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$
4	Monoclinic	P, C	2	$a \neq b \neq c$ $\alpha = \gamma = 90^\circ \neq \beta$
5	Triclinic	P	1	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$
6	Rhombohedral (Trigonal)	P	1	$a = b = c$ $\alpha = \beta = \gamma \neq 90^\circ$
7	Hexagonal	P	1	$a = b \neq c$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$

1.3 Crystal structures of cubic lattices:

There are three different types of cubical crystal lattice systems namely Simple Cubic (SC), Body-Centered Cubic (BCC) and the Face Centered Cubic (FCC).

1.3.1 Structure and packing fractions of simple cubic [SC] structure

The unit cell edge lengths of this structure along the crystallographic axes and interaxial angles are equal [i.e., $a = b = c$ and $\alpha = \beta = \gamma = 90^\circ$]. Atoms are present only at the corners of this unit cell. A corner atom is shared by eight unit cells, so that the contribution of a corner atom to a unit cell is $1/8$. The cube has eight corners, hence the contribution of eight corner atoms to a unit cell or the number of atoms per unit cell $= \frac{1}{8} \times 8 = 1$. Let ' r ' be the radius of an atom. The surfaces of the atoms touch along the cube edges. So, the distance between the centres of two neighbouring atoms or the nearest neighbour distance ($2r$) is equal to the lattice constant ' a '. In simple cubic cell, the number of nearest neighbour atoms to an atom or co-ordination number is six. Since atoms are present at a distance of ' a ' along $\pm X$, $\pm Y$ and $\pm Z$ directions. The number of nearest equidistant neighbouring atoms to an atom in the structure is called co-ordination number. Figure. 1.13 shows the simple cubic structure. Next, we find the fraction of the unit cell volume occupied by the atoms. The simple cubic structure contains only one atom per unit cell.

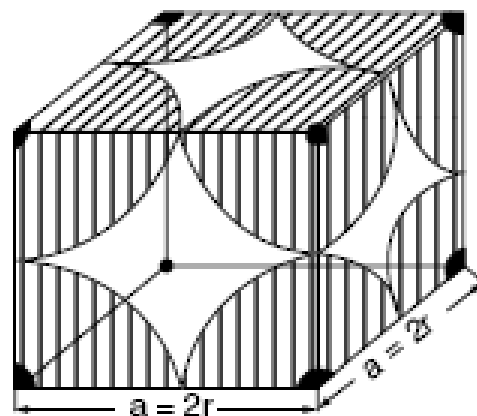
The volume occupied by atoms in the unit cell (v) $= 1 \times \frac{4}{3} \pi r^3$ and

The volume of unit cell (V) $= a^3$. Hence, the packing factor or density of packing in the unit cell (PF)

$$= \frac{v}{V} = \frac{\frac{4}{3} \pi r^3}{a^3} = \frac{4}{3} \frac{\pi r^3}{(2r)^3} = \frac{\pi}{6} = 0.52 \text{ or } 52\%$$

Atomic packing factor is defined as the fraction of the space occupied by atoms in the unit cell or it is the ratio of the volume occupied by atoms in the unit cell to the unit cell volume. An example for simple cubic structure is polonium crystal.

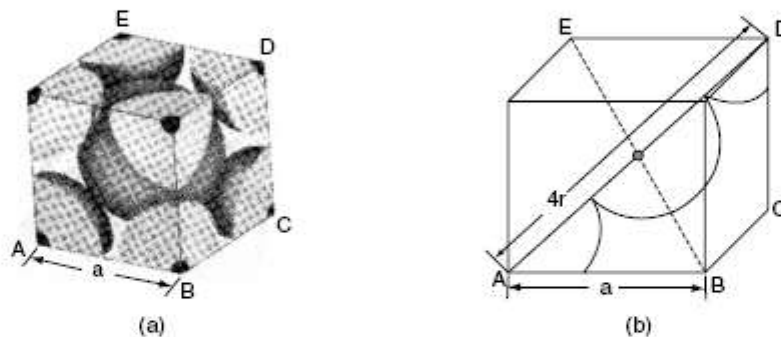
Figure 1.13 Simple cubic structure



1.3.2 Structure and packing fractions of body-centred cubic structure [BCC]

For this unit cell, atoms are present at the corners of the cube and one atom is completely present at the centre of the unit cell. The centre of the unit cell is defined as the intersecting point of two body diagonals [AD and BE as shown in Fig. 1.14]. A corner atom is shared by eight unit cells so that the contribution of a corner atom to a unit cell is $1/8$. Therefore, the number of atoms per unit cell = $(1/8) \times 8 + 1 = 2$. The centre atom is surrounded by eight corner atoms, so the coordination number is 8. The surfaces of unit cell corner atoms may not touch, but they are in contact with the centre atom i.e., the surfaces of atoms are in contact along a body diagonal of the unit cell. Half the distance between the centres of a corner atom and central atom is equal to the radius (r) of an atom. The relation between unit cell edge length (a) and radius (r) of an atom can be obtained with reference to Fig. 1.14 (b).

Figure 1.14 Body-centred cubic structure



The length of the body diagonal $AD = 4r$

$$\therefore AD^2 = AC^2 + CD^2 = AB^2 + BC^2 + CD^2 = a^2 + a^2 + a^2 = 3a^2$$

$$(4r)^2 = 3a^2$$

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

$$(\text{or}) \quad a = \frac{4}{\sqrt{3}} r$$

$$\text{Lastly, Packing factor (PF)} = \frac{\text{volume of all atoms in unit cell}}{\text{volume of unit cell}} = \frac{v}{V}$$

$$\begin{aligned} &= \frac{2 \times \frac{4}{3} \pi r^3}{a^3} = \frac{8\pi r^3}{3a^3} = \frac{8\pi r^3 3\sqrt{3}}{3(4r)^3} \\ &= \frac{\sqrt{3}\pi}{8} = 0.68 \text{ or } 68\%. \end{aligned}$$

The elements like tungsten, chromium, sodium, potassium, etc. possess bcc structure.

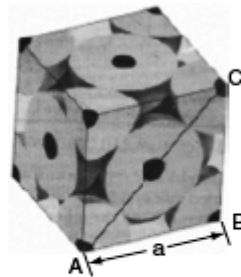
1.3.3 Structure and packing fractions of face-centred cubic [FCC] structure

Atoms are present at the corners and at the face centres of this cubic structure. The intersection of face diagonals represent face centre of the cube. A corner atom is shared by eight unit cells and a face-centred atom is shared by two unit cells. The cube has eight corners and bounded by six faces; so, the number of atoms per unit cell = $\frac{1}{8} \times 8 + \frac{1}{2} \times 6 = 4$.

Let r be the radius of an atom. The surfaces of atoms do not touch along unit cell edges but the surfaces of atoms along face diagonals of this structure are in contact. The unit cell structure is shown in Fig. 1.15. Half of the nearest neighbour distance along the face diagonal is equal to radius of an atom.

The relation between the radius of an atom and unit cell edge length of a unit cell can be obtained with reference to Fig. 1.15.

Figure 1.15 FCC structure



$$AC^2 = AB^2 + BC^2$$

$$(4r)^2 = a^2 + a^2 = 2a^2$$

$$4r = \sqrt{2}a \quad \text{or} \quad a = 2\sqrt{2}r$$

The co-ordination number is 12, and this can be explained in following way:

A face-centred atom of the cubic structure is surrounded by four corner atoms of the face of a unit cell, four surrounding face-centred atoms of the unit cell and four surrounding face-centred atoms of the adjacent unit cell. Therefore, the co-ordination number is 12. The packing factor PF of the unit cell:

$$\begin{aligned} &= \frac{\text{volume occupied by all the atoms in a unit cell}}{\text{unit cell volume}} \\ &= \frac{v}{V} = \frac{4 \times \frac{4}{3} \pi r^3}{a^3} = \frac{16\pi r^3}{3(2\sqrt{2}r)^3} \\ &= \frac{16\pi r^3}{3 \times 8 \times 2\sqrt{2}r^3} = \frac{\pi}{3\sqrt{2}} = 0.74 \text{ or } 74\% \end{aligned}$$

The packing factor of FCC structure is 74%. Examples for this structure are Cu, Ag, Al, etc.

Therefore, based on the above packing fractions information, FCC is the most closely packed structure among all the three cubic crystal lattices SC, BCC and FCC.

1.3.4 Hexagonal Closed Packed structure (HCP) :

The top and bottom faces of the unit cell consist of six atoms that form regular hexagons and surround a single atom in the center. Another plane that provides three additional atoms to the unit cell is situated between the top and bottom planes. The atoms in this mid-plane have as nearest neighbors atoms in both of the adjacent two planes. The equivalent of six atoms is contained in each unit cell; one-sixth of each of the 12 top and bottom face corner atoms, one-half of each of the 2 center face atoms, and all 3 mid-plane interior atoms. If a and c represent, respectively, the short (basal) and long (height) parameters of unit cell dimensions of Fig a, the c/a ratio should be 1.633 . The coordination number and the atomic packing factor for the HCP crystal structure are the same as for FCC: 12 and 0.74, respectively

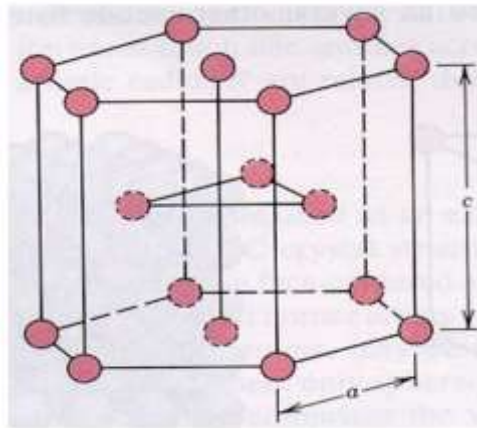


Fig 1.16: Structure of HCP

1.4. Calculation of lattice constant

The unit cell edge length of a cubic system is calculated using the density of the crystal. Let ' a ' be the edge length (or primitive) of a cubic unit cell and ' ρ ' be the density of the crystal.

The mass of the unit cell = ρa^3 _____ (1)

Let ' M ' be the molecular weight and N_A be the Avogadro number (i.e., number of molecules per kg mole of the substance) of the crystal. Then, mass of each molecule = M/N_A If each unit cell contains n molecules (or lattice points), Then the mass of unit cell = $n M/N_A$ _____ (2)

From Equation (1) and (2), we have:

$$\rho a^3 = n \frac{M}{N_A}$$

$$a^3 = \frac{nM}{\rho N_A} \quad \text{or} \quad a = \left(\frac{nM}{\rho N_A} \right)^{1/3}$$

1.5 Crystal directions, Crystal Planes and Miller Indices

When dealing with crystalline materials, it often becomes necessary to specify a particular point within a unit cell, a crystallographic direction, or some crystallographic plane of atoms. Labeling conventions have been established in which three numbers or indices are used to designate point locations, directions, and planes. The basis for determining index values is the unit cell, with a right-handed coordinate system consisting of three (x , y , and z) axes situated at one of the corners and coinciding with the unit cell edges, as shown in Figure 1.5. For some crystal systems—namely, hexagonal, rhombohedral, monoclinic, and triclinic - the three axes are *not* mutually perpendicular, as in the familiar Cartesian coordinate scheme.

A crystallographic direction is defined as a line between two points, or a vector.

The following steps are utilized in the determination of the three directional indices:

1. A vector of convenient length is positioned such that it passes through the origin of the coordinate system. Any vector may be translated throughout the crystal lattice without alteration, if parallelism is maintained.
2. The length of the vector projection on each of the three axes is determined; *these are measured in terms of the unit cell dimensions a , b , and c .*
3. These three numbers are multiplied or divided by a common factor to reduce them to the smallest integer values.
4. The three indices, not separated by commas, are enclosed in square brackets, thus: $[uvw]$. The u , v , and w integers correspond to the reduced projections along the x , y , and z axes, respectively.

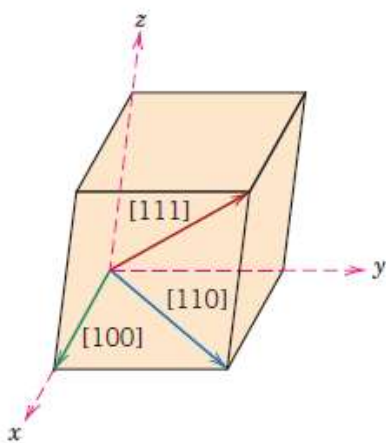


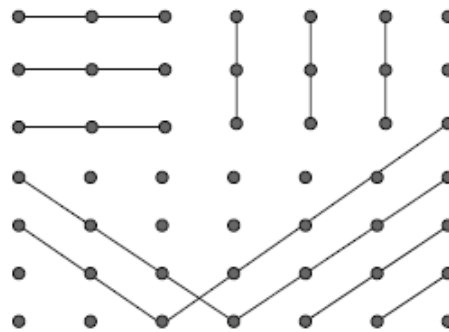
Fig. 1.17 The $[100]$, $[110]$, and $[111]$ directions within a unit cell.

For each of the three axes, there will exist both positive and negative coordinates. Thus negative indices are also possible, which are represented by a bar over the appropriate index. For example, the $[1\bar{1}1]$ direction would have a component in the $-y$ direction. Also, changing the signs of all indices produces an antiparallel direction; that is, $[\bar{1}\bar{1}\bar{1}]$ is directly opposite to $[111]$. If more than one direction (or plane) is to be specified for a particular crystal structure, it is imperative for the maintaining of consistency that a positive–negative convention, once established, not be changed.

The $[100]$, $[110]$, and $[111]$ directions are common ones; they are drawn in the unit cell shown in Figure 1.17.

Crystal planes are defined as some imaginary planes inside a crystal in which large concentration of atoms are present. Inside the crystal, there exists certain directions along which large concentration of atoms exists. These directions are called crystal directions. Figure 1.18 shows a two-dimensional lattice with different orientations of crystal planes.

Figure 1.18 A two-dimensional lattice with crystal planes

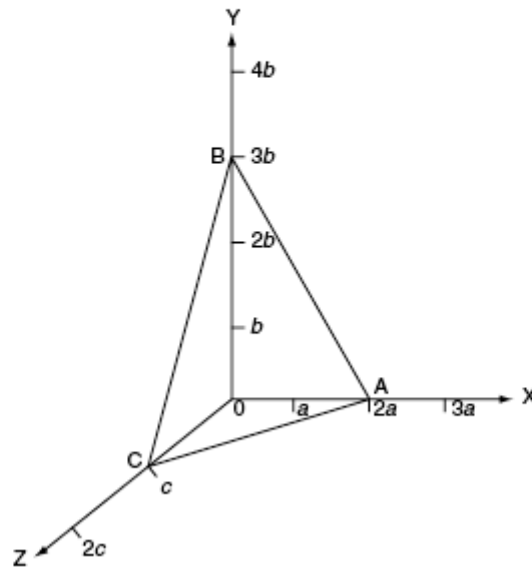


Crystal planes and directions can be represented by a set of three small integers called Miller indices [because Miller derived a method of representing crystal planes]. These integers are represented in general as h , k and l . If these integers are enclosed in round brackets as (hkl) , then it represents a plane. On the other hand, if they are enclosed in square brackets as $[hkl]$, then it represents crystal direction perpendicular to the above-said plane.

Next, we will see the way of obtaining Miller indices for a plane.

- (i) As shown in Fig. 1.19, take a lattice point as origin 'O' of crystallographic axes X, Y and Z in a space lattice. The unit cell translational distances or lattice constants along X, Y and Z directions are a , b and c , respectively. Let a crystal plane ABC intersect these three axes at $2a$, $3b$ and c . In general, the intercepts can be represented as pa , qb , and rc .
- (ii) Divide these intercepts with lattice points translational distances along the axes to obtain intercepts of the plane in terms of multiples of unit cell translational lengths.

Figure 1.19 Miller indices for a plane ABC



i.e., $\frac{2a}{a}, \frac{3b}{b}, \frac{c}{c}$
2, 3, 1

in general $\frac{pa}{a}, \frac{qb}{b}, \frac{rc}{c}$
 p, q, r

(iii) Take the reciprocals of these multiples, they are $\frac{1}{2}, \frac{1}{3}, \frac{1}{1}$; in general $\frac{1}{p}, \frac{1}{q}, \frac{1}{r}$

(iv) Clear these fractions [by multiplying with LCM] to smallest integers having the same ratio as the fractions, enclose these integers in brackets.

$$\frac{1}{2} \times 6, \frac{1}{3} \times 6, \frac{1}{1} \times 6$$

3 2 6

in general $\frac{pqr}{p}, \frac{pqr}{q}, \frac{pqr}{r}$
 $qr \quad pr \quad pq$

Miller indices of the plane ABC is (326). In general, indices of a plane are represented as $(hkl) = (qr \ pr \ pq)$

or $\frac{1}{p} : \frac{1}{q} : \frac{1}{r} = h : k : l$

Miller indices may be defined as a set of three small integers obtained by clearing the reciprocals of the three intercepts [in terms of multiples of unit cell edges] made by a plane on crystallographic axes.

Figure 1.20 Represent some important crystal planes and directions in a cubic crystal

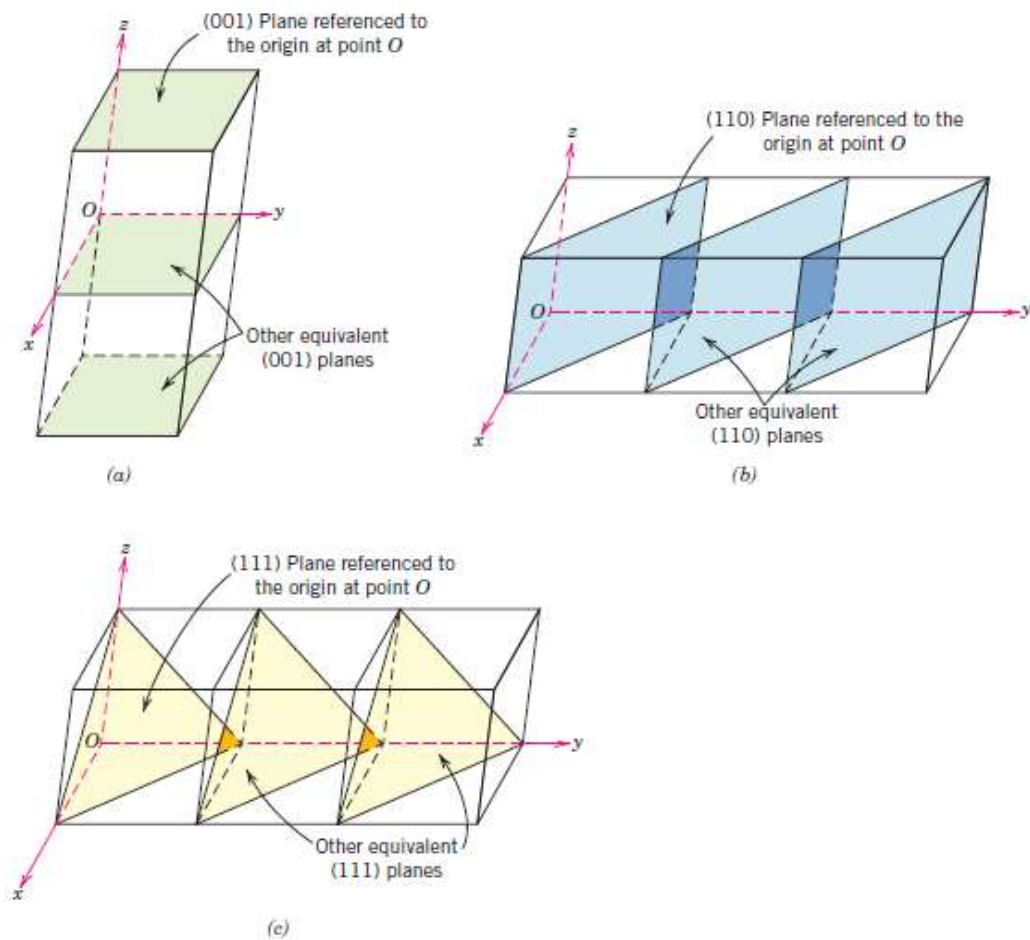
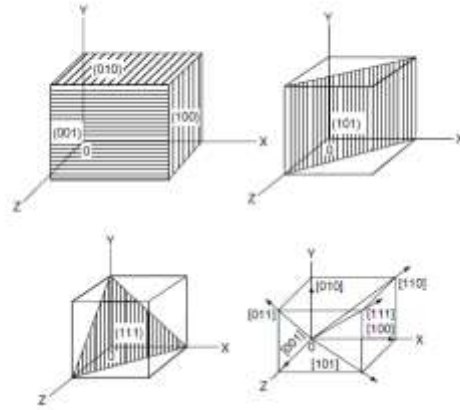
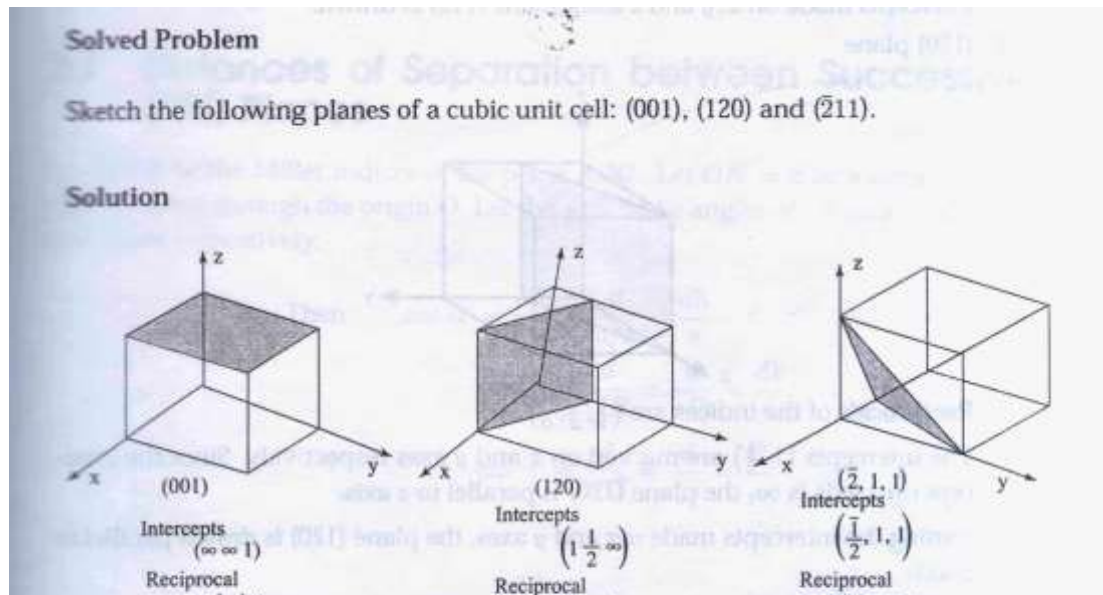


Fig. 1.21 Representations of a series each of (a) (001), (b) (110), and (c) (111) crystallographic planes.

➤ **Procedure for drawing the given plane having Miller indices (hkl):**

1. A unit cell is drawn with the given lattice parameters. After taking any convenient point as the origin O, the OX, OY and OZ crystallographic axes are to be marked. If lattice parameters are not given, then unit cubic cell of arbitrary lattice constant will be taken.
2. The reciprocals of the Miller indices $1/h$, $1/k$, $1/l$ are to be taken. These values provide the intercepts of the given plane on OX, OY and OZ axes, respectively.

3. The intercepts are marked in the unit cell and the plane is drawn.
4. If the intercept is ∞ on any axis, the plane drawn will be parallel to that axis.



Now, we will see the important features of Miller indices:

- (i) Miller indices represent a set of equidistant parallel planes.
- (ii) If the Miller indices of a plane represent some multiples of Miller indices of another plane, then these planes are parallel. For example (844) and (422) or (211) are parallel planes.
- (iii) If (hkl) are the Miller indices of a plane, then the plane divides the lattice constant ' a ' along X-axis into h equal parts, ' b ' along Y-axis into k equal parts and ' c ' along Z-axis into l equal parts.
- (iv) If a plane is parallel to one of the crystallographic axes, then the plane intersects that axis at infinity and the Miller indices along that direction is zero.
- (v) If a plane cuts an axis on the negative side of the origin, then the corresponding index is negative and is indicated by placing a minus sign above the index. For example, if the plane cuts on negative Y-axis, then Miller indices of the plane is $(h\bar{k}l)$.
- (vi) When Miller indices are enclosed in curly brackets, $\{hkl\}$, they refer to planes which in the crystal are equivalent even though their Miller indices may differ. For example in a cubic lattice, all cube faces are equivalent, they are (100), (010), (001), $(\bar{1}00)$, $(0\bar{1}0)$, $(00\bar{1})$; these planes are represented as $\{100\}$. Similarly, a full set of equivalent directions in a crystal is represented by a symbol $\langle hkl \rangle$. For example, the eight body diagonals of a cube $[111]$, $[\bar{1}\bar{1}\bar{1}]$, $[\bar{1}11]$, $[1\bar{1}1]$, $[11\bar{1}]$, $[\bar{1}\bar{1}1]$, $[1\bar{1}\bar{1}]$, $[\bar{1}1\bar{1}]$ are designated as $\langle 111 \rangle$.

➤ Distance of separation between successive hkl planes

Let (hkl) represents a set of parallel planes in a crystal with unit cell parameters a , b and c . Then we can easily prove that the distance of separation between two successive crystal planes, d , for an orthorhombic crystal is given by

$$d = \frac{1}{\sqrt{\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}} \quad (1)$$

Using Equation (1), we can determine the interplanar separation in orthorhombic crystals. For tetragonal crystal $a = b \neq c$, substitute these values in Equation (1), we have:

$$d = \frac{1}{\sqrt{\frac{h^2}{a^2} + \frac{k^2}{a^2} + \frac{l^2}{c^2}}} = \frac{1}{\sqrt{\frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}}} \quad (2)$$

For cubic crystals: $a = b = c$, substitute these values in Equation (1), we have:

$$d = \frac{1}{\sqrt{\frac{h^2}{a^2} + \frac{k^2}{a^2} + \frac{l^2}{a^2}}} \quad (\text{or}) \quad d = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \quad (3)$$

The calculation of interplanar spacing for other crystal systems is complicated, so we will not discuss them.

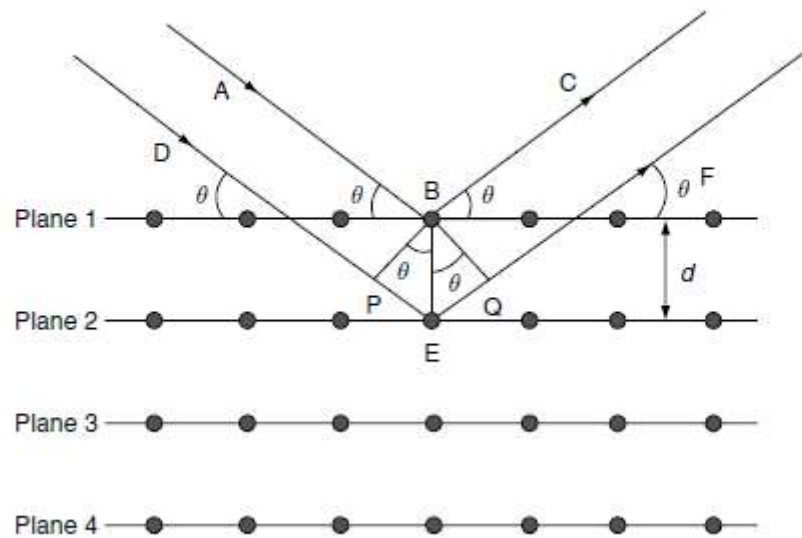
1.6 Diffraction of X-rays by crystal planes and Bragg's law

The visible light rays when pass through a sharp edge of an object can form some bright regions inside the geometrical shadow of the object. This is due to the bending nature of light, called diffraction. Diffraction of visible light rays can also be produced using plane-ruled grating. This grating consists of about 6000 lines/cm; so that the spacing between any two consecutive lines in the grating is of the order of the wavelength of visible light used to produce diffraction. The wavelength of X-rays is of the order of an angstrom, so X-rays are unable to produce diffraction with plane optical grating. To produce diffraction with X-rays, the spacing between the consecutive lines of grating should be of the order of few angstroms. Practically, it is not possible to construct such a grating. In the year 1912, a German physicist Laue suggested that the three-dimensional arrangement of atoms in a crystal can serve as a three-dimensional grating for X-rays. Inside the crystal, the spacing between the crystal planes can work as the transparent regions as between lines in a ruled grating. Laue's associates Friedrich and Knipping succeeded in diffracting X-rays by passing through a thin crystal.

In 1913, W.L. Bragg and his son W.H. Bragg gave a simple interpretation of the diffraction pattern. According to Bragg, the diffraction spots produced are due to the reflection of some of the incident X-rays by various sets of parallel crystal planes. These planes are called Bragg's planes. The Bragg's interpretation is explained in the following topic.

Bragg's law: W.L. Bragg and W.H. Bragg considered the X-ray diffraction as the process of reflection of X-rays by crystal planes as shown in Fig. 1.22. A monochromatic X-ray beam of wavelength λ is incident at an angle θ to a family of Bragg planes. Let the interplanar spacing of crystal planes is ' d '. The dots in the planes represent positions of atoms in the crystal. Every atom in the crystal is a source of scatterer of X-rays incident on it. A part of the incident X-ray beam AB, incident on an atom at B in plane 1, is scattered along the direction BC. Similarly, a part of incident X-ray DE [in parallel to AB] falls on atom at E in plane 2 and is scattered in the direction EF and it is parallel to BC. Let the beams AB and DE make an angle θ with the Bragg's planes. This angle θ is called the angle of diffraction or glancing angle.

Figure 1.22 Bragg's law



If the path difference between the rays ABC and DEF is equal to $\lambda, 2\lambda, 3\lambda, \dots$ etc. or $n\lambda$, i.e., integral multiples of wavelength, where $n = 1, 2, 3, \dots$ etc. are called first-order, second-order, third-order ... etc. maxima, respectively. As path difference is equal to $n\lambda$, then the rays reflected from consecutive planes are in phase; so, constructive interference takes place among the reflected rays BC and EF, hence the resulting diffracted ray is intense. On the other hand, if the path difference between the rays ABC and DEF is $\frac{\lambda}{2}, \frac{3\lambda}{2}, \frac{5\lambda}{2}, \dots$ etc., then the scattered rays BC and EF are out of phase so that destructive interference takes place and hence the resulting ray intensity is minimum. To find the path difference between these rays, drop perpendiculars from B on DE and EF. The intersecting points of perpendiculars are P and Q as shown in Fig. 3.11. The path difference between the rays is $PE + QE$. From the figure, we know that BE is perpendicular to plane 1 and BP is perpendicular to

AB. So, as the angle between ray AB and plane 1 is θ , then $\angle PBE = \angle QBE = \theta$. In the triangle PBE, $\sin \theta = \frac{PE}{BE} = \frac{PE}{d}$ or $PE = d \sin \theta$. Similarly, $EQ = d \sin \theta$.

\therefore For constructive interference, $PE + EQ = n\lambda$ or $d \sin \theta + d \sin \theta = n\lambda$
i.e., $2d \sin \theta = n\lambda$

The above equation is called Bragg's law.

Therefore, Bragg's law states that X-rays diffracted from different parallel planes of a crystal interfere constructively when the path difference is integral multiples of wavelength of X-rays.

From Bragg's law $n\lambda = 2d \sin \theta$, since maximum possible value for $\sin \theta$ is 1,

$$n\lambda/2d \leq 1 \text{ or}$$

$$\lambda \leq 2d.$$

This sets the limitation on the wavelength, i.e. in order to get the diffraction pattern by a crystal, the wavelength of X-rays should not exceed twice the inter-planar spacing.

Importance of Bragg's law:

1. Bragg's law is the essential condition to be satisfied by crystal planes in order to get diffraction pattern from a crystal.
2. It is used to calculate inter-planar spacing. Knowing the values of inter-planar spacing, lattice parameters can be determined.

1.7. Diffraction methods. Diffraction can occur whenever the Bragg law, $\lambda = 2d \sin \theta$, is satisfied. This equation puts very stringent conditions on λ and θ for any given crystal. With monochromatic radiation, an arbitrary setting of a single crystal in a beam of x-rays will not in general produce *any* diffracted beams. Some way of satisfying the Bragg law must be devised, and this can be done by continuously varying either λ or θ during the experiment. The ways in which these quantities are varied distinguish the three main diffraction methods:

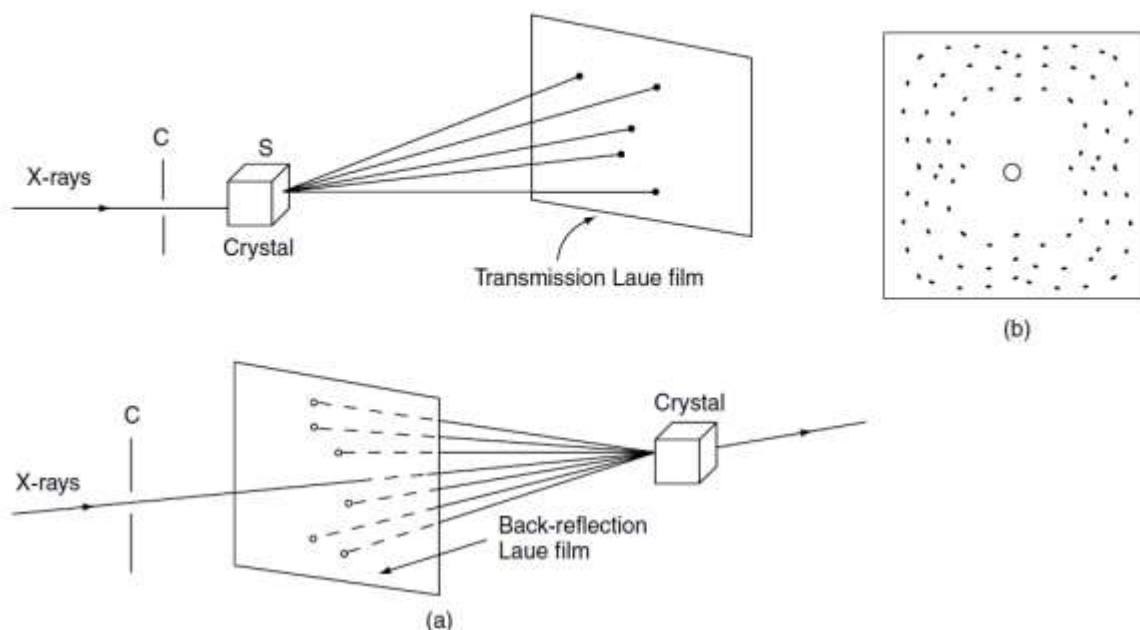
	λ	θ
Laue method	Variable	Fixed
Rotating-crystal method	Fixed	Variable (in part)
Powder method	Fixed	Variable

1. The Laue method :- applicable for single crystals
2. The Rotating crystal method :- applicable for single crystals
3. The Powder method :- used for finely divided crystalline or polycrystalline powers

1. LAUE METHOD :

The Laue method was the first diffraction method ever used. This method is used to study the orientation of crystal and to verify crystal symmetry. A beam of white radiation, the continuous spectrum from an x-ray tube, is allowed to fall on a fixed single crystal. The Bragg angle θ is therefore fixed for every set of planes in the crystal, and each set picks out and diffracts that particular wavelength which satisfies the Bragg law for the particular values of d and θ . Each diffracted beam thus has a different wavelength. There are two variations of the Laue method, depending on the relative positions of source, crystal, and film (Fig. 1.23 (a)). In each, the film is flat and placed perpendicular to the incident beam. The film in the transmission Laue method (the original Laue method) is placed behind the crystal so as to record the beams diffracted in the forward direction. This method is so called because the diffracted beams are partially transmitted through the crystal. In the back-reflection Laue method the film is placed between the crystal and the x-ray source, the incident beam passing through a hole in the film, and the beams diffracted in a backward direction are recorded. In either method, the diffracted beams form an array of spots on the film as shown in Fig. 1.23 (b) for a cubic crystal. This array of spots is commonly called a pattern, more specifically, Laue pattern, but the term is not used in any strict sense and does not imply any periodic arrangement of the spots. On the contrary, the spots are seen to lie on certain curves, as shown in Fig. 1.23 (b) for transmitted pattern. These curves are generally ellipses or hyperbolas for transmission patterns and hyperbolas for back-reflection patterns.

Figure 1.23 (a) X-ray diffraction by crystal plane; (b) Laue pattern for NaCl crystal



The spots lying on any one curve are reflections from planes belonging to one zone. This is due to the fact that the Laue reflections from planes of a zone all lie on the surface of an imaginary cone whose axis is the zone axis. The positions of the spots on the film, for both the transmission and the back-reflection method, depend on the orientation of the crystal relative to the incident beam, and the spots themselves become distorted and smeared out if the crystal has been bent or twisted in any way. The facts account for the two main uses of the Laue methods include: the determination of crystal orientation and the assessment of crystal perfection.

Therefore, the way of arrangement of spots on a film is a characteristic property of the crystal. Laue method is useful to decide the crystal symmetry and orientation of the internal arrangement of atoms/molecules in the crystal. The atomic arrangement in a crystal can be analyzed by studying the positions and intensities of spots in Laue pattern. As several wavelengths of X-rays can reflect in different orders from the same set of planes with the different order reflections superimposed on the same spot in the film, the intensity of the spots and hence the cell parameters of a crystal cannot be determined using Laue method. For transmission Laue method, the crystal should be thin. Laue method can be used to study imperfections or strains in the crystal. The presence of above defects forms streaks instead of spots in the Laue photograph.

The rotating crystal method

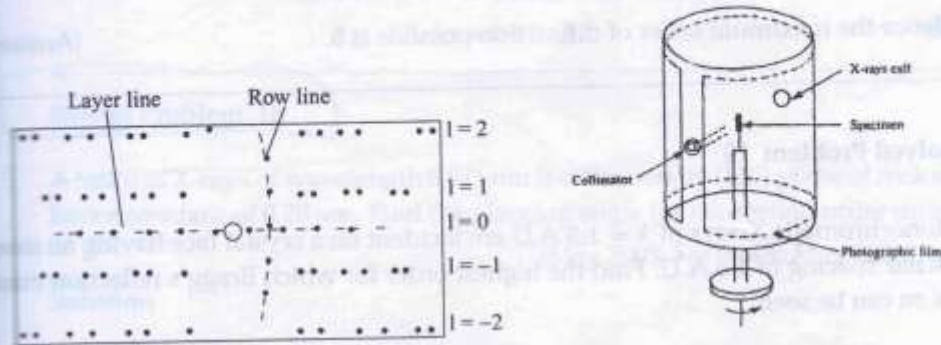


Fig. 1.24. (a) A typical rotation photograph. (b) Schematic representation of rotating crystal technique.

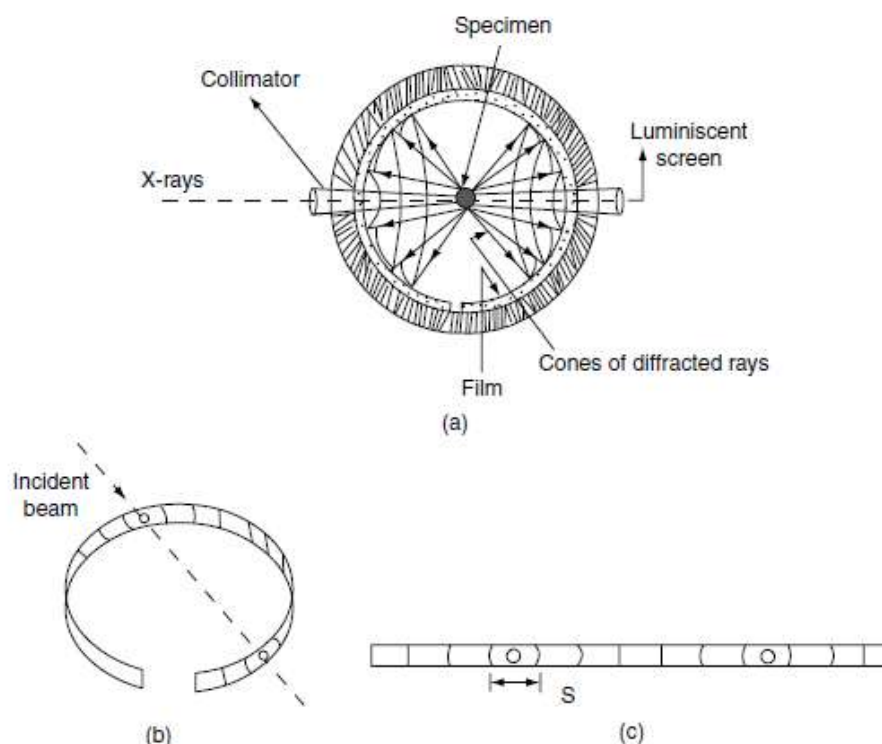
This method is very useful in determination of crystal structure when a single crystal is available. The crystal alignment is done exactly as in the case of Laue method but in this method crystal is either rotated or oscillated. A monochromatic beam of X-ray is allowed to fall on the crystal through a fine collimator. The X-ray reflections are recorded on an X-ray film loaded in a cylindrical camera. The axis of the camera is coincident with the axis of rotation (or oscillation). A schematic view of rotating crystal technique is shown in Fig. 1.24(b). A typical rotation photograph after exposure and development is also shown in Fig. 1.24(a). Analysis of the spots in rotating crystal diffraction pattern is beyond the scope of this course.

By recording the diffraction patterns (both angles and intensities) for various crystal orientations, one can determine the shape and size of unit cell as well as arrangement of atoms inside the cell.

3. Powder diffraction Method

X-ray powder method is usually carried for polycrystalline materials. The powder photograph is obtained in the following way. The given polycrystalline material is ground to fine powder and this powder can be taken either in a capillary tube made up of non-diffracting material or is just struck on a hair with small quantity of binding material and fixed at the centre of cylindrical Debye-Scherrer camera as shown in Fig. 1.25 (a).

Figure 1.25 (a) Debye-Scherrer cylindrical camera; (b) Film mounted in camera; (c) Film on stretchout



A stripe of X-ray photographic film is arranged along the inner periphery of the camera. A beam of monochromatic X-rays is passed through the collimator to obtain a narrow fine beam of X-rays. This beam falls on the polycrystalline specimen and gets diffracted. The specimen contains very large number of small crystallites oriented in random directions. So, all possible diffraction planes will be available for Bragg reflection to take place. Such reflections will take place from many sets of parallel planes lying at different angles to the incident X-ray beam. Also, each set of planes gives not only first-order reflections but also of higher orders as well. Since all orientations are equally likely, the reflected rays will form a cone whose axis lies along the direction of the incident beam and whose semi-vertical angle is equal to twice the glancing angle (θ), for that particular set of planes. For each set of planes and for each order, there will be such a cone of reflected X-rays. Their intersections with a photographic film sets with its plane normal to the incident beam, form a series of concentric circular rings. In this case, a part of the reflected cone is recorded on the film and it is a pair of arcs, the resulting pattern is shown in Fig. 1.25(c). Diameter of these rings or corresponding arcs is recorded on the film, and using this the glancing angle and interplanar spacing of the crystalline substance can be determined. Figure 1.25(b) shows the film mounted in the camera and the X-ray powder pattern obtained. The film on spread-out is shown in Fig 1.25(c). The distance between any two corresponding arcs on the film is indicated by the symbol S .

~~In case of cylindrical camera, the diffraction angle θ is proportional to S . Then,~~

$$\theta = \frac{S}{4R} \quad \text{where } R \text{ represents the radius of the camera.}$$

If $S_1, S_2, S_3 \dots$ etc. are the distances between symmetrical lines on the stretched film, then,

$$\theta_1 = \frac{S_1}{4R}, \theta_2 = \frac{S_2}{4R}, \theta_3 = \frac{S_3}{4R} \dots$$

Using these values of θ_n in Bragg's equation $n\lambda = 2 d_{hkl} \sin \theta_n$

where $n = 1, 2, 3, \dots$ etc = order of diffraction

d_{hkl} = interplanar spacing

θ_n = angle of diffraction for n th order

The interplanar spacing d_{hkl} can be calculated.

~~1.8 Reciprocal lattice~~

- Definition of the reciprocal lattice

The reciprocal lattice is a construction with vast importance for condensed matter physics. Starting with a Bravais lattice, the reciprocal lattice is the set of all wave vectors \mathbf{G} that give plane waves $e^{i\mathbf{G}\cdot\mathbf{r}}$ with the periodicity of the Bravais lattice. If the Bravais lattice is given by points \mathbf{R} , one thus have

$$e^{i\mathbf{G}\cdot(\mathbf{r}+\mathbf{R})} = e^{i\mathbf{G}\cdot\mathbf{r}}$$

The \mathbf{G} -vectors correspond to the reciprocal lattice points.

The reciprocal lattice is also a Bravais lattice.

- Construction of the reciprocal lattice

If $\mathbf{a}_1, \mathbf{a}_2$, and \mathbf{a}_3 are the primitive vectors of the direct lattice the reciprocal lattice is described by the corresponding primitive vectors

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

$$\mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

$$\mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

which corresponds to

$$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi \delta_{ij}$$

where δ_{ij} is the Kronecker delta.

• Useful facts and relations

- The reciprocal lattice of a reciprocal lattice is the original, direct lattice.
- The reciprocal lattice of a simple cubic lattice with primitive cell side a is again a simple cubic lattice, but with cell side $2\pi/a$.
- The reciprocal lattice of an *fcc* Bravais lattice with conventional cubic cell side a is a *bcc* lattice with conventional cubic cell side $4\pi/a$.
- The reciprocal lattice of an *bcc* lattice with conventional cell side a is similarly an *fcc* lattice with conventional cell side $4\pi/a$.
- The reciprocal lattice on a *simple hexagonal* Bravais lattice with lattice constants a and c is also a simple hexagonal lattice but with lattice constants $4\pi/\sqrt{3}a$ and $2\pi/c$, and rotated 30° around the c -axis.
- The volume v_g of the reciprocal lattice primitive cell is $v_g = (2\pi)^3/v_c$, where v_c is the volume of the direct lattice primitive cell. The cell volumes can be obtained from the corresponding primitive vectors by taking $v_c = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)$ and $v_g = \mathbf{b}_1 \cdot (\mathbf{b}_2 \times \mathbf{b}_3)$.
- The reciprocal lattice is the Fourier transform of the direct lattice.
- A reciprocal lattice vector $\mathbf{G}(hkl)$ is perpendicular to the plane (hkl) .
- If a function is periodic in the direct lattice, so that $f(\mathbf{r}) = f(\mathbf{r} + \mathbf{R})$ one can write

$$f(\mathbf{r}) = \sum_{\mathbf{G}} a_{\mathbf{G}} e^{i\mathbf{G} \cdot \mathbf{r}}$$

so that the sum is taken only over the reciprocal lattice points.

1.9 Applications of XRD

XRD is a nondestructive technique. Some of the uses of x-ray diffraction are;

1. Differentiation between crystalline and amorphous materials;
2. Determination of the structure of crystalline materials;
3. Determination of electron distribution within the atoms, and throughout the unit cell;
4. Determination of the orientation of single crystals;
5. Determination of the texture of poly-grained materials;
6. Measurement of strain and small grain size.....etc

Advantages and disadvantages of X-rays

Advantages;

1. X-ray is the cheapest, the most convenient and widely used method.
2. X-rays are not absorbed very much by air, so the specimen need not be in an evacuated chamber.

Disadvantage;

1. They do not interact very strongly with lighter elements.

➤ Crystal structures

Solved Problems

1. Chromium has BCC structure. Its atomic radius is 0.1249 nm. Calculate the free volume/unit cell.

(Set-4-May 2007), (Set-4-Sept. 2006)

Sol: Given data are

Atomic radius of chromium, $r = 0.1249$ nm.

Free volume/unit cell = ?

If ' a ' is the BCC unit cell edge length, then the relation between ' a ' and ' r ' is

$$a = \frac{4}{\sqrt{3}} r = \frac{4}{\sqrt{3}} \times 0.1249 \text{ nm} \\ = 0.28845 \text{ nm}.$$

$$\text{Volume of unit cell, } V = a^3 = (0.28845)^3 \text{ nm}^3 \\ = 0.024 \text{ nm}^3$$

Number of atoms in BCC unit cell = 2

$$\text{Hence volume of atoms in unit cell, } v = \frac{4}{3} \pi r^3 \times 2 = 0.01633 \text{ nm}^3$$

$$\text{Free volume/unit cell} = V - v = 0.00767 \text{ nm}^3$$

2. Lithium crystallizes in BCC structure. Calculate the lattice constant, given that the atomic weight and density for lithium are 6.94 and 530 kg/m³ respectively.

(Set-4-Nov. 2003)

Sol: Lithium crystallizes in BCC structure, so the number of atoms per unit cell, $n = 2$

Atomic weight, $M = 6.94$

Density, $\rho = 530$ Kg/m³

Lattice constant, $a = ?$

$$a^3 = \frac{nM}{\rho N_A}, \text{ where } N_A = \text{Avogadro's number}$$

$$a^3 = \frac{2 \times 6.94}{530 \times 6.02 \times 10^{26}}$$

$$= 43.50 \times 10^{-30}$$

$$a = 3.517 \times 10^{-10} \text{ m}$$

$$= 3.517 \text{ \AA}$$

3. Iron crystallizes in BCC structure. Calculate the lattice constant, given that the atomic weight and density of iron are 55.85 and 7860 kg/m³, respectively.

(Set-3–Sept. 2006), (Set-1–Nov. 2003)

Sol: Atomic weight of iron, $M = 55.85$

Density of iron, $\rho = 7860 \text{ kg/m}^3$

Find lattice constant, a in BCC iron

Number of atoms in BCC unit cell, $n = 2$

We know that:

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

$$\left[\frac{2 \times 55.85}{7860 \times 6.02 \times 10^{26}} \right]^{1/3} = 2.87 \times 10^{-10} \text{ m} = 2.87 \text{ \AA}$$

4. If the edge of the unit cell of a cube in the diamond structure is 0.356 nm, calculate the number of atoms/m³.

(Set-3–Nov. 2003)

Sol: The lattice constant of diamond, $a = 0.356 \text{ nm} = 0.356 \times 10^{-9} \text{ m}$

The number of carbon atoms per unit cell, $n = 8$

$$\text{The number of unit cells in } 1 \text{ m}^3 = \frac{1 \text{ m}^3}{a^3}$$

$$\text{and the number of atoms per m}^3 = \frac{1 \text{ m}^3}{a^3} \times 8 = \frac{1 \text{ m}^3 \times 8}{(0.356 \times 10^{-9} \text{ m})^3}$$

$$= \frac{8 \times 10^{27}}{(0.356)^3} = 177.3 \times 10^{27} \text{ atoms/m}^3$$

5. A metal in BCC structure has a lattice constant 3.5 Å. Calculate the number of atoms per sq. mm area in the (200) plane.

Sol: Lattice constant, $a = 3.5 \text{ \AA}$

The (200) plane is perpendicular to X-axis and passes through the centre of the unit cell. So, this plane contains only the central atom.

$$\therefore \text{The area per atom} = a^2 = 3.57 \text{ \AA} \times 3.5 \text{ \AA} = 12.25 \text{ \AA}^2$$

$$\text{Number of atoms per sq. mm} = \frac{1 \text{ mm} \times 1 \text{ mm}}{12.25 \text{ \AA}^2}$$

$$= \frac{10^7 \text{ \AA} \times 10^7 \text{ \AA}}{12.25 \text{ \AA}^2} = 8.16 \times 10^{12} \quad [\text{since } 1 \text{ mm} = 10^7 \text{ \AA}]$$

6. Germanium crystallizes in diamond (form) structures with 8 atoms per unit cell. If the lattice constant is 5.62 Å, calculate its density.

Sol: Number of atoms per unit cell, $n = 8$

Lattice constant, $a = 5.62 \text{ Å} = 5.62 \times 10^{-10} \text{ m}$

Atomic weight of Ge, $M = 72.59$

Density, $\rho = ?$

We know that $a^3 = \frac{nM}{\rho N_A}$, where $N_A = \text{Avogadro's number}$

$$\begin{aligned}\rho &= \frac{nM}{a^3 N_A} \\ &= \frac{8 \times 72.59}{[5.62 \times 10^{-10}]^3 \times 6.02 \times 10^{26}} \text{ Kg/m}^3 \\ &= 5434.5 \text{ kg/m}^3.\end{aligned}$$

➤ Crystal Directions, Crystal Planes, Miller Indices, X-ray diffraction

Solved Problems

1. A beam of X-rays of wavelength 0.071 nm is diffracted by (110) plane of rock salt with lattice constant of 0.28 nm. Find the glancing angle for the second-order diffraction.
(Set-1–Sept. 2007), (Set-2, Set-3–Sept. 2006), (Set-2–May 2006), (Set-3–May 2004), (Set-4–May 2003)

Sol: Given data are:

Wavelength (λ) of X-rays = 0.071 nm

Lattice constant (a) = 0.28 nm

Plane (hkl) = (110)

Order of diffraction = 2

Glancing angle $\theta = ?$

Bragg's law is $2d \sin \theta = n\lambda$

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}, \text{ because rock salt is FCC}$$

$$= \frac{0.28 \times 10^{-9}}{\sqrt{1^2 + 1^2 + 0^2}} \text{ m} = \frac{0.28 \times 10^{-9}}{\sqrt{2}} \text{ m}$$

Substitute in Bragg's equation

$$2 \times \frac{0.28 \times 10^{-9}}{\sqrt{2}} \sin \theta = 2 \times 0.071 \times 10^{-9}$$

$$\sin \theta = \sqrt{2} \times \frac{0.071}{0.28} = 0.3586$$

$$\theta = \sin^{-1}(0.3586) = 21.01^\circ \approx 21^\circ$$

2. A beam of X-rays is incident on a NaCl crystal with lattice plane spacing 0.282 nm. Calculate the wavelength of X-rays if the first-order Bragg reflection takes place at a glancing angle of $8^\circ 35'$. Also calculate the maximum order of diffraction possible.

(Set-4–Sept. 2007), (Set-3–May 2007), (Set-2–May 2004), (Set-3–May 2003)

Sol: Given data are:

NaCl crystal is FCC

Lattice plane spacing (d) = 0.282 nm

Wavelength of rays (λ) = ?

Order of diffraction (n) = 1

Glancing angle $\theta = 8^\circ 35'$

Bragg's equation is $n\lambda = 2d \sin \theta$

$$1\lambda = 2 \times 0.282 \times 10^{-9} \sin (8^\circ 35')$$

$$= 0.0842 \text{ nm}$$

Maximum order of diffraction (n_{\max}) = ?

$$2d \sin \theta = n\lambda$$

if $\theta = 90^\circ$ then $n = n_{\max}$

$$\therefore 2d = n_{\max} \lambda$$

$$n_{\max} = \frac{2d}{\lambda} = \frac{2 \times 0.282 \text{ nm}}{0.0842 \text{ nm}} = 6.7 \approx 7$$

3. The fraction of vacant sites in a metal is 1×10^{-10} at 500°C . What will be the fraction of vacancy sites at 1000°C ?
(Set-4–Sept. 2006), (Set-1–May 2004), (Set-2–May 2003)

Sol: The number of vacancies at temperature (TK) in a metal is represented by:

$$n \approx N \exp\left(\frac{-E_v}{K_B T}\right) \quad (\text{or}) \quad \frac{n}{N} = \exp\left(\frac{-E_v}{K_B T}\right)$$

The given data are:

$$\frac{n}{N} = 1 \times 10^{-10} \text{ at } 500^\circ \text{C} \quad \text{or} \quad 773 \text{ K} \quad \frac{n'}{N} = ? \text{ at } 1000^\circ \text{C} \quad \text{or} \quad 1273 \text{ K}$$

$$1 \times 10^{-10} = \exp\left(\frac{-E_v}{K_B 773}\right) \quad \text{----- (1)}$$

$$\frac{n'}{N} = \exp\left(\frac{-E_v}{K_B 1273}\right) \quad \text{----- (2)}$$

Taking logarithms on both sides of the above Equations (1) and (2), we get:

$$\ln 10^{-10} = \frac{-E_v}{773 K_B} \quad \text{----- (3)}$$

$$\ln\left(\frac{n'}{N}\right) = \frac{-E_v}{1273 K_B} \quad \text{----- (4)}$$

Dividing Equation (4) by (3),

$$\frac{\ln\left(\frac{n'}{N}\right)}{\ln 10^{-10}} = \frac{\left(\frac{-E_v}{1273 K_B}\right)}{\left(\frac{-E_v}{773 K_B}\right)} = \frac{773}{1273} = 0.60723$$

$$= \ln\left(\frac{n'}{N}\right) = \ln 10^{-10} \times 0.60723$$

$$= -23.026 \times 0.60723 = -13.982$$

Take exponential on both sides,

$$\frac{n'}{N} = \exp[-13.982] \times 10^{-7} = 8.466 \times 10^{-7}$$

The fraction of vacancy sites at 1000°C is 8.466×10^{-7} .

4. Calculate the ratios $d_{100} : d_{110} : d_{111}$ for a simple cubic structure.

(Set-2–Nov. 2004), (Set-2–Nov. 2003)

Sol: Let ' a ' be the lattice constant of cubic structure, then,

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

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

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

$$\begin{aligned} \text{The ratios } d_{100} : d_{110} : d_{111} &= a : \frac{a}{\sqrt{2}} : \frac{a}{\sqrt{3}} \\ &= 1 : \frac{1}{\sqrt{2}} : \frac{1}{\sqrt{3}} = \sqrt{6} : \sqrt{3} : \sqrt{2} \end{aligned}$$

5. The Bragg's angle in the first order for (220) reflection from nickel (FCC) is 38.2° . When X-rays of wavelength 1.54 Å are employed in a diffraction experiment. Determine the lattice parameter of nickel.

(Set-2–May 2008)

Sol: Order of diffraction, $n = 1$

Diffraction angle, $\theta = 38.2^\circ$

Wavelength of light, $\lambda = 1.54 \text{ Å}$

Plane of reflection = (220)

Lattice parameter, $a = ?$

Bragg's law is $2d \sin \theta = n\lambda$

$$d = \frac{n\lambda}{2 \sin \theta} = \frac{1 \times 1.54}{2 \times \sin 38.2} \text{ Å}$$

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

$$\begin{aligned} a &= d \times \sqrt{h^2 + k^2 + l^2} \\ &= \frac{1 \times 1.54}{2 \times \sin 38.2} \times \sqrt{2^2 + 2^2 + 0^2} \\ &= \frac{4.35578}{1.23682} = 3.522 \text{ Å} \end{aligned}$$

6. Monochromatic X-rays of $\lambda = 1.5 \text{ \AA}$ are incident on a crystal face having an interplanar spacing of 1.6 \AA . Find the highest order for which Bragg's reflection maximum can be seen.

(Set-4–May 2006)

Sol: Given data are

Wavelength of light (λ) = 1.5 \AA

Interplanar spacing (d) = 1.6 \AA

Glancing angle (θ_m) = 90°

Order of diffraction (n) = ?

Bragg's law

$$n\lambda = 2d \sin \theta$$

$$n = \frac{2d \sin \theta}{\lambda} = \frac{2 \times 1.6 \times \sin 90}{1.5} = \frac{3.2}{1.5}$$

$$= 2.13 \approx 2$$

\therefore The maximum order of diffraction is 2

7. The distance between (110) planes in a body centred cubic structure is 0.203 nm . What is the size of the unit cell? What is the radius of the atom?

(Set-3–Sept. 2007), (Set-3–May 2006)

Sol: The given data are

The distance between (110) planes of BCC structure (d_{110}) = $0.203 \text{ nm} = 0.203 \times 10^{-9} \text{ m}$

Length of unit cell (a) = ?

Volume of unit cell (a^3) = ?

Radius of the atom (r) = ?

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

$$0.203 \times 10^{-9} = \frac{a}{\sqrt{1^2 + 1^2 + 0^2}} = \frac{a}{\sqrt{2}}$$

$$a = 0.203 \times \sqrt{2} = 0.287 \times 10^{-9} \text{ m}$$

Volume of unit cell $a^3 = 0.02364 \times 10^{-27} \text{ m}^3$

$$\text{Radius of atom } (r) = \frac{\sqrt{3}a}{4} = \frac{1.732 \times 0.287 \times 10^{-9}}{4}$$

$$= 0.1243 \times 10^{-9} \text{ m}$$

8. Monochromatic X-rays of $\lambda = 1.5 \text{ \AA}$ are incident on a crystal face having an interplanar spacing of 1.6 \AA . Find the highest order for which Bragg's reflection maximum can be seen.

(Set-1–Sept. 2006)

Sol: Given data are wavelength of X-rays, $\lambda = 1.5 \text{ \AA}$

Interplanar spacing, $d = 1.6 \text{ \AA}$

For highest order of diffraction, $\theta = 90^\circ$

Highest order of diffraction, $n = ?$

Formula $2d \sin \theta = n \lambda$

$$2 \times 1.6 \times \sin 90^\circ = n \times 1.5$$

$$n = \frac{2 \times 1.6}{1.5} = 2.13 \approx 2$$

\therefore Highest order of diffraction is 2.

9. Calculate the glancing angle at (110) plane of a cubic crystal having axial length 0.26 nm corresponding to the second order diffraction maximum for the X-rays of wavelength 0.65 nm.

(Set-1–May 2007)

Sol: The given data are

Edge length of cubic system, $a = 0.26 \text{ nm}$

Wavelength of X-rays $\lambda = 0.65 \text{ nm}$

Glancing angle, for plane (110), $\theta = ?$

Order of diffraction, $n = 2$

$$\begin{aligned} \text{Separation between (110) planes of a cube, } d &= \frac{a}{\sqrt{h^2 + k^2 + l^2}} = \frac{0.26}{\sqrt{1^2 + 1^2 + 0^2}} \text{ nm} \\ &= \frac{0.26}{\sqrt{2}} = 0.184 \text{ nm} \end{aligned}$$

Bragg's law

$$2d \sin \theta = n\lambda$$

$$2 \times 0.184 \text{ nm} \times \sin \theta = 2 \times 0.65 \text{ nm}$$

$$\sin \theta = \frac{0.65}{0.184} = 0.353$$

$$\begin{aligned} \therefore \theta &= \sin^{-1}(0.353) \\ &= 20^\circ 41' 13'' \end{aligned}$$

10. The Bragg's angle for reflection from the (111) plane in a FCC crystal is 19.2° for an X-ray wavelength of 1.54 A.U. Compute the cube edge of the unit cell.

(Set-2, Set-4–May 2007)

Sol: The given data are

Bragg's angle, $\theta = 19.2^\circ$

Wavelength of X-rays, $\lambda = 1.54 \text{ \AA}$

Order of diffraction, $n = 1$

Cube edge, $a = ?$

Bragg's law

$$2d \sin \theta = n\lambda$$

$$2d \sin 19.2^\circ = 1 \times 1.54$$

$$d = \frac{1.54}{2 \times \sin 19.2^\circ} = \frac{1.54}{2 \times 0.3289}$$
$$= 2.3411 \text{ \AA}$$

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

$$\text{or } a = d\sqrt{h^2 + k^2 + l^2}$$
$$= 2.3411 \times \sqrt{1^2 + 1^2 + 1^2}$$
$$= 2.3411 \times \sqrt{3} = 4.05 \text{ \AA}$$

11. The Bragg's angle in the first order for (220) reflection from nickel (FCC) is 38.2° . When X-rays of wavelength 1.54 \AA are employed in a diffraction experiment. Determine the lattice parameter of nickel.

(Set-2-May 2008)

Sol: Order of diffraction, $n = 1$

Diffraction angle, $\theta = 38.2^\circ$

Wavelength of light, $\lambda = 1.54 \text{ \AA}$

Plane of reflection = (220)

Lattice parameter, $a = ?$

Bragg's law is $2d \sin \theta = n\lambda$

$$d = \frac{n\lambda}{2 \sin \theta} = \frac{1 \times 1.54}{2 \times \sin 38.2^\circ} \text{ \AA}$$

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

$$a = d \times \sqrt{h^2 + k^2 + l^2}$$
$$= \frac{1 \times 1.54}{2 \times \sin 38.2^\circ} \times \sqrt{2^2 + 2^2 + 0^2}$$
$$= \frac{4.35578}{1.23682} = 3.522 \text{ \AA}$$

12. Copper has FCC structure with lattice constant 0.36 nm . Calculate the interplanar spacing for (111) and (321) planes.

Sol: Given data is:

$$\text{lattice constant } (a) = 0.36 \text{ nm} = 0.36 \times 10^{-9} \text{ m}$$

Interplanar spacing (d) for (111) plane is:

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}} = \frac{0.36 \times 10^{-9}}{\sqrt{1^2 + 1^2 + 1^2}} = \frac{0.36 \times 10^{-9}}{\sqrt{3}} \text{ m}$$

$$= 0.208 \times 10^{-9} \text{ m} = 0.208 \text{ nm}$$

Interplanar spacing for (321) plane

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}} = \frac{0.36 \times 10^{-9}}{\sqrt{3^2 + 2^2 + 1^2}} = \frac{0.36 \times 10^{-9}}{\sqrt{9 + 4 + 1}} = \frac{0.36 \times 10^{-9}}{\sqrt{14}} \text{ m}$$

$$= 0.096 \times 10^{-9} \text{ m}$$

$$= 0.096 \text{ nm.}$$

13. The first-order diffraction occurs when a X-ray beam of wavelength 0.675 \AA incident at a glancing angle of $5^\circ 25'$ on a crystal. What is the glancing angle for third-order diffraction to occur?

Sol: Wavelength of X-rays (λ) = 0.675 \AA

Glancing angle for first order ($n = 1$) diffraction (θ_1) = $5^\circ 25'$

Find the glancing angle for third order ($n = 3$) diffraction (θ_3) = ?

Bragg's equation is $2d \sin \theta = n\lambda$

For first order, $2d \sin \theta_1 = 1\lambda$

$$2d \sin 5^\circ 25' = 0.675 \times 10^{-10} \text{ m}$$

$$d = \frac{0.675 \times 10^{-10}}{2 \sin 5^\circ 25'} \text{ m} = \frac{0.675 \times 10^{-10}}{0.1888} = 3.575 \times 10^{-10} \text{ m} = 3.575 \text{ \AA}$$

For third-order diffraction,

$$2d \sin \theta_3 = 3\lambda$$

$$\sin \theta_3 = \frac{3\lambda}{2d} = \frac{3 \times 0.675 \times 10^{-10}}{2 \times 3.575 \times 10^{-10}} = 0.283$$

$$\theta_3 = \sin^{-1} (0.283) = 16.45^\circ = 16^\circ 28'.$$

14. What is the angle at which the third-order reflection of X-rays of 0.79 \AA wavelength can occur in a calcite crystal of $3.04 \times 10^{-8} \text{ cm}$ spacing.

Sol: Wavelength of X-rays, $\lambda = 0.79 \text{ \AA} = 0.79 \times 10^{-8} \text{ cm}$

Interplanar spacing, $d = 3.04 \times 10^{-8} \text{ cm}$

Order of diffraction, $n = 3$

Angle of diffraction, $\theta = ?$

$$2d \sin \theta = n\lambda$$

$$\sin \theta = \frac{n\lambda}{2d} = \frac{3 \times 0.79 \times 10^{-8}}{2 \times 3.04 \times 10^{-8}} = 0.3898$$

$$\theta = \sin^{-1} (0.3898)$$

$$= 25^\circ 29' 28''$$

Bragg's law

$$2d \sin \theta = n\lambda$$

$$2d \sin 19.2^\circ = 1 \times 1.54$$

$$d = \frac{1.54}{2 \times \sin 19.2^\circ} = \frac{1.54}{2 \times 0.3289}$$
$$= 2.3411 \text{ \AA}$$

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

$$\text{or } a = d \sqrt{h^2 + k^2 + l^2}$$
$$= 2.3411 \times \sqrt{1^2 + 1^2 + 1^2}$$
$$= 2.3411 \times \sqrt{3} = 4.05 \text{ \AA}$$

11. The Bragg's angle in the first order for (220) reflection from nickel (FCC) is 38.2° . When X-rays of wavelength 1.54 \AA are employed in a diffraction experiment. Determine the lattice parameter of nickel.

(Set-2-May 2008)

Sol: Order of diffraction, $n = 1$

Diffraction angle, $\theta = 38.2^\circ$

Wavelength of light, $\lambda = 1.54 \text{ \AA}$

Plane of reflection = (220)

Lattice parameter, $a = ?$

Bragg's law is $2d \sin \theta = n\lambda$

$$d = \frac{n\lambda}{2 \sin \theta} = \frac{1 \times 1.54}{2 \times \sin 38.2^\circ} \text{ \AA}$$

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

$$a = d \times \sqrt{h^2 + k^2 + l^2}$$
$$= \frac{1 \times 1.54}{2 \times \sin 38.2^\circ} \times \sqrt{2^2 + 2^2 + 0^2}$$
$$= \frac{4.35578}{1.23682} = 3.522 \text{ \AA}$$

12. Copper has FCC structure with lattice constant 0.36 nm . Calculate the interplanar spacing for (111) and (321) planes.

Sol: Given data is:

$$\text{lattice constant } (a) = 0.36 \text{ nm} = 0.36 \times 10^{-9} \text{ m}$$

Interplanar spacing (d) for (111) plane is:

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}} = \frac{0.36 \times 10^{-9}}{\sqrt{1^2 + 1^2 + 1^2}} = \frac{0.36 \times 10^{-9}}{\sqrt{3}} \text{ m}$$

$$= 0.208 \times 10^{-9} \text{ m} = 0.208 \text{ nm}$$

Interplanar spacing for (321) plane

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}} = \frac{0.36 \times 10^{-9}}{\sqrt{3^2 + 2^2 + 1^2}} = \frac{0.36 \times 10^{-9}}{\sqrt{9 + 4 + 1}} = \frac{0.36 \times 10^{-9}}{\sqrt{14}} \text{ m}$$

$$= 0.096 \times 10^{-9} \text{ m}$$

$$= 0.096 \text{ nm.}$$

13. The first-order diffraction occurs when a X-ray beam of wavelength 0.675 \AA incident at a glancing angle of $5^\circ 25'$ on a crystal. What is the glancing angle for third-order diffraction to occur?

Sol: Wavelength of X-rays (λ) = 0.675 \AA

Glancing angle for first order ($n = 1$) diffraction (θ_1) = $5^\circ 25'$

Find the glancing angle for third order ($n = 3$) diffraction (θ_3) = ?

Bragg's equation is $2d \sin \theta = n\lambda$

For first order, $2d \sin \theta_1 = 1\lambda$

$$2d \sin 5^\circ 25' = 0.675 \times 10^{-10} \text{ m}$$

$$d = \frac{0.675 \times 10^{-10}}{2 \sin 5^\circ 25'} \text{ m} = \frac{0.675 \times 10^{-10}}{0.1888} = 3.575 \times 10^{-10} \text{ m} = 3.575 \text{ \AA}$$

For third-order diffraction,

$$2d \sin \theta_3 = 3\lambda$$

$$\sin \theta_3 = \frac{3\lambda}{2d} = \frac{3 \times 0.675 \times 10^{-10}}{2 \times 3.575 \times 10^{-10}} = 0.283$$

$$\theta_3 = \sin^{-1} (0.283) = 16.45^\circ = 16^\circ 28'.$$

14. What is the angle at which the third-order reflection of X-rays of 0.79 \AA wavelength can occur in a calcite crystal of $3.04 \times 10^{-8} \text{ cm}$ spacing.

Sol: Wavelength of X-rays, $\lambda = 0.79 \text{ \AA} = 0.79 \times 10^{-8} \text{ cm}$

Interplanar spacing, $d = 3.04 \times 10^{-8} \text{ cm}$

Order of diffraction, $n = 3$

Angle of diffraction, $\theta = ?$

$$2d \sin \theta = n\lambda$$

$$\sin \theta = \frac{n\lambda}{2d} = \frac{3 \times 0.79 \times 10^{-8}}{2 \times 3.04 \times 10^{-8}} = 0.3898$$

$$\theta = \sin^{-1} (0.3898)$$

$$= 25^\circ 29' 28''$$

List of Questions

1. Describe seven crystal systems with diagrams.
2. Obtain the relations between the edge of the unit cell and atomic radius for the BCC and FCC lattices.

3. What are Bravais lattices?
4. Describe FCC crystal structure.
5. Define crystal lattice, unit cell, lattice parameter and coordination number.
6. Explain the unit cell and lattice parameters. What is a primitive cell and how does it differ from unit cell.
7. Explain the terms: (i) basis, (ii) space lattice, (iii) lattice parameters and (iv) unit cell.
8. Describe BCC structure, with suitable example.
9. Describe in detail, the seven crystal systems with diagrams.
10. Tabulate the characteristics of the unit cells of different crystal systems.
11. Illustrate Bravais lattices.
12. Illustrate simple cubic, FCC and BCC crystal structures.
13. What is space lattice? Find the packing fraction for BCC and FCC crystals.
14. Classify various lattice types in the crystal system.
15. What is a Bravais lattice? What are the different space lattices in the cubic system?
16. Describe FCC crystal structure.
17. Obtain an expression for the packing factor of FCC structure.
18. Define crystal lattice, unit cell, lattice parameter and coordination number.
19. Explain the unit cell and lattice parameters. What is a primitive cell and how does it differ from unit cell.
20. Describe the crystal structure of CsCl.
21. Consider a body centred cubic lattice of identical atoms having radius 'R' compute (i) the number of atoms per unit cell (ii) The coordination number and (iii) the packing fraction
22. Explain the terms: (i) basis, (ii) space lattice, (iii) lattice parameters and (iv) unit cell.
23. Describe BCC structure, with suitable example.
24. Describe in detail, the seven crystal systems with diagrams.
25. Tabulate the characteristics of the unit cells of different crystal systems.
26. Illustrate Bravais lattices.
27. What is space lattice? Find the packing fraction for BCC and FCC crystals.
28. Classify various lattice types in the crystal system.
29. Describe in detail the structure of ZnS.
30. What is a Bravais lattice? What are the different space lattices in the cubic system?
31. Deduce the expression for the interplanar distance in terms of Miller indices for a cubic structure.
32. Sketch the following planes of a cubic unit cell: (001), (120) and (211).

33. Define Miller indices. Sketch the following atomic planes in a simple cubic structure (010), (110) and (111).
34. How can the interplanar spacing of a set of Miller planes be calculated in terms of Lattice parameters?
35. What is Bragg's law? Explain.
36. What are Miller Indices? Draw (111) and (110) planes in a cubic lattice.
37. Draw the (112) and (120) planes and the [112] and [120] directions of a simple cubic crystal.
38. Sketch the following planes of a cubic unit cell: (001), (120) and (211).