

2.1 INTRODUCTION

Materials science deals with the study of structure and properties of materials. It helps to select materials for particular applications, to design new materials and to improve the existing ones. When we want to fabricate an engineering part, like a hacksaw blade, we must go in search of a material, like high speed steel which possesses desirable properties as will permit the blade to perform its functions successfully while in use.

2.2 CRYSTAL SYSTEMS AND BRAVAIS LATTICES

Solids can be classified into crystalline solids or crystals and amorphous solids.

Crystals	Amorphous solids
<ol style="list-style-type: none"> 1. In each crystal, the atoms or molecules are arranged in a regular and orderly manner in a three dimensional pattern, called lattice. 2. They possess internal spatial symmetry of atomic or molecular orientation. 3. When a crystal breaks, the broken pieces are all having regular shape. 4. The crystals have directional properties and therefore called anisotropic substances. 	<ol style="list-style-type: none"> 1. In an amorphous solid, molecules which are the basic units are arranged in an irregular manner, otherwise there is no lattice structure. 2. These do not possess any internal spatial symmetry. 3. When an amorphous solid breaks, the broken pieces are irregular in shape. 4. These solids have no directional properties and therefore called isotropic substances.
<p>Examples:</p> <ol style="list-style-type: none"> (i) Metallic crystals: Copper, Silver, Aluminium, etc. (ii) Non-metallic crystals: Diamond, Silicon, Germanium, Sodium Chloride, etc. 	<p>Examples</p> <p>Glass, Plastics, Rubber, etc.</p>

(ii) To find the packing factor of HCP structure

Area of the base = 6 × area of the triangle ABO

$$= 6 \times \frac{1}{2} \times AB \times OY$$

$$V = 3 \times a \times \left(\frac{\sqrt{3}}{2} a \right) = \frac{3\sqrt{3} a^2}{2} c$$

Hence the volume of the unit cell of the HCP structure = Area of the base × c

Volume = 3

Considering the top layer which has totally seven atoms, each corner atom contributes 1/6 atom to the unit cell and the centre atom contributes 1/2 atom to the unit cell. Hence the total contribution by the top layer to the unit cell is $1/6 \times 6 + 1/2 = 3/2$ atoms. Similarly the bottom layer also contributes the same $3/2$ atoms. The central layer contributes 3 atoms fully because all the central layer atoms are well inside the unit cell.

Therefore total number of atoms per unit cell

$$= \frac{6}{6} + \frac{6}{2} + 3 = 6$$

Packing fraction

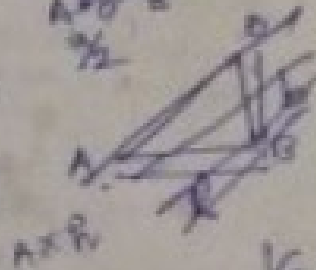
$$\frac{V}{V} = \frac{6 \times \frac{4}{3} \pi r^3}{\frac{3\sqrt{3} a^2 c}{2}}$$

Substituting $2r = a$ and $c = \sqrt{8/3} a$, we get

Packing factor = $\frac{\pi}{3\sqrt{2}} = 0.74$

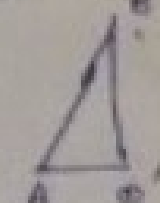
Thus the density of packing is 74% and hence it is a close packed structure. So most of the metals like zinc and magnesium crystallize in this structure.

$$AO = \frac{1}{2} AO' + OO'c$$



$$\frac{1}{2} ab$$

$$\frac{1}{2} AB \times OY$$



✓ Corner $1 + 1 = 2$
 ✓ Center $2 \times \frac{1}{2} = 1$

$$6 \times \frac{1}{6} = 1$$

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

3

5.17 SODIUM CHLORIDE (NaCl) STRUCTURE

5.17.1. Structure

Sodium chloride (NaCl) is an ionic crystal. In the NaCl structure, positive charged sodium ion (Na^+) and negative charged chlorine ion (Cl^-) are situated in an alternative lattice position as shown in Fig. 5.35. The radius of chlorine ion is about 1.81 \AA and the radius of sodium ion is about 0.98 \AA .

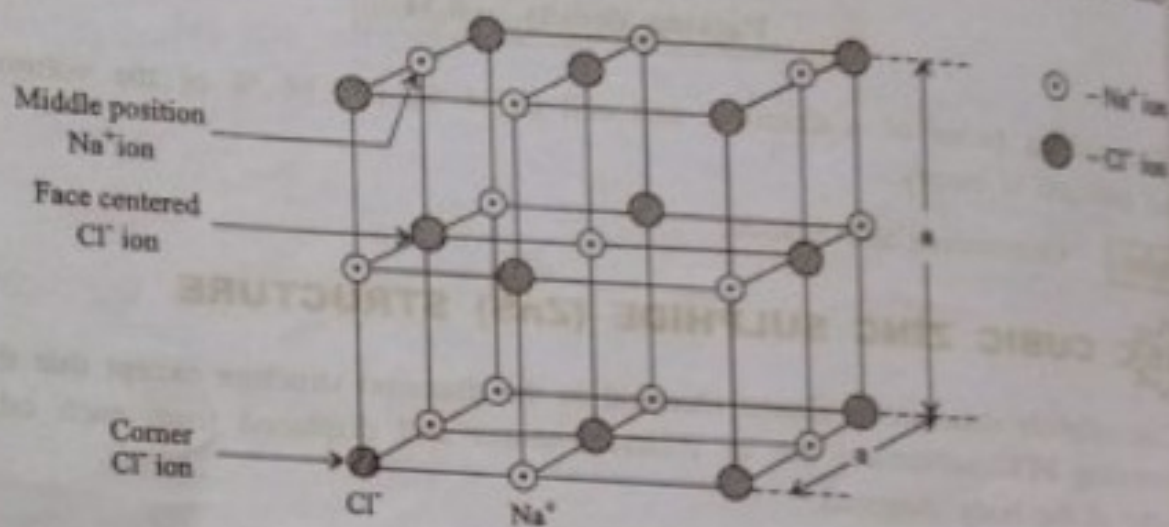


Fig. 5.35. Sodium Chloride (NaCl) Structure

It has two face centered cubic (FCC) sub-lattices. In the face centered cubic lattice basis of one Na^+ ion and one Cl^- ion are separated by one - half the body diagonal of the unit cell. The Na^+ ions are situated at the middle position of the axial length of the unit cell and the Cl^- ions are situated at the corners and the center of faces of the cube.

2. Number of Molecules per Unit Cell

There are four Na^+ ions and four Cl^- ions in one unit cell. Therefore, the total number of NaCl molecules per unit cell is four with ions in the positions:

$$\text{Na}^+ \text{ ions} : \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right), \left(0, 0, \frac{1}{2} \right), \left(0, \frac{1}{2}, 0 \right), \left(\frac{1}{2}, 0, 0 \right)$$

$$\text{Cl}^- \text{ ions} : \left(0, 0, 0 \right), \left(\frac{1}{2}, \frac{1}{2}, 0 \right), \left(\frac{1}{2}, 0, \frac{1}{2} \right), \left(0, \frac{1}{2}, \frac{1}{2} \right)$$

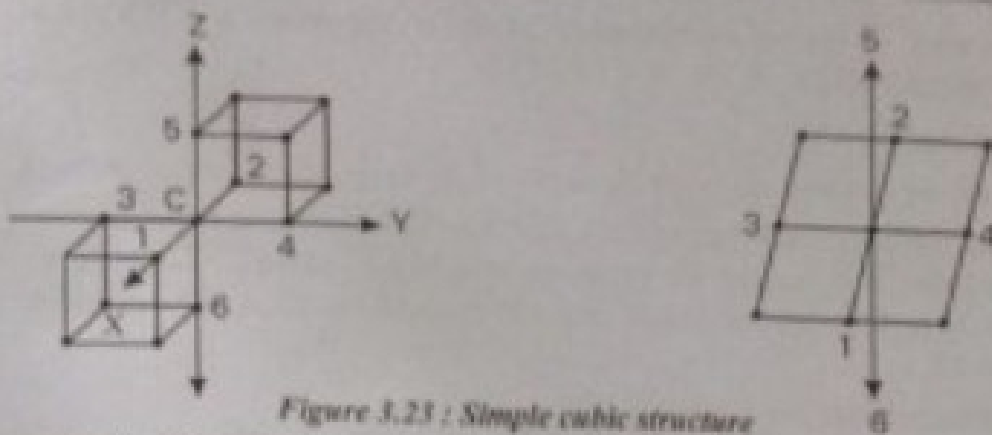


Figure 3.23 : Simple cubic structure

(b) Body centered cubic structure

In this structure, there will be one atom at the body centre and eight atoms at the 8 corners of the unit cell figure 3.24. Thus, for an atom C at the body centre obviously, there are 8 nearest neighbours (corner atoms). Hence, the co-ordination number of an atom in body centered cubic structure is 8. The corner atoms do not touch each other. But, each corner atom touches the body centre along the body diagonal.

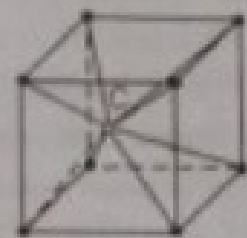


Figure 3.24

Alternative method

The coordination number can also be determined in another way as follows.

We know that in a BCC structure, each corner atom is surrounded by eight other body centered unit cells. Therefore, the nearest adjacent neighbours are the body centered atoms of the eight surrounding unit cells.

Thus, the coordination number is 8.

(c) Face centered cubic structure

In this system, there are 8 corner atoms and six face centered atoms one at the centre of each face.

To calculate the coordination number, consider any corner atom C. In its own plane it has 4 face centered atoms as nearest neighbour. In a plane which lie just above this corner atom, it has 4 more face centre atoms as nearest neighbours and similarly, in a plane which lie just below this corner atom it has 4 more face centered atoms as nearest neighbours.

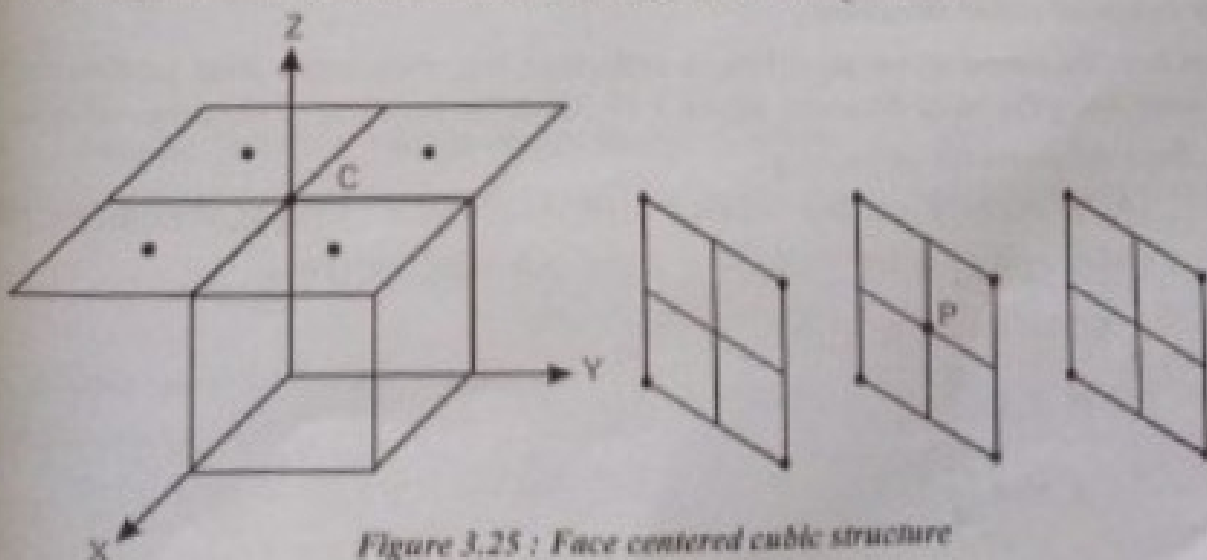


Figure 3.25 : Face centered cubic structure

(e) Diamond cubic structure:

Germanium, Silicon and Carbon (Diamond) possess this structure which is a combination of two interpenetrating FCC sub-lattices.

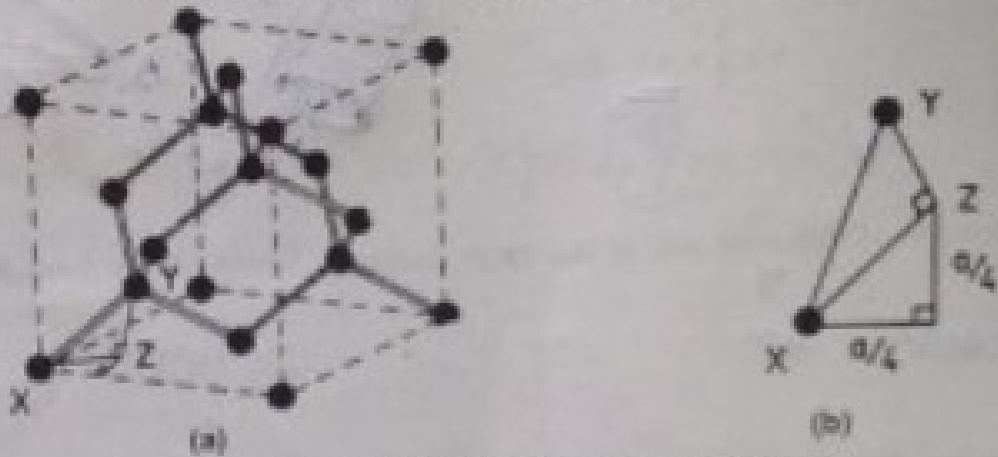


Fig. 2.17: Diamond cubic structure

As seen from the unit cell of diamond cubic structure (figure 2.17 (a)) one sub-lattice say 'X' has its origin at $(0,0,0)$ and the other say 'Y' at a point one quarter of the way along the body diagonal, i.e. at the $(a/4, a/4, a/4)$ point. The structure is loosely packed since each atom has only four nearest neighbours, i.e. its coordination number is 4. In the unit cell, in addition to the eight corner atoms, there are six face centred atoms and four more atoms located inside the unit cell as shown in the figure. Each corner atom is shared by eight adjacent unit cells and each face centred atom is shared by two unit cells. Hence the total number of atoms per unit cell

$$= \frac{1}{8} \times 8 + \frac{1}{2} \times 6 + 4 = 8$$

From the figure 2.17(b), $XZ^2 = \left(\frac{a}{4}\right)^2 + \left(\frac{a}{4}\right)^2 = \frac{a^2}{8}$

Further $XY^2 = XZ^2 + YZ^2 = \frac{a^2}{8} + \frac{a^2}{16} = \frac{3a^2}{16}$

But $XY = 2r$

Therefore $(2r)^2 = \frac{3a^2}{16}$

(or) $a = \frac{8}{\sqrt{3}} r$

$$\therefore \text{Packing factor} = \frac{8 \times \frac{4}{3} \pi \left[\frac{a\sqrt{3}}{8} \right]^3}{a^3}$$

$$= \frac{\sqrt{3} \pi}{16} = 0.34$$

\therefore Packing density = 0.34

The packing factor of a diamond unit cell is 34 %, i.e. 66 % of the volume of a diamond unit cell is empty.

Examples Germanium and Silicon.

5.16 CUBIC ZINC SULPHIDE (ZnS) STRUCTURE

Zinc sulphide structure is almost identical to the diamond structure except that the two interpenetrating FCC sublattices are of different atoms and displaced from each other by one-quarter of the body diagonal.

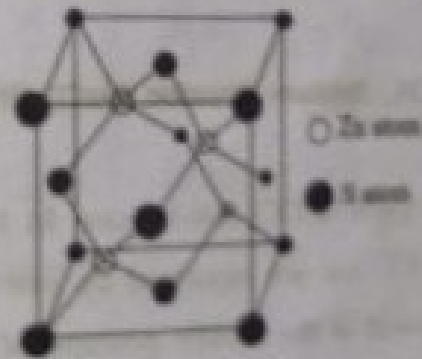


Fig. 5.34. Zinc Sulphide (ZnS) Structure

The cubic zinc sulphide structure results when Zinc atoms are placed in one FCC lattice and S atoms on the other FCC lattice as shown in Fig. 5.34. The conventional cell of this structure is a cube. There are four molecules per unit cell. Therefore, the coordination number is 4. For each atom, there are four equally distant atoms of opposite kind arranged in a regular tetrahedron.

Examples CdS and InSb have this type of structure.

(d) Hexagonal Close Packed (HCP) structure

Figure 2.15(a) shows the unit cell of a hexagonal crystal. Even though the volume of this unit cell is great, the number of atoms in an unit cell is only 2. Further its packing factor is low and hence metals do not crystallize in this simple hexagonal structure. Figure 2.15(b) shows the unit cell of the close packed hexagonal structure.

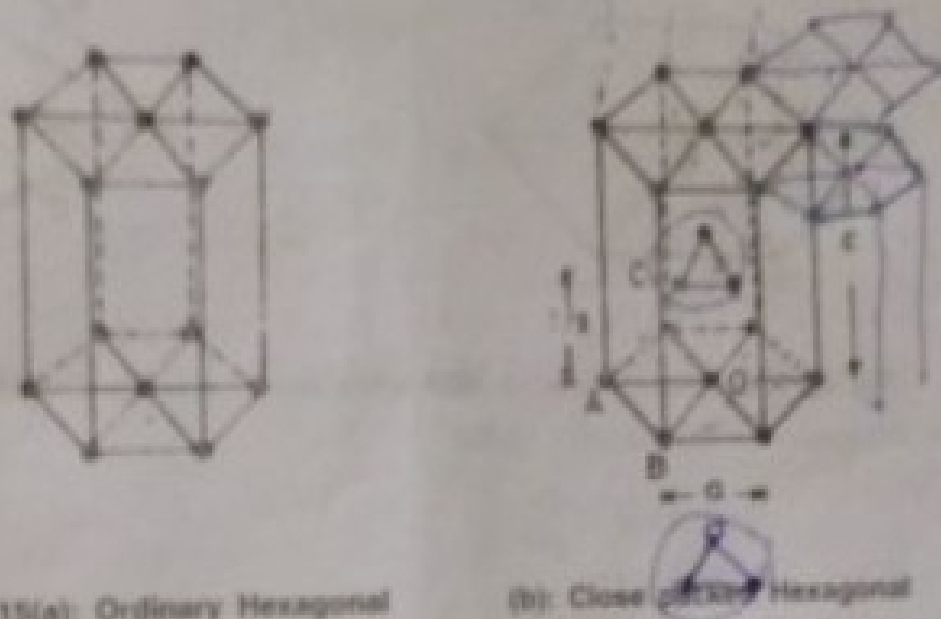


Fig. 2.15(a): Ordinary Hexagonal

(b): Close packed Hexagonal

There are three layers of atoms in it. At the bottom layer central atom has 6 nearest neighbouring atoms in the same plane. Further the second layer, which is at a distance $\frac{c}{2}$ from the bottom layer, has three atoms as shown in the figure. Third layer is similar to the bottom layer in the arrangement of atoms and it is at a distance c from the bottom layer. Thus it has the stacking sequence of AB AB. ... So it is a 2-layer structure.

i) Calculation of coordination number for HCP structure

Let us calculate the number of nearest neighbouring atoms for each atom in the HCP structure. If we take the bottom layer, the central atom has 6 nearest neighbouring atoms in the same plane. Further at a distance $\frac{c}{2}$ from the bottom layer there are two layers, one is above and another is below the bottom layer containing three atoms in each layer. So totally there are about 12 nearest neighbouring atoms (6) the coordination number is 12. So it is a close packed structure. Further from the figure the nearest neighbouring distance, $2r = a$.

ii) Calculation of c/a ratio in hexagonal close packed structure

Consider the figure 2.15. Let c be the height of the unit cell and a be the distance between two neighbouring atoms. Consider the triangle ABO in the bottom

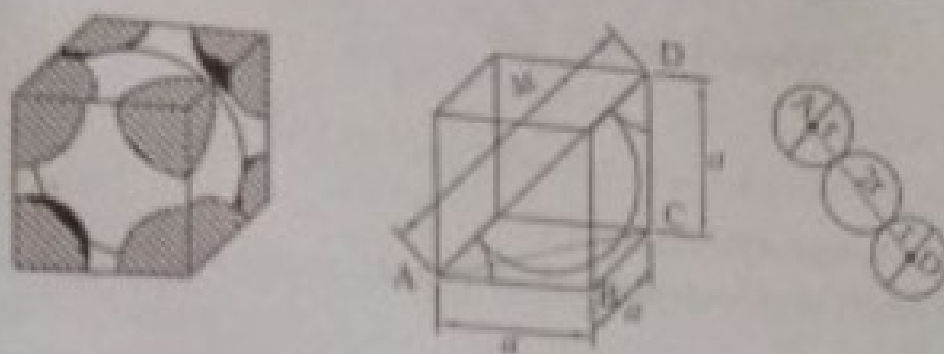


Figure 3.27: Body centered cubic structure

(c) Face centered structure

In face-centered cubic structure, the atoms touch each other along the diagonal of any face of the cube. The diagonal of the cube AC is $4r$.

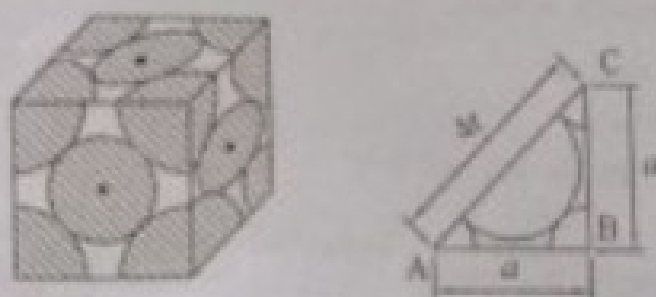


Figure 3.28

But, from the geometry of the figure 3.28,

$$(AC)^2 = (AB)^2 + (BC)^2 = a^2 + a^2 = 2a^2$$

$$\therefore AC = a\sqrt{2} \quad ; \quad \text{But, } AC = 4r$$

Hence,

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

or

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

3.9 Atomic Packing Factor of the Cubic System

The packing factor or packing density of the three cubic systems can be calculated as follows:

$$APF = \frac{\text{No. of atoms per unit cell} \times \text{Volume of one atom}}{\text{Volume of the unit cell}} \quad \text{--- [1]}$$

(a) Simple cubic structure

In simple cubic,

$$\text{The number of atoms per unit cell} = 1$$

$$\begin{aligned}\text{Volume of 1 atom} &= \frac{4}{3} \pi r^3 \\ &= \frac{4}{3} \pi \left[\frac{a}{2} \right]^3 \quad [\because r = a/2]\end{aligned}$$

$$\text{Volume of the unit cell} = a^3$$

Therefore, density of packing or packing factor as per equation (1) is,

$$\text{APF} = \frac{1 \times \frac{4}{3} \pi \left(\frac{a}{2} \right)^3}{a^3}$$

$$\therefore \text{APF} = \frac{\pi}{6} = 0.52.$$

\therefore 52% of the volume is occupied by atoms and remaining 48% volume is vacant.
Thus, the packing density is 52%.

(b) *Body centered cubic structure*

In body centered cubic structure,

$$\text{The number of atoms per unit cell} = 2$$

$$\therefore \text{Volume of 2 atoms} = 2 \times \frac{4}{3} \pi r^3 = \frac{8\pi}{3} \left[\frac{a\sqrt{3}}{4} \right]^3 = \pi a^3 \frac{\sqrt{3}}{8} \quad \left[\because r = \frac{a\sqrt{3}}{4} \right]$$

$$\text{Volume of the unit cell} = a^3$$

$$\therefore \text{APF} = \frac{\pi a^3 \frac{\sqrt{3}}{8}}{a^3} = \pi \frac{\sqrt{3}}{8}$$

$$\text{APF} = 0.68.$$

\therefore 68% of the volume is occupied by atoms and remaining 32% volume is vacant.
Thus, the packing density is 68%.

(c) *Face centered cubic structure*

In face centered cubic structure,

$$\text{The number atoms per unit cell} = 4$$

$$\therefore \text{Volume of 4 atoms} = 4 \times \frac{4}{3} \pi r^3 = \frac{16\pi}{3} \left[\frac{a\sqrt{2}}{4} \right]^3 = \frac{\pi a^3 \sqrt{2}}{6} \quad \left[\because r = \frac{a\sqrt{2}}{4} \right]$$

$$\text{Volume of the unit cell} = a^3$$

Example 3.13 : Find the Miller indices of a set of parallel planes which make intercepts in the ratio $2b : 7c$, and are parallel to x -axis; a , b , and c being primitive vectors of the lattice

Solution :

Given $OB = 2b$ and $OC = 7c$ and $OA = \infty$

$$(hkl) = ?$$

The numerical value of intercepts along the three axis are $(\infty, 2, 7)$

Therefore, Miller indices are $\left(\frac{1}{\infty} \frac{1}{2} \frac{1}{7}\right) = (0 \ 7 \ 2)$.

3.8 Crystal Structure of Materials

Let us know some important parameters which are used to describe the crystal structure.

1. Number of atoms per unit cell or Effective number

The total number of atoms present in an unit cell is known as number of atoms per unit cell.

2. Co-ordination number

Definition - 1 : It is the number of nearest neighbouring atoms to a particular atom.

Definition - 2 : Co-ordination number is the number of nearest neighbours directly surrounding a given atom.

3. Atomic radius

It is defined as half of the distance between two nearest neighbours in a crystal of a pure element.

It is usually expressed in terms of cube edge a . Any two nearest neighbouring atoms touch each other.

4. Atomic packing factor (Packing density or Density of packing)

It is defined as the ratio of the volume of atoms per unit cell to the total volume occupied by the unit cell.

$$\text{i.e., APF} = \frac{\text{Volume of atoms per unit cell}}{\text{Volume of the unit cell}}$$

$$\text{or APF} = \frac{\text{No. of atoms per unit cell} \times \text{Volume of one atom}}{\text{Volume of the unit cell}}$$

All the above parameters are briefly explained one by one for a simple cubic structure.

3.8.1 Number of atoms per unit cell

This number varies from structure to structure. We shall evaluate the number of atoms per unit cell for the three cubic system.

(a) Simple cubic structure

The figure 3.20 shows the unit cell of a simple cubic structure. In this case, there are only 8 atoms, one at each corner of the cube or the unit cell.

In actual crystals, each and every corner atom is shared by 8 adjacent unit cells. Therefore, each and every

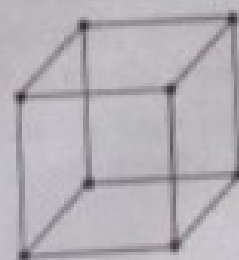


Figure 3.20 : Simple cubic

corner atom contributes $\frac{1}{8}$ of its part to one unit cell.

Total number of corner atoms = 8

\therefore The total share of all the corner atoms/unit cell = $8 \times \frac{1}{8} = 1$

\therefore Number of atoms/unit cell = 1.

In other words, the effective number of lattice points in a simple cubic structure is one. A simple cubic is a primitive cell.

(b) Body centered cubic structure

In this case, there are 8 atoms one at each corner of the unit cell plus one atom at the centre of the unit cell, figure 3.21.

Each and every corner atom is shared by 8 adjacent unit cells.

\therefore The total share of all the corner atoms per unit cell is $8 \times \frac{1}{8} = 1$.

The atom at the body centre is not shared by any other unit cell.

\therefore Number of unshared atoms/unit cell = 1.

Hence, total number of atoms/unit cell = $1 + 1 = 2$.

(c) Face-centered cubic structure

In this case, there are 8 atoms, one at each corner of the unit cell and six atoms at the centres of six faces of unit cell figure 3.22.

The total share of all the corner atoms per unit cell is $8 \times \frac{1}{8} = 1$.

Now, consider the atoms at the face centre of the unit cell. Each such atom is shared by only two unit cells, which lie on either side of the plane in which the atom is located.

\therefore The total share of all the face centered atoms per unit cell = $6 \times \frac{1}{2} = 3$.

Hence, the total number of atoms/unit cell is $1 + 3 = 4$.



Figure 3.21: Body centered cubic structure

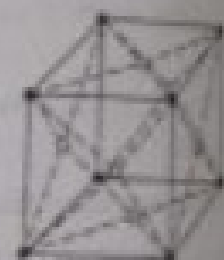


Figure 3.22: Face centered cubic structure

3.8.2 Co-ordination number

The coordination number for the three types of cubic crystal structure can be calculated as follows:

(a) Simple cubic structure

Simple cubic unit cell consists of 8 corner atoms. Let us consider any one corner atom, figure 3.23.

For this particular atom C there are 4 nearest neighbours (shown as 1, 2, 3 and 4) in the same plane (horizontal plane) and there are 2 more nearest atoms, one directly above and the other directly below (shown as 5 and 6).

Except these six atoms all the other atoms lie at greater distances from C. The coordination number for an atom in simple cubic is 6.

\therefore The total number of nearest atoms to any corner atoms is $4 + 4 + 4 = 12$.
coordination number is 12.

Alternative method

The co-ordination number can also be determined in another way as follows.

Let us consider 3 planes as shown in figure 3.25. Consider the face centered atom P in one plane. It is seen that all the corner atoms irrespective of the 3 planes to which it belongs are at same distance from P. There are 4 such atoms in each plane. Thus, the number of atoms to P is $3 \times 4 = 12$.

Hence, the coordination number is 12.

3.8.3 Relation between Atomic radius and Lattice constant

It is possible to express the lattice constant a in terms of the atomic radius r . All atoms are assumed to be spherical in shape. For the three cubic structures it can be calculated as follows.

(a) Simple cubic structure

Let us consider one face of the simple cubic structure, figure 3.26. In this structure the atoms touch each other along the edges.

Hence, the nearest neighbour distance is $2r = a$.

Therefore, $r = a/2$.

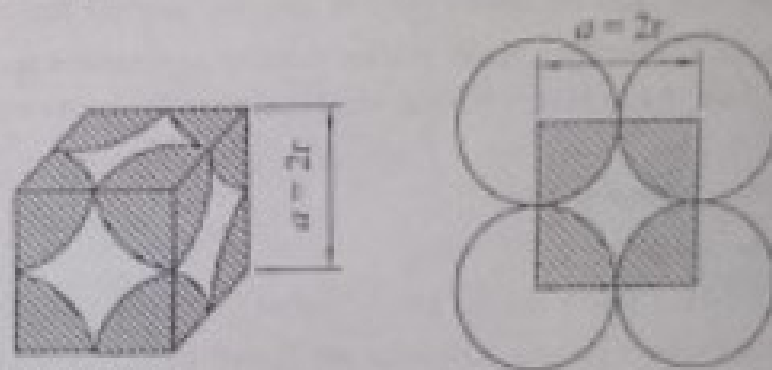


Figure 3.26 : Simple cubic structure

(b) Body centered cubic structure

In this structure, the corner atoms do not touch each other. But, each corner atom touches the body centered atom along the body diagonal, figure 3.27. Thus, the diagonal of the cube AD is 4r.

But, from the geometry of the cube,

$$(AD)^2 = (AC)^2 + (CD)^2 = (AB)^2 + (BC)^2 + (CD)^2 \quad [\because (AC)^2 = (AB)^2 + (BC)^2]$$

$$(AD)^2 = r^2 + r^2 + r^2 = 3a^2 \quad [\because AB = BC = CD = a]$$

$$\text{or} \quad AD = a\sqrt{3}; \text{ But, } AD = 4r$$

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

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

Miller indices are the set of three integers used to describe the orientation of a crystal plane.

- The use of Miller indices for notation of crystallographic planes is universal.
- Miller indices of a plane are given by the reciprocal of its three numerical parameters expressed as whole numbers.
- The general form for miller indices of a plane is $(h\ k\ l)$

Procedure for finding Miller indices:

- (a) Choose a system of three coordinate axes, preferably along the crystallographic axes.
- (b) Find the intercepts of the plane (whose Miller indices are desired) on the three coordinate axes. Let these be x', y', z' , along x, y and z axes respectively.
- (c) Then express them in terms of the axial units or primitives. Let them be $x' = pa, y' = qb$ and $z' = rc$.
- (d) Next take the numerical parameters of the plane i.e. $p : q : r$. The numerical parameters must be in whole numbers.
- (e) Find the ratio of their reciprocals $\left(\frac{1}{p} : \frac{1}{q} : \frac{1}{r}\right)$
- (f) Convert these reciprocals into whole numbers by multiplying each with the L.C.M. to get the smallest whole number. This gives the Miller indices $(h\ k\ l)$ of the plane.

For example, the plane ABC of figure 2.4 has intercepts of 2 axial units on x -axis and 2 axial units on y -axis and 1 axial unit on z -axis. In other words, the numerical

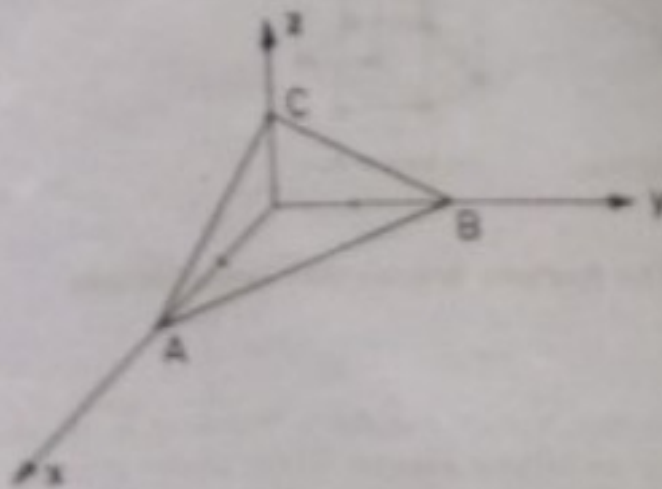


Fig. 2.4: Plane ABC in a crystal

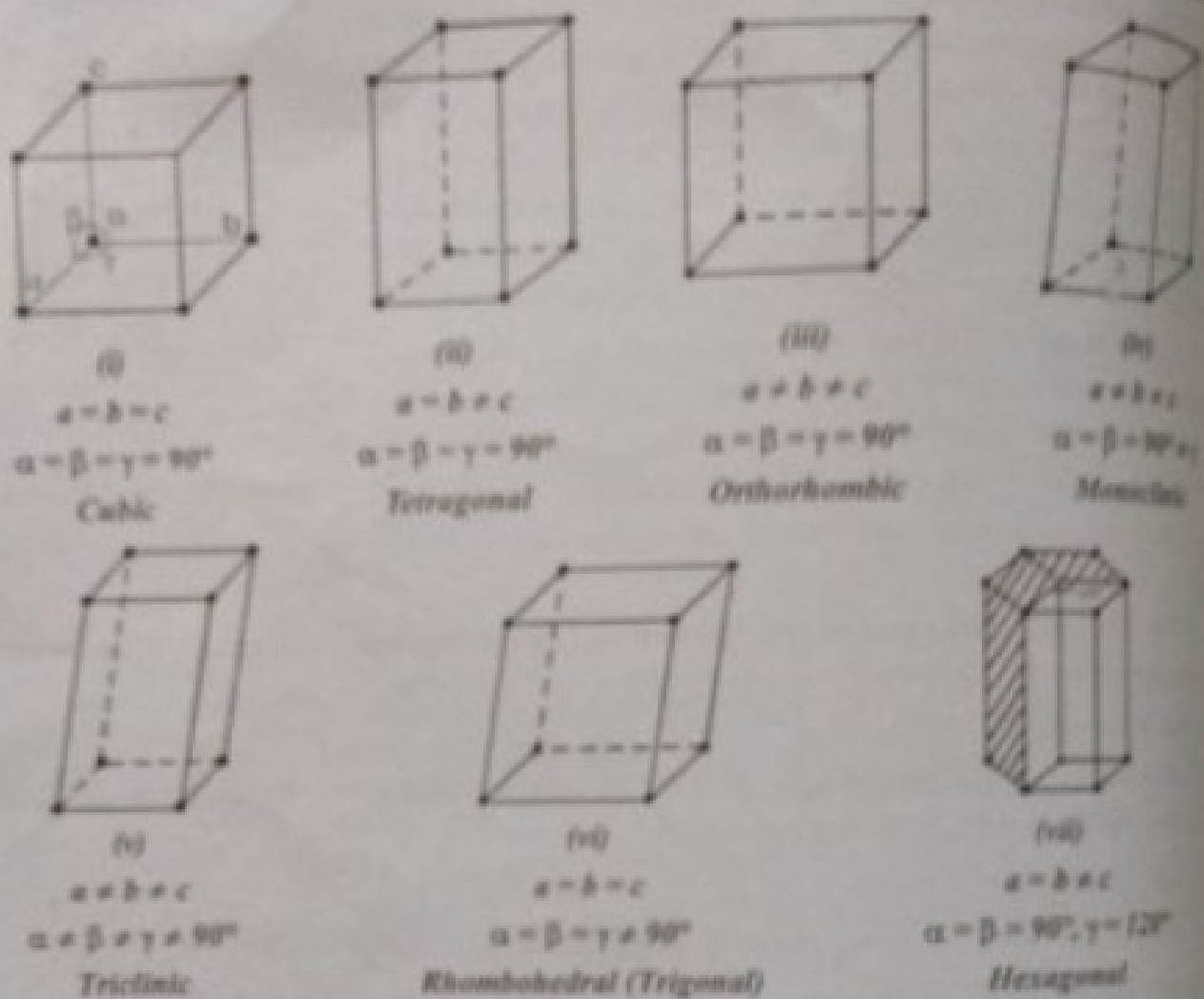


Figure 3.7 : The seven crystal system

3.4.2 Bravais lattice

Bravais in 1850 showed that there are 14 possible types of space lattices in the 7 crystal systems of crystal. According to Bravais, there are only 14 possible ways of arranging points in one lattice such that, all the lattice points have exactly the same surroundings. That is these 14 lattices are called *the Bravais lattices*. The possible types of Bravais lattices of the 7 crystal systems are explained in brief in this section and is also listed in Table 3.1.

Table 3.1

System	Bravais Lattice	
Cubic	3	SC or P, BCC
Tetragonal	2	SC or P, BCC
Orthorhombic	4	SC or P, BCC, FCC and Base centered (C)
Monoclinic	2	SC or P, Base centered (C)
Triclinic	1	SC or P
Trigonal	1	SC or P
Hexagonal	1	SC or P
Total	14	

Table 2.1 shows the details of the fourteen Bravais lattices of seven crystal systems along with their primitives, interfacial angles and examples and figure 2.1 shows the fourteen types of Bravais lattices.

Table 2.1 Crystal systems and Bravais lattices

Sl. No.	Name of Crystal system	Relation between primitives and the values of interfacial angles	Type of Bravais lattice	Examples
1.	Cubic	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$	P	Po (at certain temperature range)
			I	Na, W, α -Fe, Co_2O
			F	Ag, Au, Pb, Cu
2.	Tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	P	TiO_2 , SnO_2
			I	KH_2PO_4
3.	Orthorhombic (rhombic)	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	P	$\text{C}_{12}\text{H}_{20}\text{O}_7$
			C	PbCO_3 , BaSO_4
			F	KNO_3 , K_2SO_4
			I	α -S
4.	Monoclinic	$a \neq b \neq c$ $\alpha = \beta = 90^\circ \neq \gamma$	P	$\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$ (gypsum)
			C	$\text{K}_2\text{MgSO}_4 \cdot 6\text{H}_2\text{O}$
5.	Triclinic	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90^\circ$	P	$\text{K}_2\text{Cr}_2\text{O}_7$ $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$
6.	Rhombohedral (trigonal)	$a = b = c$ $\alpha = \beta = \gamma \neq 90^\circ$ (but less than 120°)	P	Calcite, As, Sb, Bi
7.	Hexagonal	$a = b \neq c$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$	P	Quartz, Zn, Cd

(Note: \neq means 'not necessarily equal to and generally different from')

Unit Cell of a crystal is the smallest volume of a solid or geometric figure from which the entire crystal is built up by translational repetition in three dimensions. It may be considered as the brick of a wall where the latter represents the crystal. Since the unit cell reflects the structure and properties of the crystal, it is enough to study the unit cell alone to get the clear idea about the whole crystal.

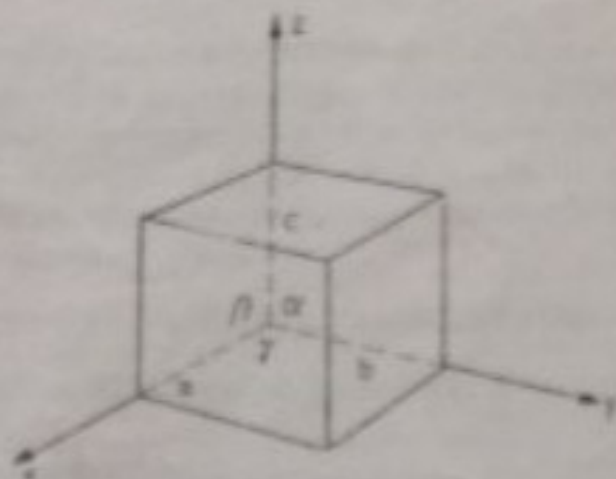


Fig. 2.1: Lattice parameters of an unit cell.

Lattice parameters of an unit cell

Figure 2.1 shows the lattice parameters of an unit cell. As shown in the figure, the lines drawn parallel to the lines of intersection of any three faces of the unit cell which do not lie in the same plane are called **crystallographic axes** x , y and z .

The angles between the three crystallographic axes represented by α , β and γ are called **interfacial angles** or **interaxial angles**.

The intercepts a , b and c , which define the dimensions of an unit cell, on the respective crystallographic axes are called **primitives** of the unit cell.

Thus the three primitives a , b and c and three interfacial angles α , β and γ are the **lattice parameters** which determine the form and actual size of the unit cell and hence the crystal.

The unit cell, formed by the primitives a , b and c and having only one lattice point is called **primitive cell**.

Example: The unit cell of a simple cubic crystal lattice is a primitive cell.

Space lattice is an infinite three dimensional array of points showing how atoms or molecules are arranged in a crystal. In the lattice array, every point has surroundings or environments identical to that of every other point in the array.

$$\therefore \text{APF} = \frac{\pi a^3 \frac{\sqrt{2}}{6}}{a^3} = \pi \frac{\sqrt{2}}{6} = 0.74$$

\therefore 74% of the volume is occupied by atoms and remaining 26% volume is vacant.

Thus, the packing density is 74%.