



**ANNAI WOMEN'S COLLEGE**  
(Affiliated to Bharathidasan University , Tiruchirapalli-24)



TNPL ROAD, PUNNAMCHATRAM, KARUR

**DEPARTMENT OF PHYSICS**  
**MATERIAL SCIENCE-16SMBEPH1**

**UNIT-I**

**PART-A**

**1. How solids are classified?**

- Crystalline solids (or) Crystals
- Non-Crystalline solids (or) Amorphous solids

**2. What is meant by crystal? Give examples.**

The regular periodic arrangement of atoms in a three dimension is called crystal.

**Examples:** Copper, silver, aluminium

**3. What is meant by amorphous solids? Give examples.**

In amorphous solids atoms are not arranged in an orderly fashion.

**Examples:** plastics, rubber, glass

**4. What is meant by crystallography?**

The branch of physics which deals with the geometric form and other physical properties of crystals using x – rays, electron beam, neutron beam etc., is called as crystallography.

**5. Distinguish between Crystalline and Non-Crystalline solids.**

S. No.	Crystalline Solids	Amorphous Solids
1.	They have definite and regular geometrical shape.	They do not have definite and regular geometrical shape.
2.	They are anisotropic.	They are isotropic.
3.	They are more stable.	They are less stable.
4.	They have sharp melting point.	They do not have sharp melting point.
5.	<b>Examples:</b> Diamond, NaCl, KCl, Copper etc.	<b>Examples:</b> Glass, plastic, rubber etc.

**6. Define lattice or space lattice.**

An array of points in the three dimensional pattern is known as space lattice.  
In the space lattice every point has identical surroundings to that of every other point.

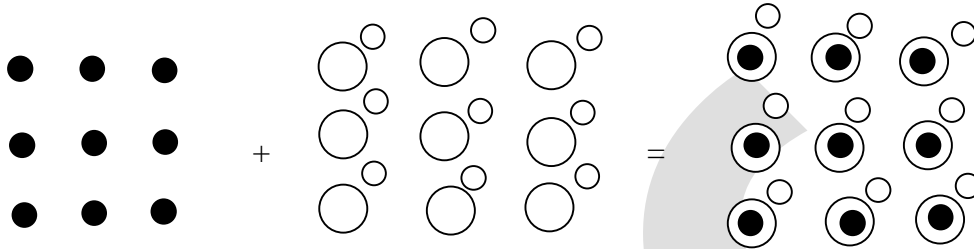
### 7. Define Lattice points?

The points in the space lattice are called lattice points.

### 8. Define basis.

The unit assembly of atoms associated with every lattice point is called a basis.

**Lattice + Basis = Crystal Structure**



### 9. Define unit cell?

Unit cell is defined as the smallest geometric figure, the repetition of which gives the actual crystal structure.

(or)

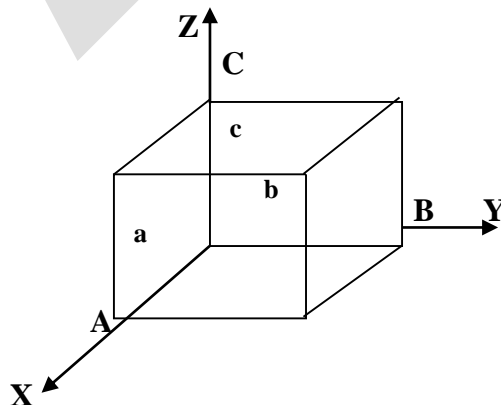
A unit cell in three dimension is defined as that volume of the solid, from which the entire crystal can be formed by the translational repetition in three dimension.

### 10. Define lattice planes.



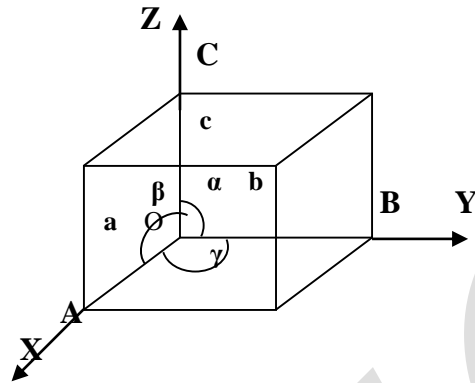
A set of parallel and equally spaced planes in a space lattice are called lattice planes.

### 11. Define Crystallographic axes.



The lines drawn parallel to the edges of a unit cell are known crystallographic axes.

**12. What is meant by lattice parameters?**



From the fig.  $OA = a$ ,  $OB = b$ ,  $OC = c$  are the intercepts i.e., edges of the unit cell which defines the dimensions of an unit cell. These intercepts are known as **primitives (or) translational vector (or) axial lengths**.

From the fig.  $\alpha$ ,  $\beta$ ,  $\gamma$  are the angles between Y & Z, Z & X and X & Y axes respectively. These three angles are known as **interfacial angles (or) interaxial angles**.

Both the intercepts a, b, c and interfacial angles  $\alpha$ ,  $\beta$ ,  $\gamma$  are the lattice parameters of the unit cell.

**13. Define primitive cell.**

A Primitive cell is the simplest type of unit cell which contains only one lattice point per unit cell. (Contains lattice points at its corner only).

**Example:** Simple Cubic (SC)

**14. What are Miller indices?**

A set of three numbers which is used to designate a plane in a crystal is known as Miller indices.

**15. Define Atomic radius (r).**

It is defined as the half of the distance between the nearest neighbouring atoms in a crystal.

**16. Define Co-ordination Number.**

It is the number of nearest neighboring atoms to a particular atom.

**17. Define Packing density (or) Atomic packing factor (APF).**

It is defined as the ratio of volume of all the atoms in the unit cell to the volume of the unit cell.

$$\text{Packing Factor} = \frac{\text{Volume of all the atoms in the unit cell}(v)}{\text{Volume of the unit cell}(V)}$$

**18. What is meant by Bravais lattice?**

S.No.	System	No. of Bravais lattices	Bravais Lattice
1.	Cubic	3	Simple (or) Primitive, Face centered and Bodycentered
2.	Monoclinic	2	Simple (or) Primitive, Base Centered
3.	Orthorhombic	4	Simple (or) Primitive, Base Centered, Face centered and Body centered
4.	Tetragonal	2	Simple (or) Primitive and Body Centered
5.	Hexagonal	1	Simple (or) Primitive
6.	Trigonal (Rhombohedral)	1	Simple (or) Primitive
7.	Triclinic	1	Simple (or) Primitive
	<b>Total</b>	14	

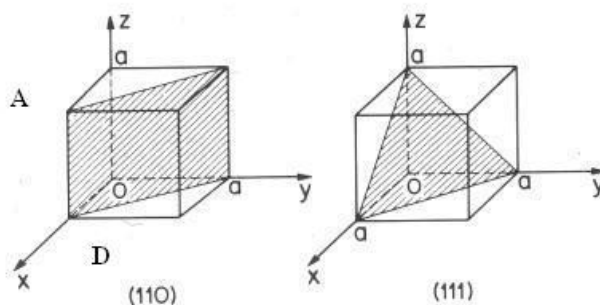
According to Bravais, there are only 14 possible ways of arranging points in space lattice from the 7 crystal systems such that all the lattice points have exactly the same surroundings. These 14 space lattices are called **Bravais lattices**.

**19. Define inter-atomic distance and interplanar distance.**

**Interatomic distance:** The distance between any two atoms is called inter-atomic distance.

**Interplanar distance:** The distance between any two planes is called inter planar distance.

**20. Draw the planes having Miller indices (110) and (111) in cubic system.**

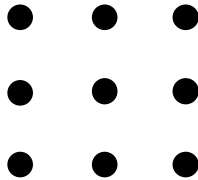


## PART-B

### CRYSTALLOGRAPHIC TERMS

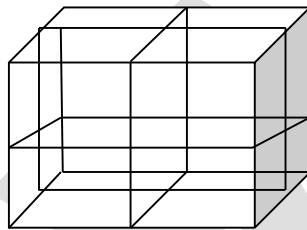
#### Lattice Points

It denotes the position of regular and periodic arrangement of atoms.



#### Space lattice

An array of points in the three dimensional pattern is known as space lattice. In the space lattice every point has identical surroundings to that of every other point.

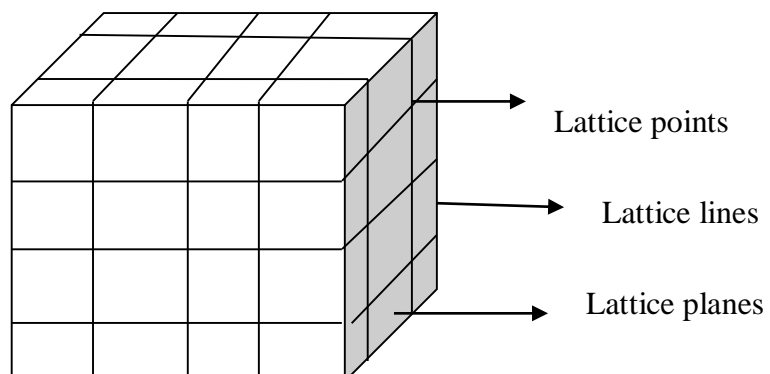


#### Lattice lines or directions

The lines joined between the lattice points are called lattice lines or lattice directions.

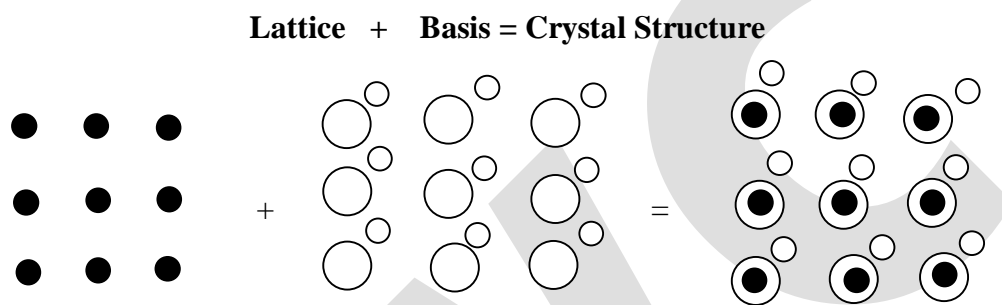
#### Lattice planes

A plane containing lattice points is known as a lattice plane or atomic plane. (or) A set of parallel and equally spaced planes in a space lattice are called lattice planes.



## Basis

The unit assembly of atoms or molecules which are identified with respect to the position of lattice points. The basis must be identical in composition, arrangement and orientation. When the basis is repeated with correct with periodicity in all directions gives the actual crystal structure. Therefore a space lattice is combined with a basis to get a crystal structure.



## UNIT CELL

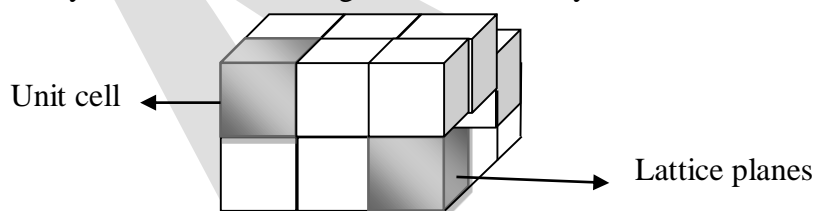
Unit cell is defined as the smallest geometric figure, the repetition of which gives the actual crystal structure.

(or)

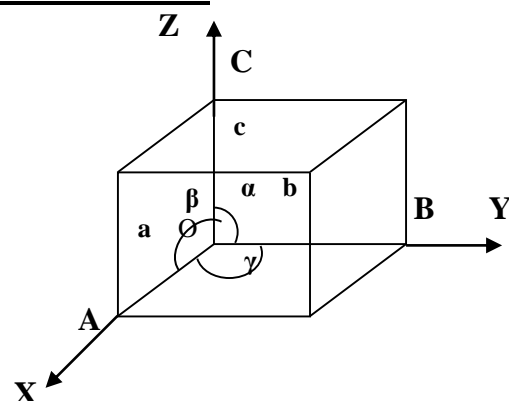
A unit cell in three dimension is defined as that volume of the solid, from which the entire crystal can be formed by the translational repetition in three dimension.

(or)

It is the smallest unit and fundamental building block of a crystal. Which, when repeated indefinitely in three dimension gives the whole crystal structure.



## Lattice parameters of a unit cell



From the fig.  $OA = a$ ,  $OB = b$ ,  $OC = c$  are the intercepts i.e., edges of the unit cell which defines the dimensions of an unit cell. These intercepts are known as **primitives (or) translational vector (or) axial lengths**.

From the fig.  $\alpha$ ,  $\beta$ ,  $\gamma$  are the angles between Y & Z, Z & X and X & Y axes respectively. These three angles are known as **interfacial angles (or) interaxial angles**.

Both the intercepts a, b, c and interfacial angles  $\alpha$ ,  $\beta$ ,  $\gamma$  are the lattice parameters of the unit cell.

### **Primitive cell**

It is defined as unit cell which contains lattice points at corner only. (or) It is the simplest type of unit cell contains only one lattice point per unit cell.

Eg: Simple cubic

If there is more than one lattice point in a unit cell it is called a non-primitive cell. All primitive cells are unit cells, but, all unit cell are not primitive cells.

### **THE SEVEN CRYSTAL SYSTEM**

Crystals are classified into 7 crystal systems on the basis of lattice parameters. The basic crystal systems are

1. Cubic
2. Tetragonal
3. Orthorhombic
4. Monoclinic
5. Triclinic
6. Rhombohedral or Trigonal
7. Hexagonal.

### **What are Bravais Lattices? Describe the Bravais lattice structures based on seven crystal system with neat sketch.**

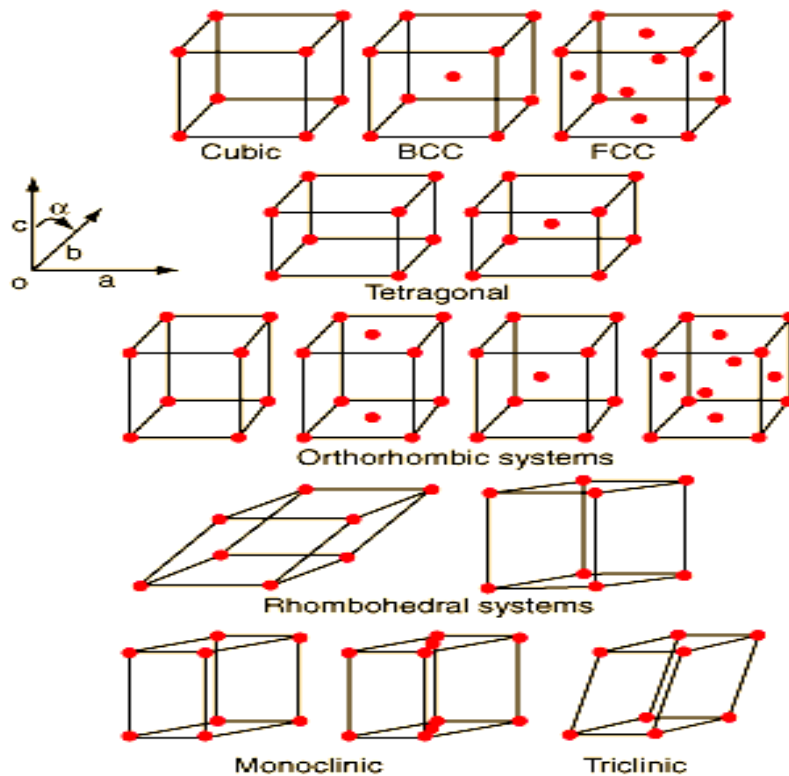
It is found that the point symmetry of crystal lattice can lead to 14 different types of lattices in three dimensional spaces. These 14 different types of arrangement are called Bravais lattices. Each type of this arrangement can be represented by a unit cell. The Bravais lattices formed by unit cells are marked by the following symbols:

Primitive Lattice - P  
Body Centred Lattice - I  
Face Centred Lattice - F  
Base Centred Lattice - C

The 14 Bravais lattices are illustrated in the figure.

The occurrences of the 14 Bravais lattices are given in the following table.

S.No.	System	No.of Bravais lattices	Bravais Lattice
1.	Cubic	3	Simple cubic(SC) (or Primitive (P), Face centered cubic(FCC) and Bodycentered cubic (BCC)
2.	Monoclinic	2	Simple (or) Primitive, Base Centered
3.	Orthorhombic	4	Simple (or) Primitive, Base Centered, Face centered and Body centered
4.	Tetragonal	2	Simple (or) Primitive and Body Centered
5.	Hexagonal	1	Simple (or) Primitive
6.	Trigonal (Rhombohedral)	1	Simple (or) Primitive
7.	Triclinic	1	Simple (or) Primitive
	Total	14	





### Miller Indices:

A set of three numbers which is used to designate a plane in a crystal is known as Miller indices.

Miller indices are certain numbers which are used to represent crystal planes.

It is also defines as the reciprocals of the intercepts are made by the plane on the crystallographic axes when reduced to smallest numbers. They are always whole number. A set of parallel planes are represented by the same Miller indices.

The common notations used to represent a plane in the Miller indices are h,k,l. They are commonly written as (h k l).

### Steps for finding Miller indices:

The steps in determining the Miller indices of a plane are illustrated below.

Let us consider a plane ABC which cuts 3 units along the x – axis, 1 unit along the y – axis and 2 units along the z – axis.

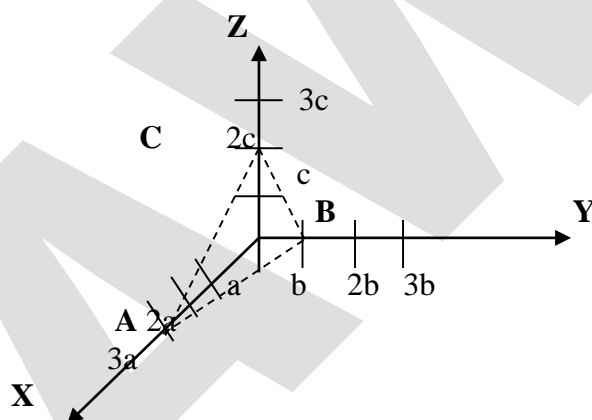
#### Step 1

Find the intercepts made by the plane ABC along the three axes and express the intercepts in terms of multiples of axial lengths (multiples of the fundamentals vectors) i.e.,

$$OA : OB : OC = pa : qb : rc$$

In this case from figure (p = 3, q = 1, and r = 2),

∴ The intercepts are 3a: 1b: 2c



#### Step 2

Find the coefficients of the intercepts i.e., 3, 1, 2

#### Step 3

Find the reciprocal of these numbers  $\frac{1}{p} : \frac{1}{q} : \frac{1}{r}$  i.e.,  $\frac{1}{3} : \frac{1}{1} : \frac{1}{2}$

#### Step 4

Convert these reciprocals into whole numbers by multiplying each and every reciprocal with their least common multiplier (LCM).

$$\text{Since 6 is the LCM in this case, we get } 6 \times \frac{1}{3} \quad 6 \times \frac{1}{1} \quad 6 \times \frac{1}{2}$$

$$\therefore \text{ We have } = 2 \quad 6 \quad 3$$

#### Step 5

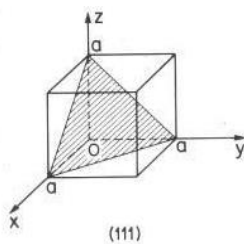
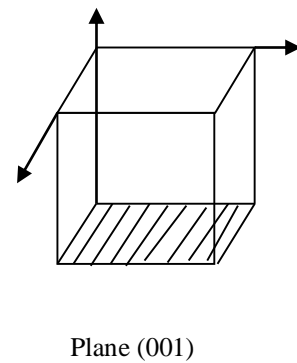
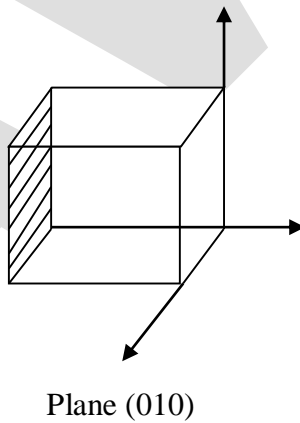
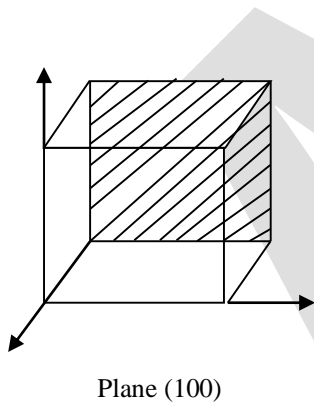
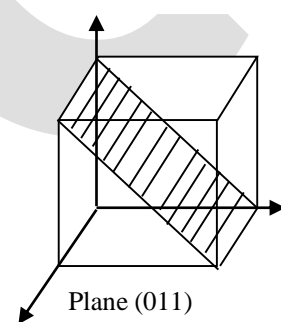
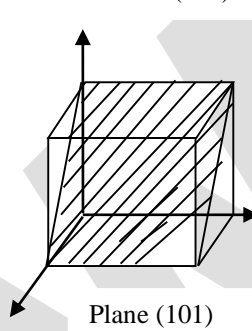
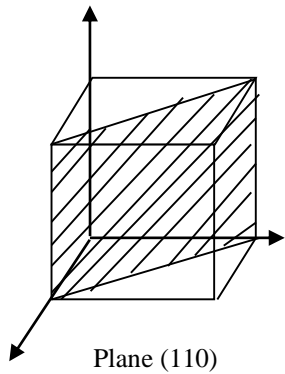
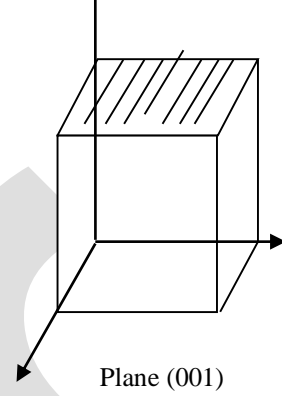
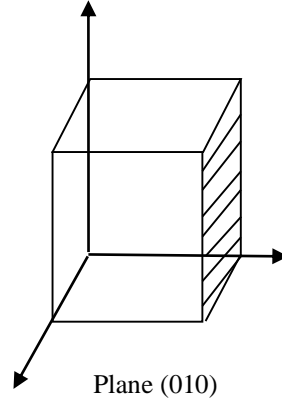
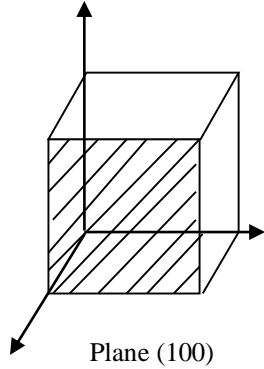
Enclose these numbers in a bracket like this ( ) i.e., (2 6 3). This represents the indices of the given plane and is called the Miller indices of the plane.

Miller indices is generally denoted by (hkl).

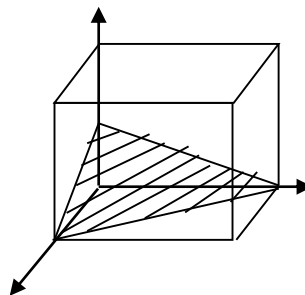
Thus, we can write

$$h:k:l = \frac{a}{p} : \frac{b}{q} : \frac{c}{r} \text{ for any system and } h:k:l = \frac{a}{p} : \frac{a}{q} : \frac{a}{r} \text{ for cubic system.}$$

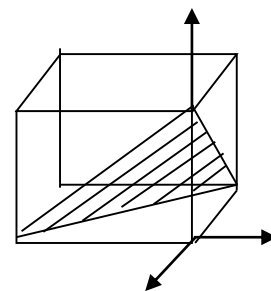
**Important features of the Miller indices: Miller indices for some crystal planes**



Plane(111)



Plane(112)



Plane(111)

- All equally, spaced parallel planes have the same index numbers (hkl)
- A plane parallel to one of the co-ordinate axes has an intercept of infinity.
- If the miller indices of two planes have the same ratio, then the planes are parallel to each other.
- If a normal is drawn to a plane (hkl), the direction of the normal is  $[hkl]$

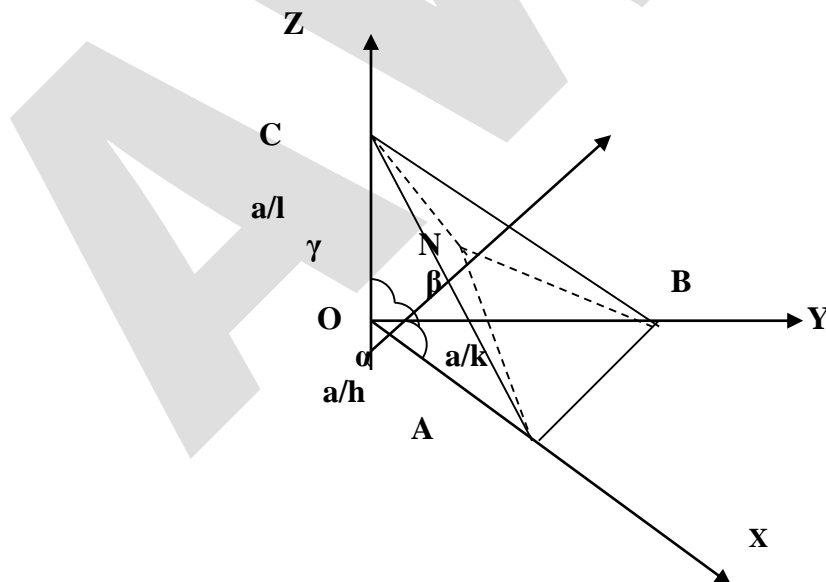
### RELATION BETWEEN THE INTERPLANER SPACING, MILLER INDICES AND THE CUBE EDGE

#### Definition:

'd' spacing (or) interplanar distance is the distance between any two successive planes.

#### 'd' spacing in cubic lattice:

Let us consider the plane ABC. The plane ABC belongs to a family of planes whose Miller indices are (h k l). Let ON = d i.e., the perpendicular distance to the plane from the origin. Let OA, OB, and OC be the intercepts made by the plane on X, Y and Z axis respectively. Let  $\alpha$ ,  $\beta$ ,  $\gamma$  represents the angle between ON and X, Y and Z axis respectively.



Then the intercepts of the plane on the three axes are,

$$OA = \frac{a}{h}; OB = \frac{a}{k}; OC = \frac{a}{l}$$

Where 'a' is the length of the cube edge.

$$\text{From } \triangle \text{ ONA, } \cos \alpha = \frac{ON}{OA} = \frac{d}{a/h} = \frac{dh}{a}$$

$$\text{From } \triangle \text{ ONB, } \cos \beta = \frac{ON}{OB} = \frac{d}{a/k} = \frac{dk}{a}$$

$$\text{From } \triangle \text{ ONC, } \cos \gamma = \frac{ON}{OC} = \frac{d}{a/l} = \frac{dl}{a}$$

From the law of direction cosines,  $\cos^2\alpha + \cos^2\beta + \cos^2\gamma = 1$

$$\therefore \left(\frac{dh}{a}\right)^2 + \left(\frac{dk}{a}\right)^2 + \left(\frac{dl}{a}\right)^2 = 1$$

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

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

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

## **IMPORTANT PARAMETERS IN CRYSTAL STRUCTURE**

About 90% of available metal elements crystallize only into three densely packed crystal structures namely body-centered (BCC), face centered (FCC), and hexagonal close-packed (HCP) structures.

Let us now examine in detail the arrangement of atoms in simple cubic (SC) structure and also in the three (BCC, FCC, and HCP) principal crystal structure unit cells.

### **1. Number of atoms per unit cell (N)**

The number of atoms possessed by a unit cell is known as number of atoms per unit cell. This can be determined if the arrangement of atoms inside the unit cell is known.

### **2. Co-ordination Number (CN)**

Every atom in a crystal structure is surrounded by other atoms. The term coordination number is defined as the number of nearest equidistant neighbours that an atom has in the given structure. When the coordination number is large the structure is closely packed.

### 3. Atomic radius (AR)

Atomic radius is defined as half of the distance between any two nearest neighbor atoms which have direct contact with each other.

### 4. Packing density (or) Atomic packing factor (APF).

It is defined as the ratio of volume of all the atoms in the unit cell to the volume of the unit cell.

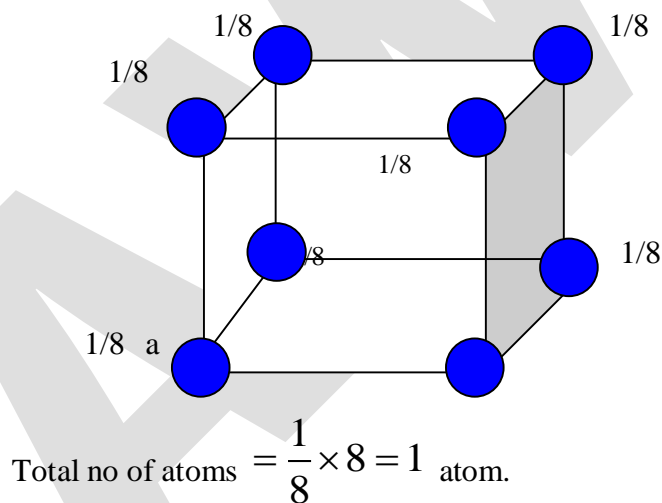
$$\text{Packing Factor} = \frac{\text{Volume of all the atoms in the unit cell}(v)}{\text{Volume of the unit cell}(V)}$$

### Simple Cubic structure (SC):

#### 1. Number of atoms per unit cell:

The diagram shows the unit cell of SC structure. In this structure the atoms are only at the corners of the cube.

To form full crystal structure each corner atom is shared by 8 adjoining unit cells. Hence  $1/8^{\text{th}}$  part of an atom is present in every corner of the cube. Since there are eight corners.



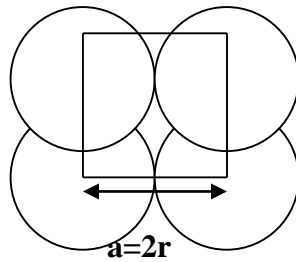
#### 2. Co-ordination Number:

Consider one corner atom in a SC structure. This atom is surrounded by 4 nearest neighboring atoms in the same plane and one vertically above the atom and one exactly below the atom.

Hence the coordination number is  $4 + 1 + 1 = 6$ .

#### 3. Atomic Radius:

Each corner atom touches each other along the edges of the cube. If 'r' is the atomic radius and 'a' is the side of the cube, then from the fig.



$$a = 2r$$

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

#### **4. Packing Factor:**

$$\text{Packing Factor} = \frac{\text{Volume of all the atoms in the unit cell}(v)}{\text{Volume of the unit cell}(V)}$$

$$\text{Packing Factor} = \frac{\text{number of atoms present in a unit cell} \times \text{Volume of one atom}}{\text{Volume of the unit cell}(V)}$$

No. of atoms present in the unit cell (SC) = 1

Volume of unit cell,  $V = a^3$

$$\text{Volume of atoms in the unit cell, } v = \frac{4\pi r^3}{3} \times 1 = \frac{4\pi}{3} \left(\frac{a}{2}\right)^3 = \frac{\pi a^3}{6}$$

$$\begin{aligned} \text{Packing Factor} &= \frac{v}{V} = \frac{4\pi r^3}{3a^3} \\ &= \frac{\pi a^3 / 6}{a^3} = \frac{\pi}{6} = 0.52 \\ &\text{(or) } 52\% \end{aligned}$$

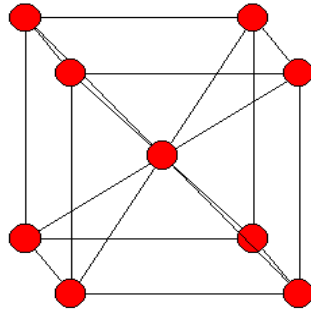
This means that 52% of the space in the unit cell is occupied and the remaining 48% is unoccupied. Therefore, the stability of the crystal forming simple cubic structure is less.

**Example: Polonium**

#### **Body Centred Cubic structure (BCC):**

##### **1.Number of atoms per unit cell:**

The diagram shows the unit cell of BCC structure. In this structure the atoms are at the corners of the cube and there is one atom at the centre of the cube. To form full crystal structure each corner atom is shared by 8 adjoining unit cells. Hence  $1/8^{\text{th}}$  part of an atom is present in every corner of the cube. Therefore,



$$\text{Contribution of corner atoms} = \frac{1}{8} \times 8 = 1 \text{ atom.}$$

$$\text{Contribution of centre atoms} = \frac{1}{2} \times 2 = 1 \text{ atom.}$$

$$\text{Total number of atoms / unit cell} = 1+1 = 2 \text{ atoms.}$$

## 2. Co-ordination Number:

Consider the body centre atom in a BCC structure. This atom is surrounded by the corner atoms only. So the nearest neighbor for a body centre atom is the 8 corner atoms.

Hence the coordination number = 8

## 3. Atomic Radius:

In this structure the unit cell has 8 atoms at the corners of the cube and 1 atom at the centre of the cube. Here the corner atoms do not touch each other, but each corner atom touches the central atom. If 'r' is the atomic radius and 'a' is the side of the cube, then from the fig.

In triangle  $\Delta ADC$ ,

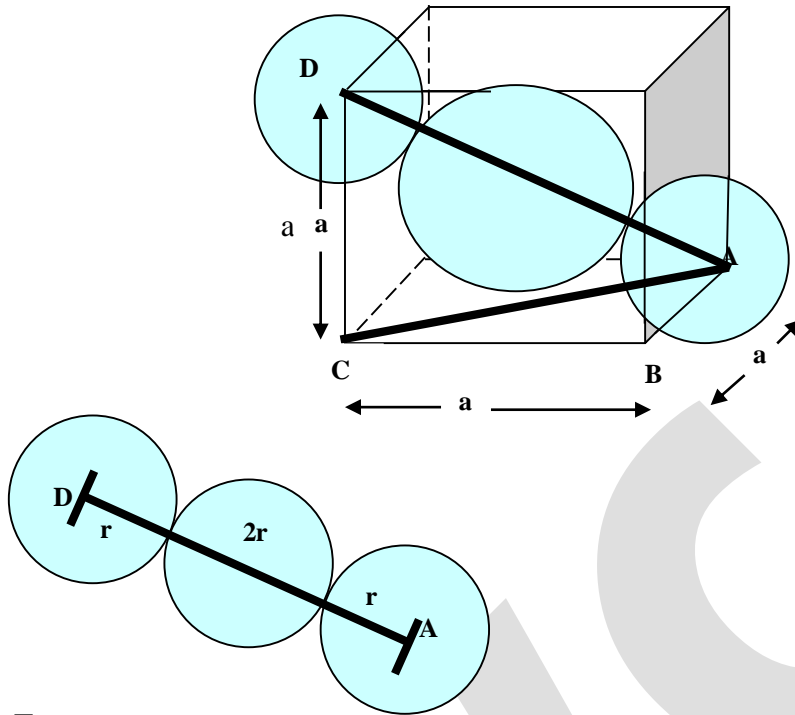
$$\begin{aligned} AD^2 &= AC^2 + DC^2 \\ &= AB^2 + BA^2 + DC^2 \quad (\text{from } \Delta ABC) \end{aligned}$$

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

$$16r^2 = 3a^2$$

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

$$\therefore \text{atomic radius } r = \frac{\sqrt{3}}{4} a$$



#### 4. Packing Factor:

$$\text{Packing Factor} = \frac{\text{Volume of all the atoms in the unit cell}(v)}{\text{Volume of the unit cell}(V)}$$

No. of atoms present in the unit cell (BCC) = 2

$$\text{Volume of one atom} = \frac{4}{3} \pi r^3$$

Volume of unit cell =  $a^3$  (where 'a' is the side of the cube)

$$\text{PF} = \frac{2 \times \frac{4}{3} \pi r^3}{a^3}$$

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

Substitute the value of 'r' in the above equation, we get

$$\text{PF} = \frac{\frac{8}{3} \pi \left( \frac{\sqrt{3}a}{4} \right)^3}{a^3} = \frac{\sqrt{3}}{8} \pi = 0.68$$

In this case 68% of the space is occupied and 32% of the space is unoccupied. The stability of the crystal structure is more than that of the simple cubic structure.

This structure is not a closely packed one.

**Examples: Tungsten, sodium, iron, and chromium.**

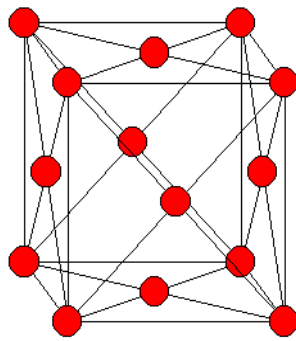


## Face centred cubic structure (FCC):

### 1. Number of atoms per unit cell:

The diagram shows the unit cell of FCC structure. In this structure the atoms are at the corners of the cube and there are six atoms at the face centers of the cube. To form full crystal structure each corner atom is shared by 8 adjoining unit cells. Hence  $1/8^{\text{th}}$  part of an atom is present in every corner of the cube. Along with this each face centered atom is shared by 2 adjoining unit cells. Therefore,

$$\text{Contribution of corner atoms} = \frac{1}{8} \times 8 = 1 \text{ atom.}$$



$$\text{Contribution of face centered atoms} = \frac{1}{2} \times 6 = 3 \text{ atoms.}$$

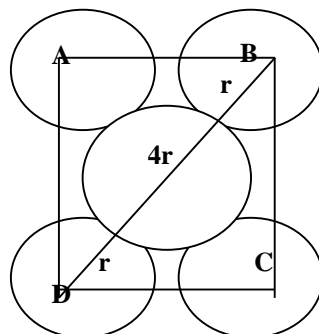
$$\text{Total number of atoms / unit cell} = 1 + 3 = 4 \text{ atoms.}$$

### 2. Co-ordination Number:

In this structure the nearest neighbors of any corner atom are the face centered atoms of the surrounding unit cells. Any corner atom has four such atoms in its own plane, four in the plane above it and four in the plane below it.

$$\text{Hence the coordination number} = 4 + 4 + 4 = 12$$

### 3. Atomic Radius:



$$\text{In } \Delta BCD, \\ BD^2 = BC^2 + DC^2$$

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

$$16r^2 = 2 a^2$$

$$r^2 = \frac{a^2}{8}$$

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

$$(or) \quad a = 2r\sqrt{2}$$

#### 4. Packing Factor:

$$\text{Packing Factor} = \frac{\text{Volume of all the atoms in the unit cell}(v)}{\text{Volume of the unit cell}(V)}$$

$$\text{Volume of the unit cell, } V = a^3 \quad \text{----- (1)}$$

$$\text{Number of atoms in the unit cell} = 4$$

$$\text{Volume of atoms in the unit cell } v = 4 \times \frac{4\pi}{3} r^3$$

$$v = \frac{16\pi}{3} \times \frac{a^3}{(2\sqrt{2})^3}$$

$$v = \frac{16\pi}{3} \times \frac{a^3}{8 \times 2\sqrt{2}}$$

$$v = \frac{\pi a^3}{3\sqrt{2}} \quad \text{----- (2)}$$

$$\therefore \text{Atomic packing factor} = \frac{v}{V} \quad \text{----- (3)}$$

Substitute equation (1) and (2) in equation (3)

$$\text{Atomic packing factor} = \frac{\pi a^3 / 3\sqrt{2}}{a^3} = \frac{\pi}{3\sqrt{2}}$$

$$= 0.74 \text{ (or)}$$

$$= \mathbf{74\%}$$

In this structure, 74% of the unit cell is occupied by the atoms. When compared with simple cube and body centered cube, this has highest packing factor.

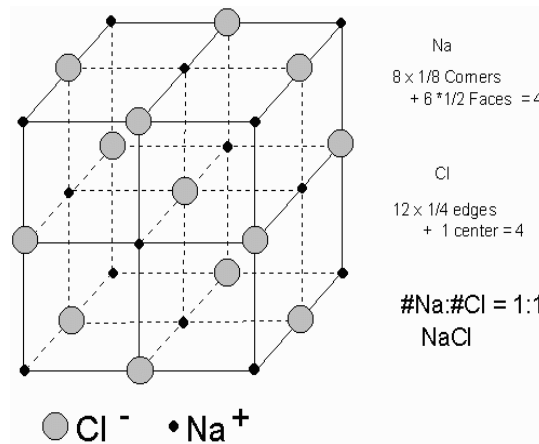
Examples: copper, aluminum, and silver

## OTHER CUBIC STRUCTURES

Although many elements solidify in one of the structures described above, several other elements and components possess combination of the structures discussed below.

### (a) Sodium chloride structure (NaCl):

Sodium chloride is an ionic crystal. It has **FCC structure** with a basis of one  $\text{Na}^+$  ion and one  $\text{Cl}^-$  ion in an alternate fashion. Most of the alkali halides and sulphides exhibit this type of structure.



### Structure Composition:

The  $\text{Cl}^-$  ions are situated at the corners as well as at the centers of the faces of the cube. The  $\text{Na}^+$  ions are situated exactly at the midpoint of the axial length of the unit cell along each axis. Thus, NaCl crystal can be thought to be composed of two FCC sub lattices. One of  $\text{Cl}^-$  ion having the origin of (0, 0, 0) and the other of  $\text{Na}^+$  ion having the origin (1/2, 0, 0).

Let us discuss the important parameters of the NaCl crystal.

### Number of Atoms per Unit Cell:

In this NaCl structure, we have two types of ions namely  $\text{Na}^+$  and  $\text{Cl}^-$ . Let us find the number of sodium ions and chlorine ions separately.

#### **(i) Number of $\text{Na}^+$ ions per unit cell**

Here we have two types of  $\text{Na}^+$  ions, namely,

**(a) Midpoint  $\text{Na}^+$  ions**

**(b) Body centered  $\text{Na}^+$  ion**

(a) Each  $\text{Na}^+$  ion situated at the mid point of the axial length is shared by 4 unit cells. Similarly, we have 12 midpoint  $\text{Na}^+$  ions.

$$\therefore \text{Number of midpoint } \text{Na}^+ \text{ ions per unit cell} = \frac{1}{4} \times 12 = 3 \text{ ions.}$$

(b) Each body centered  $\text{Na}^+$  ion is shared by that particular unit cell alone.

$$\therefore \text{Number of body centered } \text{Na}^+ \text{ ion per unit cell} = \frac{1}{1} \times 1 = 1 \text{ ion.}$$

∴ Total number of  $\text{Na}^+$  ions per unit cell =  $3 + 1 = 4$  ions.

**(ii) Number of  $\text{Cl}^-$  ions per unit cell**

Here, we have two types of  $\text{Cl}^-$  ion namely,

**(a) Corner  $\text{Cl}^-$  ions**

**(b) Face centered  $\text{Cl}^-$  ions**

(a) Each corner  $\text{Cl}^-$  ions is shared by 8 unit cells. Similarly, we have 8 such corner ions.

∴ Number of corner  $\text{Cl}^-$  ions per unit cell =  $\frac{1}{8} \times 8 = 1$  ion.

(b) Each face centered  $\text{Cl}^-$  ions is shared by 2 unit cells. Similarly, we have 6 face centered  $\text{Cl}^-$  ions.

∴ Number of face centered  $\text{Cl}^-$  ions per unit cell =  $\frac{1}{2} \times 6 = 3$  ions.

∴ Total number of  $\text{Cl}^-$  ions per unit cell =  $3 + 1 = 4$  ions.

**Thus, there are 4  $\text{Na}^+$  ions and 4  $\text{Cl}^-$  ions per unit cell in a NaCl crystal.**

**Coordination number:**

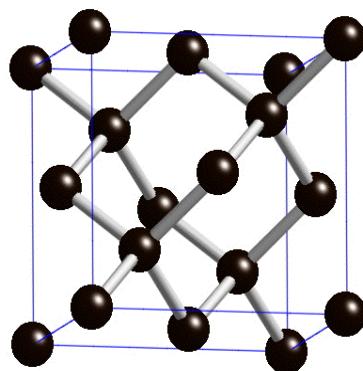
Each  $\text{Cl}^-$  ions has 6  $\text{Na}^+$  ions as nearest neighbors. Similarly, each  $\text{Na}^+$  ion has 6  $\text{Cl}^-$  ions as nearest neighbors. Hence, the coordination number of NAACO for opposite kind of ions is 6.

**Atomic radius:**

The distance between any two nearest neighbors is  $a/2$ .

**Examples: KCl, KBr, CaO, etc.**

**(b) Diamond cubic structure :**



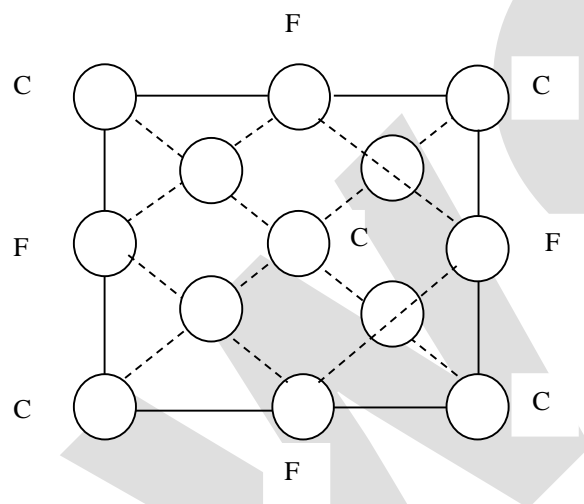
Silicon (Si), Germanium (Ge) Carbon (c) and Tellurium (Te) possess this structure which is a combination of two interpenetrating FCC sub lattices.

As seen from the unit cell of diamond in figure, one sub – lattice has its origin at (0, 0, 0) and the other at a point  $\frac{1}{4}$  of the way along the body diagonal i.e., at  $\left(\frac{a}{4}, \frac{a}{4}, \frac{a}{4}\right)$  point. This structure is loosely packed structure since each atom has only 4 nearest neighbours.

**Number of Atoms per Unit Cell:**

In diamond we have 3 types of atoms viz.,

- (i) Corner atoms, represented by ‘c’
- (ii) Face centered atoms represented by ‘F’
- (iii) Four atoms present inside the unit cell represented as 1, 2, 3, and 4.



**(i) Number of corner atoms per unit cell**

Each corner atom is shared by 8 unit cells. Similarly, we have 8 corners atoms in an unit cell.

$$\therefore \text{Number of corner atoms per unit cell} = \frac{1}{8} \times 8 = 1 \text{ atom.}$$

**(ii) Number of face centered atoms per unit cell**

Each face centered atom is shared by 2 unit cell. Similarly, we have 6 face centered atoms.

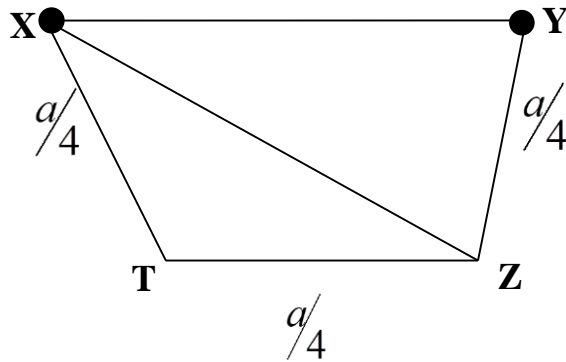
$$\therefore \text{Number of face centered atoms per unit cell} = \frac{1}{2} \times 6 = 3 \text{ atoms.}$$

**(iii) Number of atoms inside the unit cell**

Inside the unit cell we have 4 atoms, represented by 1, 2, 3, 4 which is shared by that particular unit cell alone.

$$\therefore \text{Total number of atoms per unit cell} = 1 + 3 + 4 = 8 \text{ atoms.}$$

**Atomic radius:**



Here, the corner atoms do not have contact with each other and the face centered atoms also do not have contact with the corner atoms. But both the face centered atoms and the corner atoms has contact with the 4 atoms (1, 2, 3, 4) situated inside the unit cell.

In figure, we can see that the nearest two neighbours which has direct contact are atoms 'X' and 'Y'.

Let us draw perpendicular to the Y atom, which meets the unit cell at a point 'Z' as shown in figure, which is at a distance of  $a/4$ .

From the diagram,

$$\begin{aligned}
 (XY)^2 &= (XZ)^2 + (ZY)^2 \\
 &= \left[ (XT)^2 + (TZ)^2 \right] + (ZY)^2 \\
 &= \left( \frac{a}{4} \right)^2 + \left( \frac{a}{4} \right)^2 + \left( \frac{a}{4} \right)^2 \\
 &= \frac{a^2}{16} + \frac{a^2}{16} + \frac{a^2}{16} \\
 \therefore (XY)^2 &= \frac{3a^2}{16}
 \end{aligned}$$

Since  $XY = 2r$ ,

We can write,

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

$$4r^2 = \frac{3a^2}{16}$$

$$r^2 = \frac{3a^2}{64}$$

$\therefore$  Atomic radius

$$r = \frac{a\sqrt{3}}{8}$$

$\therefore$  The lattice constant

$$a = \frac{8r}{\sqrt{3}}$$

**Coordination number:**

From the figure the number of nearest atoms for Y atom is 4. Therefore, the **coordination number of diamond is 4.**

**Atomic Packing factor:**

$$\text{Packing Factor (APF)} = \frac{\text{Volume occupied by the atoms per unit cell (v)}}{\text{Volume of the unit cell (V)}} \text{----- (1)}$$

$$\text{Volume occupied by 1 atom (spherical)} = \frac{4}{3} \pi r^3$$

In diamond we have 8 atoms per unit cell

$$\text{Therefore volume occupied by all the 8 atoms per unit cell (v)} = 8 \times \frac{4}{3} \pi r^3$$

$$\text{We know atomic radius for diamond structure } r = \frac{a\sqrt{3}}{8}$$

$$\therefore \text{Volume occupied by the atoms per unit cell (v)} = 8 \times \frac{4}{3} \pi \frac{a^3 3\sqrt{3}}{8^3}$$

$$v = \frac{\pi a^3 \sqrt{3}}{16} \text{----- (2)}$$

$$\text{Since diamond has cubic structure, the volume of the unit cell (v)} = a^3 \text{----- (3)}$$

Substituting equations (2) and (3) in (1) we get,

$$(APF) = \frac{\pi a^3 \sqrt{3}}{16a^3}$$

$$\therefore APF = \frac{\pi \sqrt{3}}{16}$$

$$\text{Atomic packing factor} = 0.34$$

$$\text{Packing density} = 34 \%$$

Thus it is a loosely packed structure.

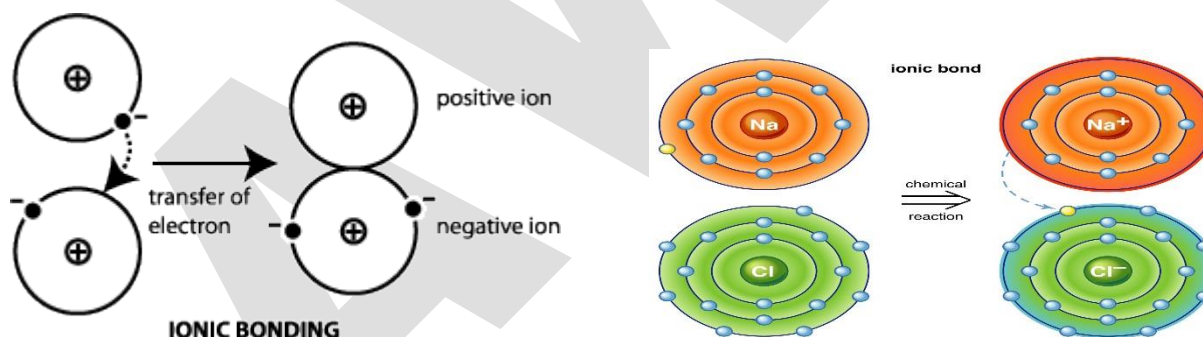
Thus we can say that 34% volume of the unit cell in diamond cubic structure is occupied by atoms and the remaining 66% volume is vacant.

## Distinguish between Ionic bonds and Covalent bonds.

S. No.	Ionic bonds	Covalent bonds
1.	Ionic solids are formed when the atoms of two different elements transfer the electrons among them to become positive and negative ions.	Covalent solids are formed between the atoms of same elements by sharing of electrons between them.
2.	The bonds are non-directional.	The bonds are directional
3.	The bonds are relatively stronger	The bonds are relatively weaker
4.	possess high melting point and high boiling point	Comparatively lower melting point and low boiling
5.	Soluble in polar solvents	Soluble in nonpolar solvents
6.	Not very hard	Very hard
7.	Examples: NaCl, KBr, Al <sub>2</sub> O <sub>3</sub>	Examples: Diamond.

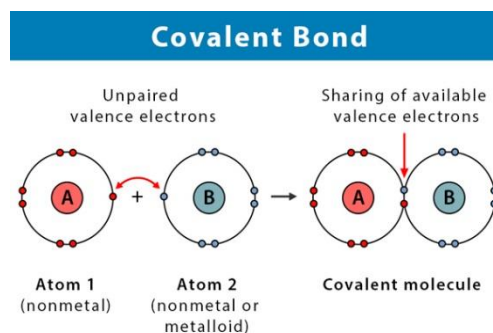
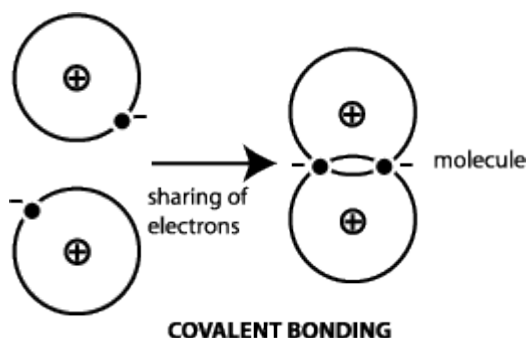
## Ionic bonding

An ionic bond is formed when valence electrons are transferred from one atom to the other to complete the outer electron shell.



## Covalent bonding

A covalent bond is formed when the valence electrons from one atom are shared between two or more particular atoms





**AWNC**