

5.8.a) CRYSTAL IMPERFECTIONS

In ideal crystal (perfect crystal) the atomic arrangement is perfectly regular and continuous thought.

But in real crystal due to some reasons the regular orientation of atoms may be disturbed at a point, along a line or in a region.

Definition

The disturbance occurred in the regular orientation of atoms is called crystal defect of imperfections.

Some properties of crystal defects are structure sensitive i.e., properties such as mechanical strength, ductility, crystal growth, magnetic hysteresis, dielectric strength are greatly affected by relatively minor changes in crystal structure caused by imperfections.

Some other properties of crystals are structure-insensitive i.e. properties such as stiffness and density are not affected by the presence of imperfections.

Classification of crystal imperfections (or) Defects

Crystalline imperfections are classified on the basis of their geometry as follows.

1. Point Defects

- (a) Vacancies
- (b) Interstitials
- (c) Impurities

2. Line Defects

- (a) Edge dislocations
- (b) Screw dislocations

3. Surface Defects

- (a) Grain boundaries

- (b) Tilt boundaries
- (c) Twin boundaries
- (d) Stackingfaults

4. Volume Defects

- (a) Cracks

1. Point Defects

Point defects are crystalline irregularities of atomic dimensions. They are imperfect points like regions in crystal. One or two atomic diameter is the typical size of point imperfection.

Point defect takes place due to imperfect packing of atoms during crystallisation.

They produced distortion in side the crystal structure.

Types of Point Defects

- (a) Vacancies

- (b) Intersititials

- (c) Impurities

(a) Vacancy

In crystallography, a vacancy is simplest a type of point defect in a crystal. A defect in which an atom is missing from one of the lattice sites is known as a "vacancy" defect.

Whenever one or more atoms are missing from a normally occupied position as shown in figure, the defect caused is known as vacancy.

The atoms surrounding the vacancies are displaced inward thereby distorting the regularity of arrangement. There are different kinds of vacancies like Frenkel defect, Schottky defect, Colour centre, etc.

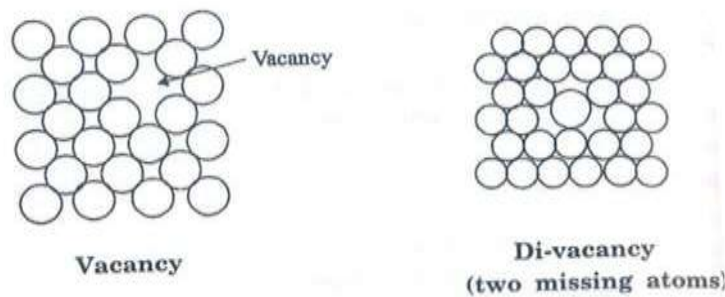


Fig:5.8.1 Vacancy

(i) **Schottky Defect**

It refers to the missing of pair of positive and negative ions in an ionic crystal.

A neutral defect that involves paired vacancies on the cation and anion sub lattices is called a **Schottky defect**.

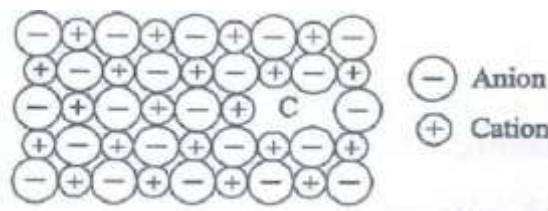


Fig 5.8.2 Schottky Defect

(ii) **Frankel Defects**

A vacancy associated with interstitial impurity is called Frenkel defect.

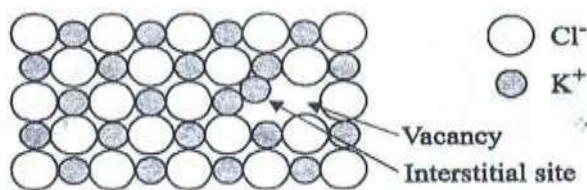


Fig 5.8.3 Frankel Defects

Here a missing atoms occupies interstitial position .This defect always occurs in ionic crystal, If a positive ion moves into an interstitial site in an ionic crystal, a cation vacancy is created in normal site, this *vacancy- interstitial* pair is known as **Frenkel defect**.

(b) Interstitial Defect

When an extra atoms occupies interstitial space with in the crystal structure without removing parent atom,the defect is called interstitial defect.

Types of interstitial defect

(i) Self-interstitial

(ii) Foreign interstitial

(i) Self-interstitial

If an atom from same crystal occupies interstitial site,then it is called self-interstitial.

(ii) Foreign interstitial

If impurity atom(foreign atom) occupies the interstitial position without replacing the parent atom, it is called foreign interstitial.

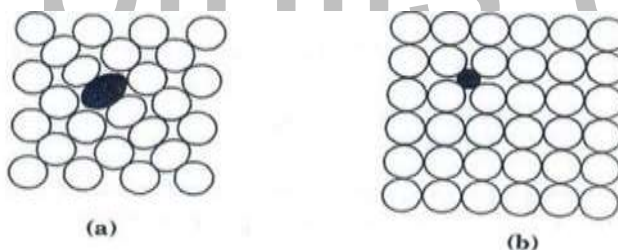


Fig 5.8.4 Foreign interstitial

- These can exist only ionic and covalent crystals.
- Here the impurity atom has very small size as that of the host atoms.

(c) Impurities

When the foreign atoms(impurities) are added to crystal lattices,they are known as impurities.The defect is called impurity defect.

The impurity atoms may fit in the structure in two ways giving rise to two kinds of impurities defects. They are

- (i) Substitutional impurity defect
 - (ii) Interstitial impurity defect
- (i) **Substitutional Impurities**

A substitutional impurity refers to a foreign atom that replaces a parent atom in the Lattice.

Substitutional impurities changes the electrical properties enormously.

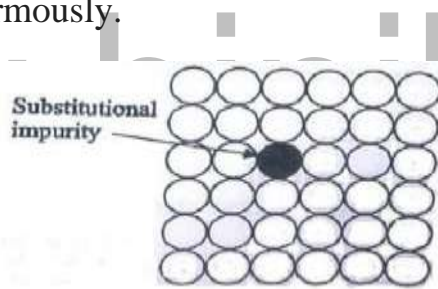


Fig 5.8.5- Substitutional impurities

Example

1. n-type and p-type semiconductor have substitutional impurities from Vth group and IIIrd group elements. This is used to producing many electronic devices like diode and transistors.
2. During the production of brass alloy, zinc atoms are doped in copper lattice. Here zinc atoms are called as substitutional impurities.

ii) Interstitial impurity defect



Fig 5.8.6- Interstitial impurity defect

An interstitial impurity is a small size atom occupying the empty space(interstitial) in the parent crystal, without dislodging any of the parent atoms from their sites.

An atom can enter into interstitial or empty space only when it is substantially smaller than parent atom.

Example

In FCC iron, the atomic radius of iron atom is 0.225nm. The carbon atoms with atomic radius 0.078nm can occupy empty space in FCC lattice as interstitial impurities.

5.1. Line defect or dislocation: (one dimensional Effect)

This defect due to dislocation or distortion of atoms along a line are known as

line defects.

In line defect, a portion of line of atoms is missing or displaced from its regular site.

Types of line defects

There are two types of line defects

(a) Edge dislocation and

(b) Screw dislocations

(a) Edge Dislocation

An edge dislocation arises when one of the atomic planes forms only partially and does not extend through the entire crystal.

The atomic plane AB abruptly terminates at B. It is viewed as an extra plane inserted in between a set of parallel planes.

The edge of such a plane forms a line defect and it is called an edge dislocation.

The atomic row 1 passing through point B has one atom more than row 2 adjacent to it.

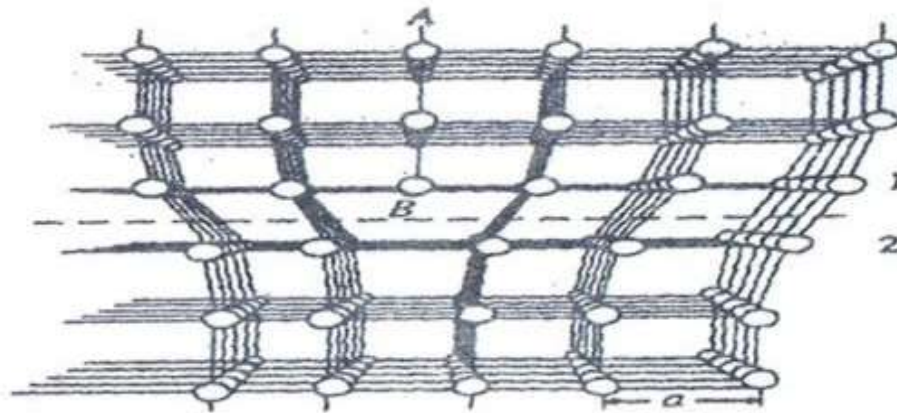


Fig 5.8.7- Edge Dislocation

Classification of edge dislocation

Edge dislocations are symbolically represented by or depending on whether the incomplete plane starts from top or bottom of the crystal.

There are two configurations are referred as

- (i) Positive edge dislocation
- (ii) Negative edge dislocations

(i) Positive edge dislocation

If the extra plane of atoms is above the slip plane of the crystal than the edge dislocation is called positive as shown in figure. It is denoted by the symbol \perp .

(ii) Negative edge dislocations

If the extra plane of atoms is below the slip plane than the edge dislocation is called negative. It is denoted by the symbol \top .

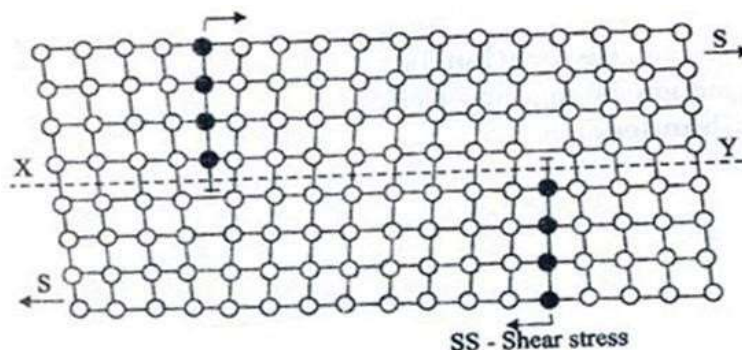


Fig 5.8.8- Negative edge dislocations

(iii) Screw dislocations

Screw dislocation is due to a displacement of atoms in one part of a crystal relative to rest of the crystal.

The displacement terminates within crystal. This dislocation forms a spiral ramp around dislocation line.

In screw dislocation, the realignment of atoms about which crystal planes are warped to give an effect similar to threads of screw.

The row of atoms marking the termination of the displacement is the screw dislocation. EF indicates the dislocation line

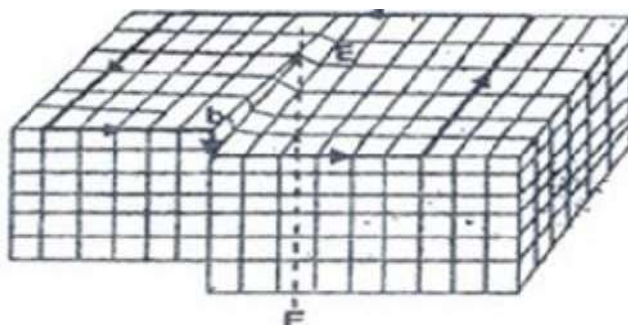


Fig 5.8.9- Screw dislocations

The term screw represents that one part of the crystal is moving in spiral

manner about dislocation line.

BURGER'S VECTORS

The dislocation lines are expressed by a burger vector. It indicates the amount and direction of shift in lattice on slip plane. The figure shows a perfect crystal and crystal with a positive edge dislocation.

Consider a point starting from p in figure (b) which moves in particular direction as shown and it completes atomic distance in the form of a circuit called Burger circuit or burger loop.

If the same circuit is drawn starting from pin figure. Then the circuit would not complete, this is because of the presence of a dislocation.

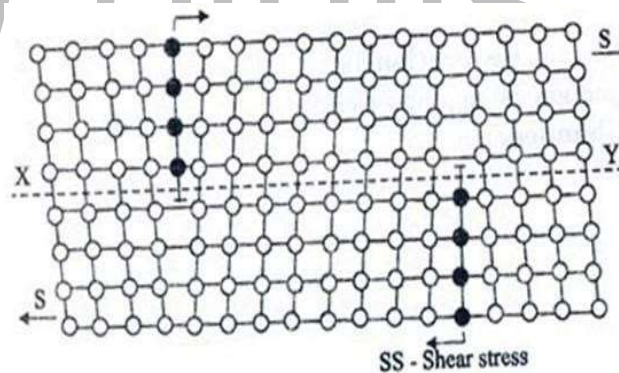


Fig 5.8.9- Burger's vectors

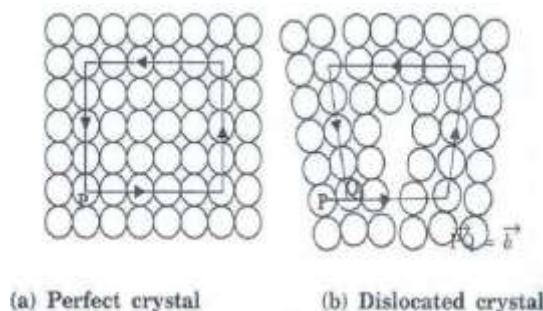


Fig 5.8.10 –a)Perfect Crystal and b)Dislocated Crystal

If we wish to arrive at starting point p from Q, then we must move an extra distance as shown in figure. The vector $b+PQ$ connects end point with starting point. This is Burger's vector of the dislocation.

SURFACE DEFECTS(PLANE DEFECTS)

The defects on the surface of material are called as surface defect or plane defects.

They are also known as two dimensional imperfections.

Surface defects are due to a change in the stacking of atomic planes on or across a boundary. Some important internal surface defects.

- (i) Grain boundaries
- (ii) Tilt and twist boundaries
- (iii) Twin boundaries
- (iv) Stacking fault
- (v) Grain boundaries

(i) Grain boundaries

Whenever the grains of different orientations separate the general pattern of atoms and exhibits a boundary the defect caused is called grain boundary.

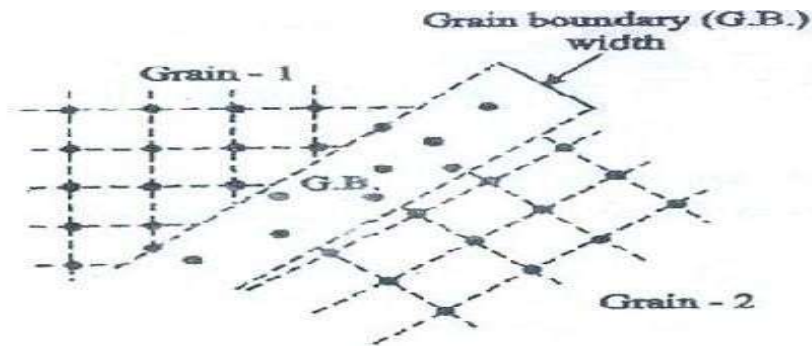


Fig 5.8.11- Grain boundaries

A grain boundary is formed when two growing grain surface meet. The shape of the grains is usually influenced by the presence of surrounding grains.

(i) **Tilt and twist boundaries**

Tilt boundary is another surface imperfection. It is an array of parallel edge dislocations of same sign (i.e. either) arranged one above other in an array or series.

Tilt boundary is a type of low angle boundary (less than 10°)

By rotation of an axis in the boundary, it is possible to bring the axis of two bordering grains into coincidence, then

$$\text{Angle of tilt, } \tan \theta = \frac{b}{D}$$

D - dislocation spacing

b - length of Burger's vector

When angle very small, then $\tan \theta = \theta$,

$$\theta = \frac{b}{D}$$

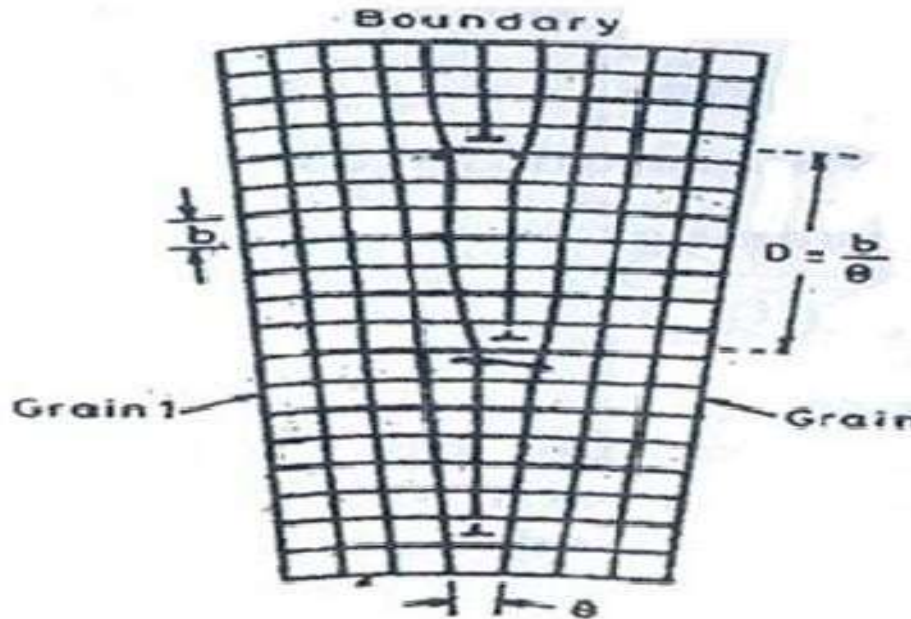


Fig 5.8.12- Tilt and twist boundaries

Twist boundaries

Twist boundaries are another type of low angle boundaries. It consists of at least two sets of parallel screw dislocations lying in the boundary. In two boundaries, the rotation is about an axis normal to the boundary.

(ii) Twin boundaries

Twin boundaries are another surface imperfections

If the boundary in which the atomic arrangement on one side of the boundary is somewhat a mirror image of the arrangement of atoms of the other side. This defect caused is called twin boundary.

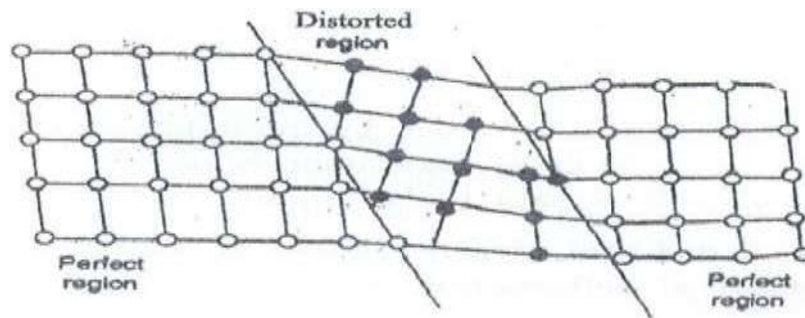


Fig 5.8.13- Twin boundaries

STACKING FAULTS

It is the kind of surface imperfection. Whenever the stacking of atoms is not in proper sequence though the crystal, defect caused is called stacking effect.

Explanation

Figure shows that the proper sequences of atomic plans if we read from bottom to top A-B-C-A-B-C-A-B-C.

But figure(b) shows the sequence of atomic planes as A-B-C-A-B-A-B-A-B-C

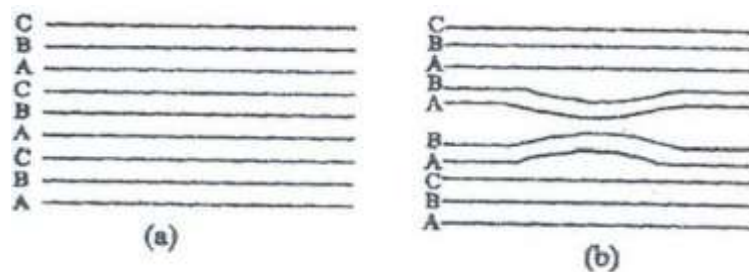


Fig:5.8.14 - stacking faults

The region in which the stacking fault occurs (A-B-A-B) forms a thin region of hexagonal close packing in FCC crystal.

5.8-b)ROLE OF IMPERFECTION IN PLASTIC DEFORMATION

Dislocation sand plastic deformation

Suppose a crystal is deformed by the application of stresses. Now it returns to its original state upon removal of the stresses, then the deformation is said to be elastic.

However, it does not return to its original state, i.e., retains a certain amount of deformation is said to be elastic.

It is generally believed that in most of the crystals the plastic deformation results from the slip of one part of the crystal relative to another.

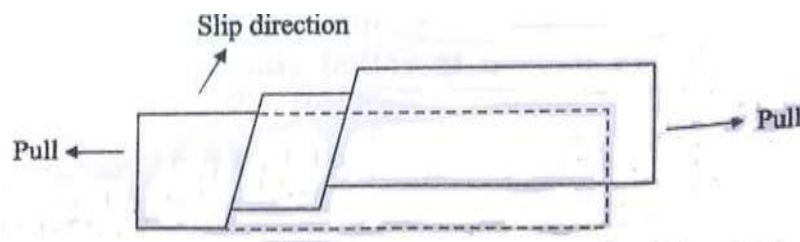


Fig:5.8.14 - Dislocation

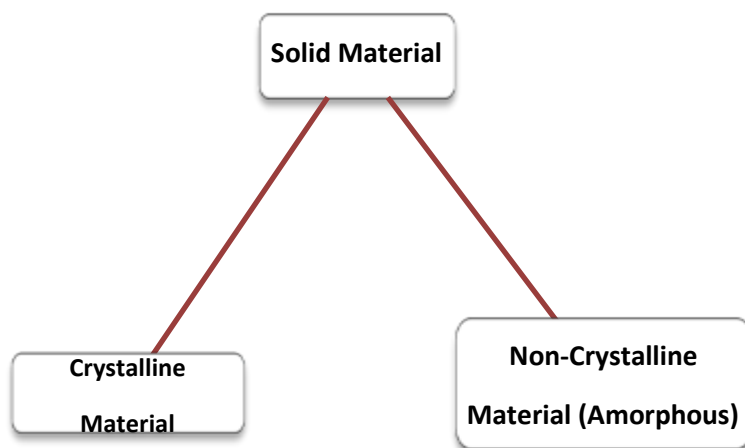
If we confine ourselves with the plastic deformation which is composed of an increase in length only, then the figure is used to explain how such a process may lead to an increase in length of a crystal under the influence of tension.

Since slip is caused by the presence of dislocation, connections between plastic deformation and dislocations must obviously exist.

5.1 CRYSTAL PHYSICS

Introduction

Many of the properties of solid materials depend mainly on their crystal structures. Based on the arrangement of atoms and molecules, the solid material classified as follows



Crystalline Material

The periodic arrangement of atoms in all three dimensions space is called crystal.

It has regular shape and when it is broken, all broken pieces have the same regular shape. It has sharp melting point. The physical properties of the crystal vary with direction and therefore they are called *anisotropic* substances. It may be made up of metallic crystals or non-metallic crystals.

Examples: Cu, Al, W, Mg, Carbon, crystalized polymer and plastics.

Non-Crystalline Material

Random arrangement of atoms in all three dimensions space is called non-crystalline material or amorphous. They have no directional properties and therefore they are called *isotropic* substances. They do not possess any regular shape and they have a wide range of melting points.

Examples: Glass and Rubber.

Fundamental Definitions

Space Lattice

A regular and periodic arrangement of infinite number of points in three dimensions space is known as space lattice. Every point in this arrangement is identical to that of every other point.

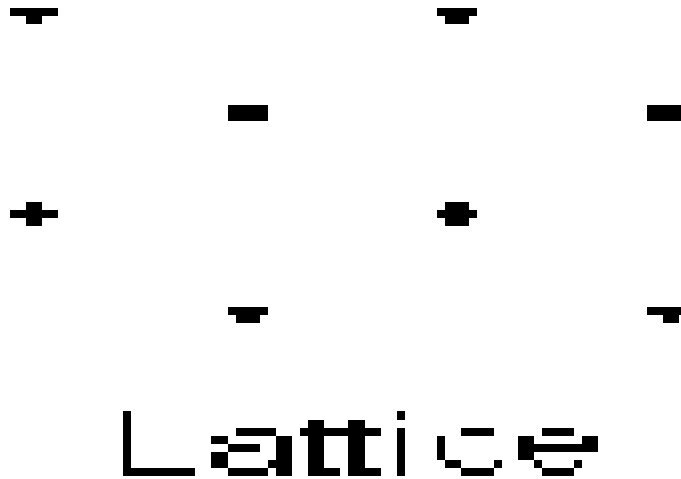


Fig: 5.1.1 Lattice

Basis (Motif)

A group of atoms in every lattice point is called basis or motif.



Fig: 5.1.2 - Basis

Crystal

A crystal is defined as regular and periodic arrangements of atoms or molecule in three dimensional spaces.

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

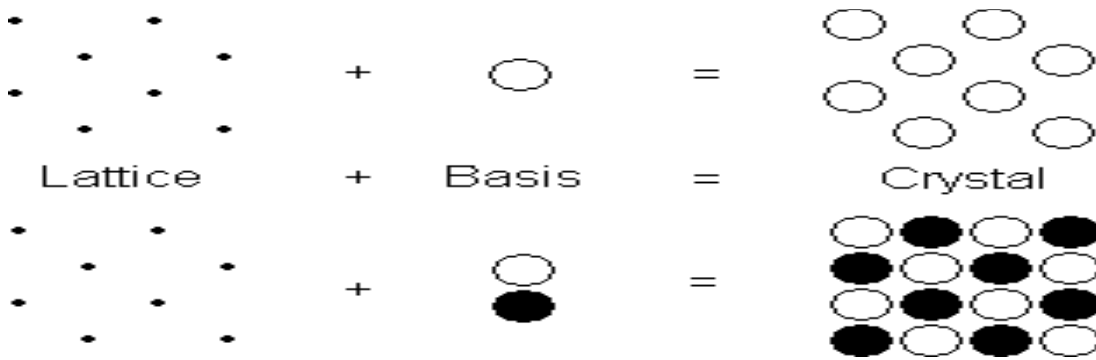


Fig: 5.1.3 – Crystal Structure

It can be classified into two types. They are,

1. Single Crystal
2. Polycrystalline Material

1. Single Crystal

The entire crystalline material consists of only one crystal is known as single crystal.

Example: KDP, ADP.

2. Polycrystalline Material

A collection of many small crystals are separated by well-defined boundaries is called polycrystalline materials.

Example: GaP, GaAs, ZnO and ZnS.

Fundamental translation vector

Mathematical representation of position vector in the space lattice is called fundamental translation vector.

In two dimension $R = n_1a + n_2b$

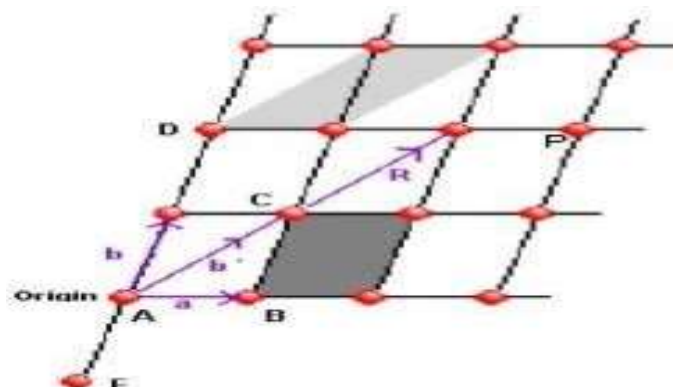


Fig: 5.1.4 –Lattice

In three dimension $R = n_1a + n_2b + n_3c$

Where, a , b and c are the fundamental translation vectors and n_1 , n_2 and n_3 are the integers.

Interfacial angle

The angles between the three crystallographic axes are known as interfacial angles.

Generally it's are represented as α , β and γ respectively.

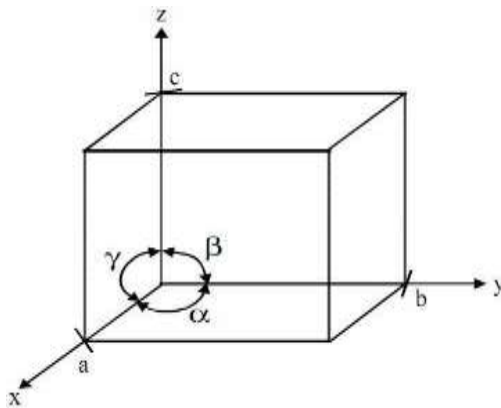


Fig :5.1.5- Interfacial angle α , β and γ

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5.6 DIAMOND CUBIC STRUCTURE

Diamond is one of the allotropic forms of carbon. In diamond, carbon atoms are arranged tetrahedrally. Each carbon is attached to four other carbon atoms 1.544 Å away with a C-C-C bond angle of 109.5° . Diamond structure is formed due to the combination of two interpenetrating FCC sublattices having the origin (000) and $(\frac{a}{4}, \frac{a}{4}, \frac{a}{4})$ along the body diagonal.

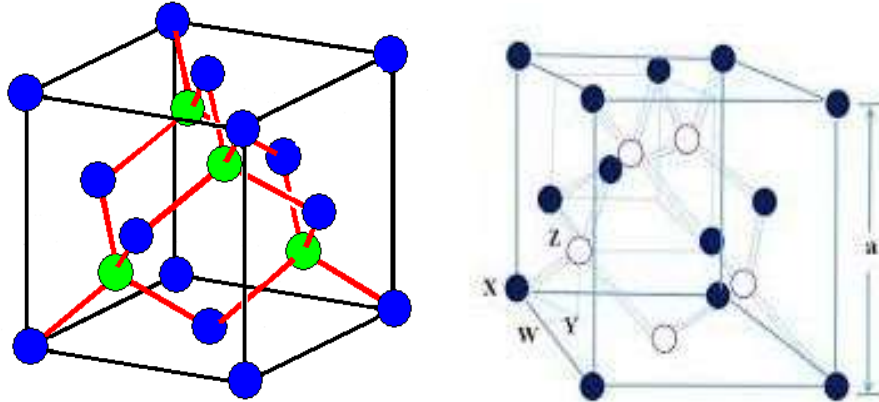


Figure:5.6.1- Diamond structure.

NUMBER OF ATOMS PER UNIT CELL

Number of atoms per unit cell in diamond carbon atoms is present at three different positions of the unit cell.

- The corner atoms represented by 'C'. There are corner atoms in the unit cell. Each corner atom is shared by 8 unit cells. The total number of corner atoms per unit cell $= 8 \times \frac{1}{8} = 1$ atom

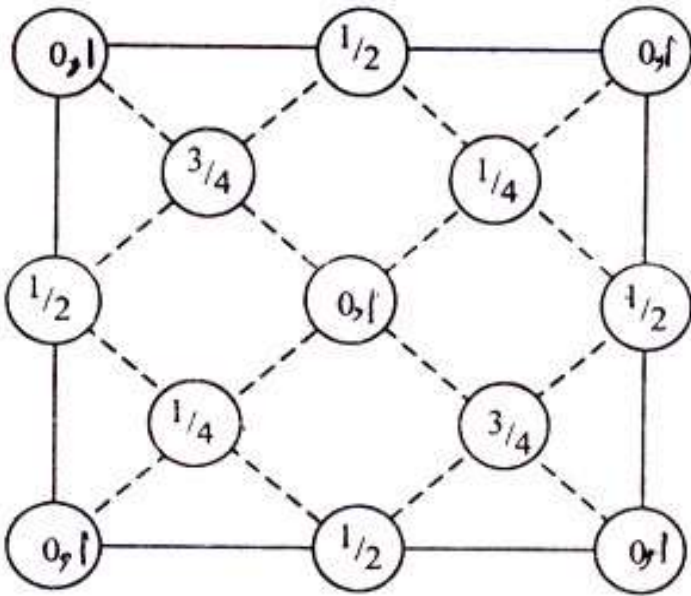


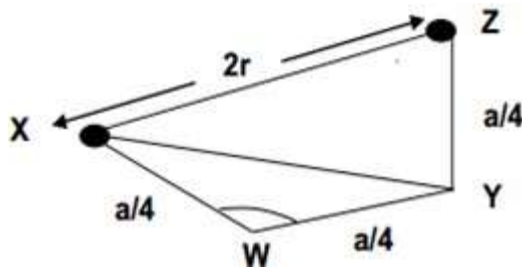
Figure:5.6.2- Diamond structure.

- Face centered atoms represented by 'F'. There are 6 face centered atoms. Each face centered atom is shared by 2 unit cells. Number of face centered atoms per unit cell = $6 \times \frac{1}{2} = 3$ atoms
- Number of atoms present inside the unit cell = 4 atoms

Total number of atoms per unit cell = $1 + 3 + 4 = 8$ atoms

Atomic Radius (R)

The corner atoms and face centered atoms don't touch each other. But both the corner atoms and face centered atoms have direct contact with the 4 atoms present inside the unit cell.



From fig,

$$XZ^2 = XW^2 + WZ^2$$

$$XZ^2 = XW^2 + WY^2 + YZ^2$$

$$(2r)^2 = \left(\frac{a}{4}\right)^2 + \left(\frac{a}{4}\right)^2 + \left(\frac{a}{4}\right)^2$$

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

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

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

CO-ORDINATION NUMBER

The co-ordination number is the nearest neighboring atom to a particular atom. The four atoms present inside the unit cell are the nearest neighbors for the corner atom.

The co-ordination number =4

ATOMIC PACKING FACTOR

$$\text{Atomic Packing Factor (APF)} = \frac{u \dots\dots\dots}{v} \quad (1)$$

Where,

u = Total number of atoms per unit cell X volume of one atom

v = Total volume of the unit cell
Volume of an atom (spherical) is $= \frac{4}{3} \pi r^3$ In diamond, we have 8 atoms per unit cell

We know that the atomic radius of diamond structure is

$$\therefore r = \frac{a\sqrt{3}}{8} \dots\dots\dots(2)$$

Volume occupied by the total number of atoms per unit cell is

$$= 8 \times \frac{4\pi r^3}{3} \dots\dots\dots (3)$$

since diamond has cubic structure, the volume of the unit cell is

$$v = a^3 \dots\dots\dots(4)$$

Substitute equation (3) and (4) in equation (1) we get,

$$APF = \frac{8 \times \frac{4}{3} \pi r^3}{a^3}$$

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

$$\frac{8 \times 4 \times \frac{\pi \left[\frac{\sqrt{3}a}{8} \right]^3}{3}}{a^3} = \frac{\pi \sqrt{3}}{16} = 0.34$$

$$APF = 34\%$$

The APF is 34%. Since the packing density is very low, it is a loosely packed structure.

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5.4 Face Centred Cubic Structure (FCC)

A face centred cubic (FCC) structure unit cell consists of eight corner atoms and six face centred atoms. A face centred cubic unit cell is shown in given figure.

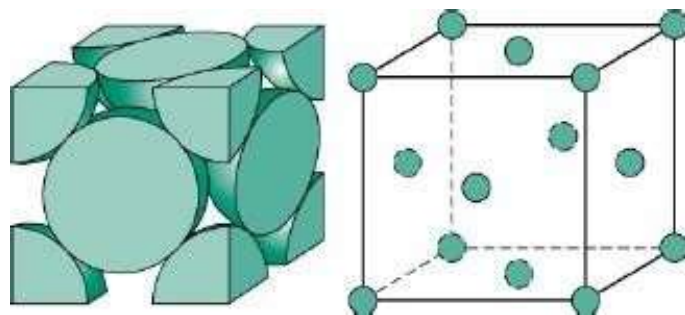


Fig 5.4.1- Face Centred Cubic Structure

Number of atoms per unit cell

Each and every corner atom is shared by eight adjacent unit cells. Therefore, each and every corner atom contributes $\frac{1}{8}$ of its part to unit cell.

Hence, the total number of atoms contributed by the corner atom is $= \frac{1}{8} \times (\text{total number of corner atoms})$

$$= \frac{1}{8} \times 8$$

Each and every face centred atom is shared by two unit cells. Therefore, a face centred atom contributes half of its part to one unit cell.

Hence,

the total number of atoms contributed by the face centred atom is $= \frac{1}{2} \times 6$

Total number of atoms per unit cell in FCC is $= 1 + 3$

$$= 4$$

Atomic Radius

In FCC structure, the corner atoms do not touch each other. But each corner atom touches the face centred atoms along the diagonal of the face of the cube as shown in figure

Therefore, the two corner atoms (A and C) situated at the opposite ends of the same face can be joined by drawing a diagonal as shown in above figure.

From the geometry of the figure, we can write

$$\begin{aligned} (AC)^2 &= (AB)^2 + (BC)^2 \\ &= a^2 + a^2 \end{aligned}$$

–

$$(AC)^2 = 2a^2$$

$$AC = a\sqrt{2}$$

But from figure, the diagonal of the cube is

$$AC = 4r \dots \dots \dots (2)$$

From equation (1) and (2) we can write

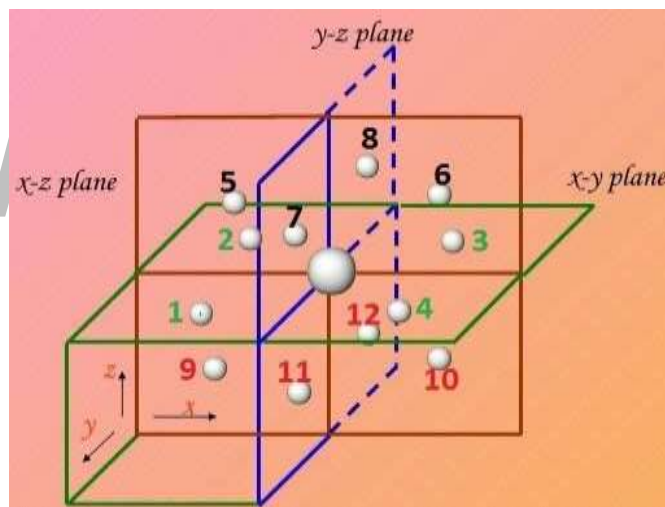
$$4r = a\sqrt{2}$$

$$\text{Atomic radius } r = \frac{a\sqrt{2}}{4}$$

Co-Ordination Number

In this system, there are eight corner atoms, and six face centred atoms, one at the centre of each face. To calculate the coordination number, for FCC, let us consider a corner atom (X) as shown in figure.

Fig 5.4.2-planes to find cocodination number



In its own plane it has four face centred atoms (1, 2, 3 and 4) as nearest neighbours. In a plane which lies just above this corner atom, it has four more face centred atoms (5, 6, 7 and 8) as nearest neighbours. And, similarly in a plane which lies just below this corner atom it has four more face centred atoms, (9, 10, 11 and 12) as nearest neighbours. The total number of nearest atoms to any corner atom is $4+4+4=12$. Hence, *the coordination number is 12.*

Packing factor

$$APF = \frac{u}{v} \dots \dots \dots (1)$$

Where

u = Total number of atoms per unit cell X volume of one atom

v = Total volume of the unit cell

The number of atoms per unit cell = 4

Volume of one atom (spherical) is $= \frac{4}{3}\pi r^3$ (2)

We know that, the atomic radius of FCC is $r = \frac{a\sqrt{2}}{4}$ (4)

Volume occupied by the atoms per unit cell is $u = 4 \times \frac{4}{3}\pi r^3$

Volume occupied by the atoms per unit cell is $u = 4 \times \frac{4}{3}\pi \left(\frac{a\sqrt{2}}{4}\right)^3$

Substitute equation (3) in (4) we get,

$$u = \frac{\pi a^3\sqrt{2}}{6}$$

Volume of the unit cell for a cubic system is $v = a^3$

Substitute equation (5) and (6) in equation (1) we get,

$$\text{Atomic packing factor (APF)} = \frac{\frac{\pi a^3\sqrt{2}}{6}}{a^3}$$

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

$$\text{APF} = 0.74 \text{ (7)}$$

Therefore, we can say that 74% volume of the unit cell of FCC is occupied by atoms and remaining 26% volume is vacant. Thus, the packing density is 74%. Since the packing density is very high, the FCC structure has closely or tightly packed structure.

Unit V-Crystal Physics

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5.7. Miller Indices

5.7.1. Procedure for finding Miller indices

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5.7.3. Interplanar distance (or) 'd' spacing in cubic lattice

5.7. Miller Indices

Miller indices are a symbolic vector representation for the orientation of an atomic plane in a crystal lattice. It is defined as the reciprocal of the fractional intercepts which the plane makes with the crystallographic axes.

5.7.1. Procedure for finding Miller indices

1. Find the intercepts of the plane along the co-ordinate axes X, Y and Z.
2. Take reciprocal of these intercepts.
3. Reduce the reciprocals into whole numbers using least common multipliers (LCM).
4. Write these integers within parentheses to get Miller indices.

For example, consider a crystal plane as shown in given figure

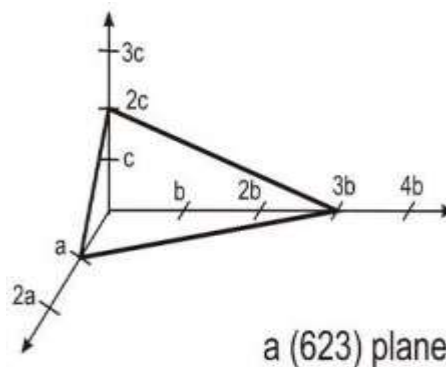


Fig 5.7.1. Plane ABC

1. Intercepts are 1, 3, 2.

2. Reciprocal of these intercepts are $\frac{1}{1}, \frac{1}{3}, \frac{1}{2}$

3. LCM of denominators 1, 3, and 2. Hence, multiplying by 6, we have $\frac{6}{1}, \frac{6}{3}, \frac{6}{2}$. The Miller indices of this plane is (6 2 3).

5.7.2. Features of Miller Indices

1. Plane passing through the origin has non zero intercepts.

2. All equally spaced parallel planes have same Miller indices.

3. Miller indices do not define a particular plane, but it defines a set of parallel planes.

4. If the plane is parallel to any one of the coordinate axes, then its intercepts will be at infinity.

Therefore, the miller index of that particular axis is zero.

5. If a plane cuts the axis on the negative side, then the corresponding Miller indices will be negative.

Some common Planes

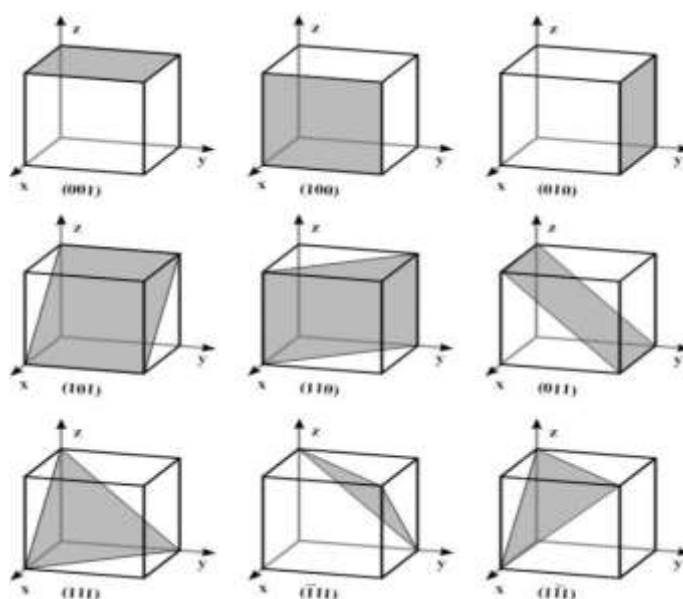


Fig 5.7.2. Different planes of a crystal

5.7.3. Interplanar distance (or) 'd' spacing in cubic lattice

Definition: The distance between any two successive planes is called d spacing or interplanar distance.

Let us consider a cubic lattice of length „a” with two planes ABC and A' B' C'. Let d1 and d2 be the distance between the origin and the first (ABC) and second plane (A' B' C'). Let d be the distance between the two planes ABC and A' B' C'

Let us assume that the second plane lies in the origin. So we can find the distance between the origin and first plane instead of finding the distance between the two planes.

The plane AB makes the intercepts OA,OB and OC on X,Y and Z axis respectively.

$$OA:OB:OC = \frac{1}{h} : \frac{1}{k} : \frac{1}{l}$$

Multiply by lattice constant „a”

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

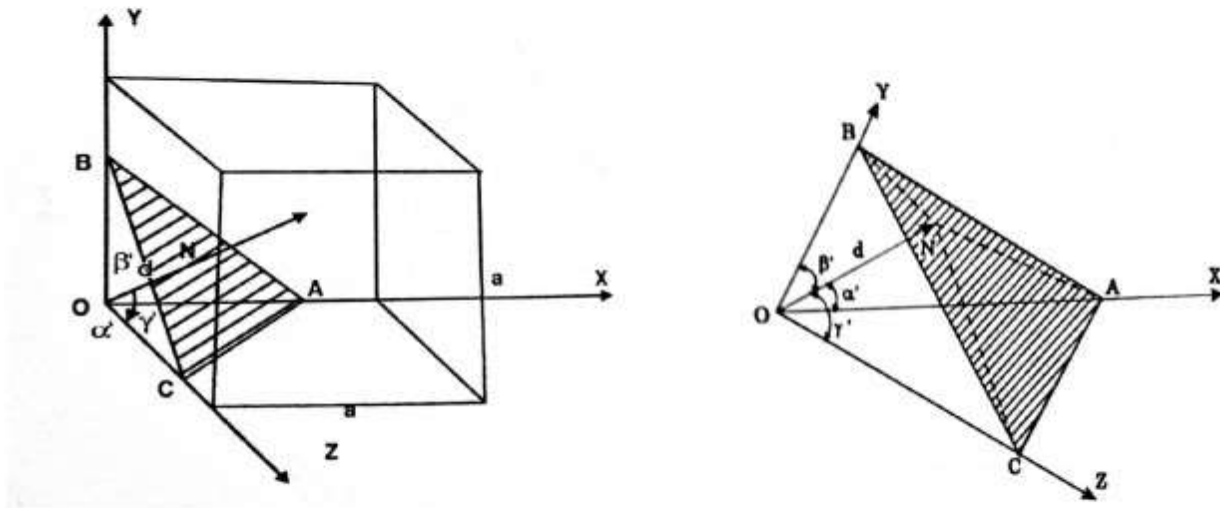


Fig 5.7.3 Inter planar spacing

From the figure

$$\cos \alpha' = \frac{ON}{OA} = \frac{d}{\frac{a}{h}} = \frac{dh}{a}$$

$$\cos \beta' = \frac{ON}{OB} = \frac{d}{\frac{a}{k}} = \frac{dk}{a}$$

$$\cos \gamma' = \frac{ON}{OC} = \frac{d}{\frac{a}{l}} = \frac{dl}{a}$$

According to the law of conservation of energy

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

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

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

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

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

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

The above equation gives the expression for interplanar spacing d .

5.3-a) STRUCTURE OF CUBIC

Cubic system

The cubic crystal structure is the simplest type and the atoms can take positions at the corners, faces and also at the centre of the cube. Based on the positions of the atom in the cubic system, it can be classified in to three types. They are,

1. Simple Cubic (SC) or Primitive(P)
2. Body Centred Cubic (BCC) and
3. Face Centred Cubic (FCC)

Simple Cubic Structure (SC)

A simple cubic unit cell consists of eight corner atoms as shown in given figure.

Example: polonium

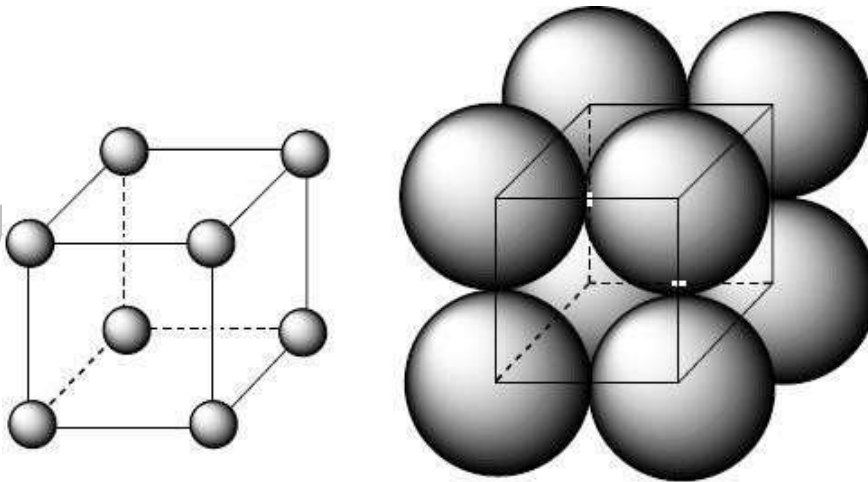


Fig :5.3.1- Simple Cubic Structure

Number of Atoms per unit cell

In actual crystal, each and every corner atom touches with each other and is shared by eight adjacent unit cells. Therefore, one corner atom contributes 1/8 of its part to one unit cell. Hence,

$$\begin{aligned} \text{Total number of atoms per unit cell is} &= \frac{1}{8} \times (\text{total number of corner atoms}) \\ &= \frac{1}{8} \times 8 \end{aligned}$$

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

Atomic Radius

In simple cubic (SC) structure the corner atoms touch each other along the edges. Let us consider one face (front face) of the simple cubic structure as shown in figure.

Here, the nearest neighbour distance is the lattice constant

$$a = 2r$$

$$\text{Atomic radius } r = \frac{a}{2}$$

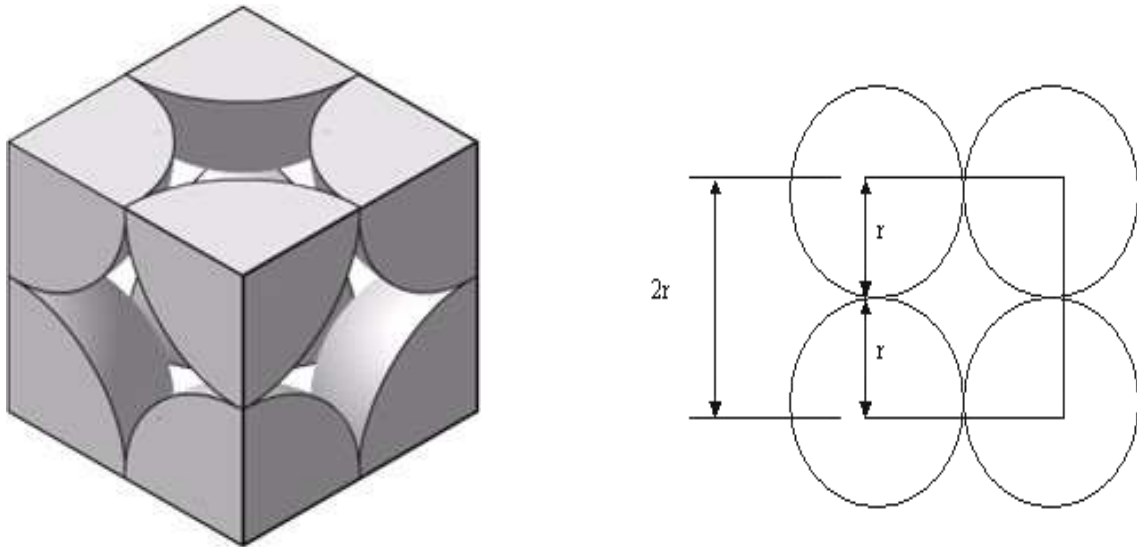


Fig :5.3.2- Atomic radius r

Co-ordination Number

Simple cubic unit cell consists of eight corner atoms. Let us consider any one

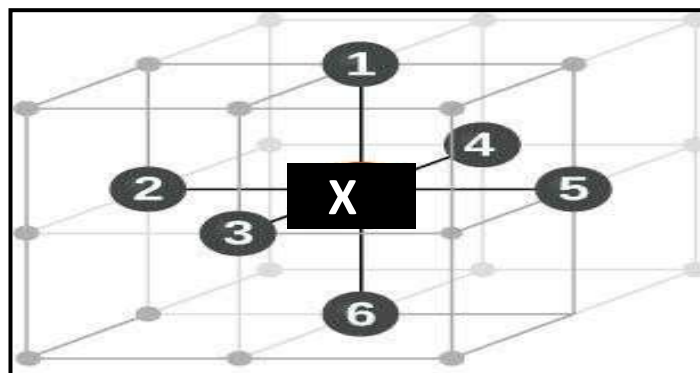


Fig :5.3.3- Co-ordination Number

corner atom say X, shared by 8 unit cells as shown in figure.

For this particular atom 'X' there are four nearest neighbour atoms, shown as 2, 3, 4 and 5 in its own plane (horizontal plane) and there are two more nearest atoms, one directly above (atom 1) and the other one directly below (Atom 6). All the atoms, other than these six atoms lie at greater distances from the X atom. The total number of nearest neighbours for X-atom is 4+2= 6. Hence, the coordination number for simple cubic is six.

Packing factor

$$\text{APF} = \frac{u}{v} \text{-----(1)}$$

Where

u - Total number of atoms per unit cell X volume of one atom

v - Total volume of the unit cell

The number of atoms per unit cell = 1

Volume of one atom (spherical) is = $\frac{4}{3}\pi r^3$ -----(2)

We know that, the radius of atom in simple cubic is

$$r = \frac{a}{2} \text{-----(3)}$$

Volume occupied by the total number of atoms per unit cell is

$$u = 1 \times \frac{4}{3}\pi r^3 \text{-----(4)}$$

substitution (3) in(4)

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

$$u = \frac{4\pi a^3}{24}$$

$$u = \frac{\pi a^3}{16}$$

Volume of the unit cell (v) = length x breadth x height

We know that for a cubic system,

length = breadth = height = a

$$v = a \times a \times a$$

$$v = a^3 \dots\dots\dots (6)$$

Substitute equation (5) and (6) in equation (1) we get, atomic packing factor (APF) is,

$$APF = \frac{\pi \frac{a^3}{6}}{a^3}$$

$$APF = \pi/6$$

(Or) $APF = 0.52 \dots\dots\dots (7)$

Therefore, we can say that 52% volume of the unit cell of SC is occupied by atoms and remaining 48% volume is vacant. Thus, the packing density is 52%. Since the packing density is very low, SC has loosely packed structure.

5.3-b) Body Centre Cubic Structure (BCC)

A body centred cubic structure has eight corner atoms and one body centred atom. The diagrammatic representation of a body centred cubic structure is shown in given figure.

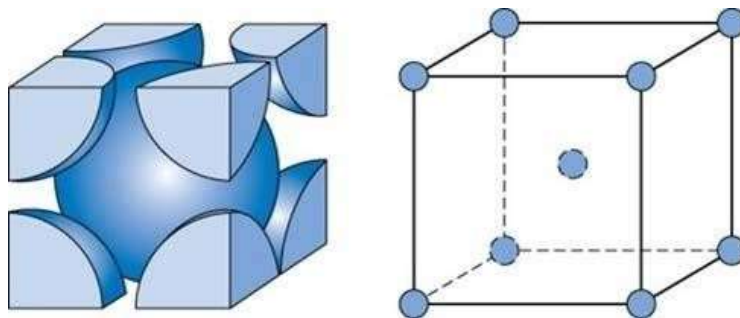


Fig : 5.3.4 BCC Structure.

Examples: Tungsten, Chromium, Molybdenum, etc

Number of Atoms per unit cell

In a body centred crystal structure, the body centred atom touch along the diagonal of the body.

In bcc unit cell, each and every corner atom is shared by eight adjacent unit cells.

The total number of corner atoms per unit cell is

$$\begin{aligned} \text{Total number of atoms per unit cell is} &= \frac{1}{8} \times (\text{total number of corner atoms}) \\ &= \frac{1}{8} \times 8 \end{aligned}$$

Total number of atoms per unit cell in BCC is = 1 + 1 = 2

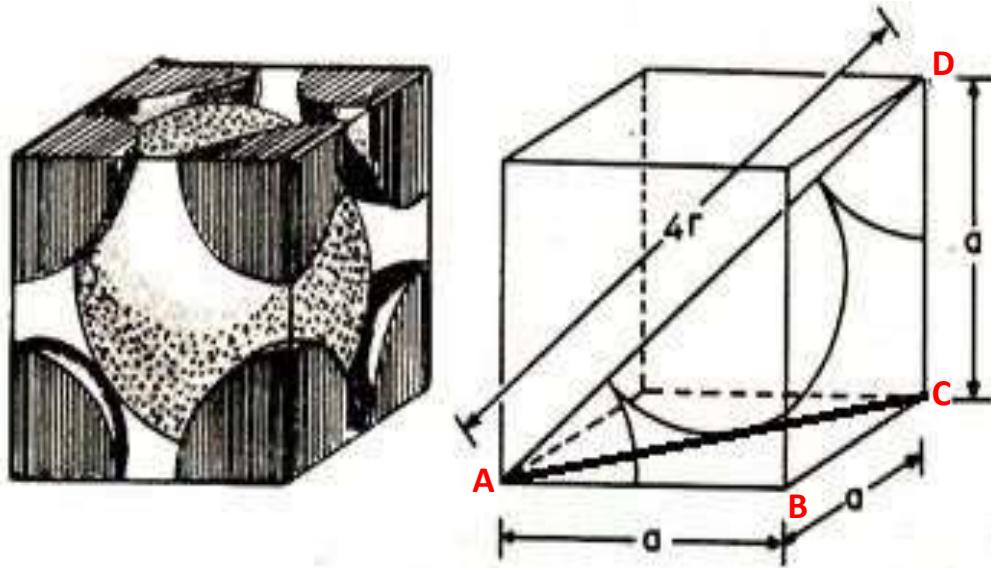


Fig : 5.3.5-Geometry to find atomic radius

From the geometry of the figure, we can write

$$(AD)^2 = (AC)^2 + (CD)^2$$

$$(AD)^2 = a^2 + a^2 + a^2 = 3a^2$$

$$AD = a\sqrt{3} \text{ -----(1)}$$

From figure,

The diagonal of the cube $AD = 4r$

$$AD = a\sqrt{3} \text{ -----(2)}$$

From equation (1) and (2) we can write

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

$$\text{Atomic radius } r = \frac{a\sqrt{3}}{4} \text{ -----(3)}$$

Co-Ordination Number

In BCC structure, there will be one body centred atom at the centre of the unit

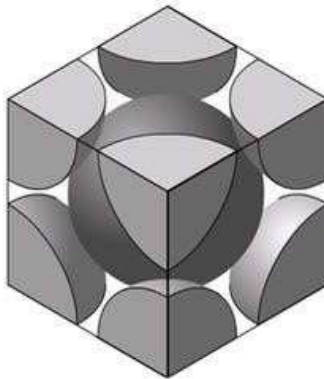


Fig : 5.3.6- structure to find Co-Ordination Number

cell and eight atoms at the 8 corners of the unit cell as shown in figure.

The corner atoms do not touch each other. But each corner atom touches the body centred atom along the body diagonal. Thus, the body centre atom has eight nearest neighbour atoms (corner atoms). Hence, *the co-ordination number body centred cubic structure is eight.*

Packing factor

$$APF = \frac{u}{v} \text{-----} (1)$$

Where

u - Total number of atoms per unit cell X volume of one atom

v - Total volume of the unit cell

The number of atoms per unit cell = 2

Volume of one atom (spherical) is = $\frac{4}{3}\pi r^3$ ----- (2)

We know that, the radius of atom in simple cubic is

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

Volume occupied by the total number of atoms per unit cell is

$$u = 2 \times \frac{4}{3} \pi r^3 \text{-----(4)}$$

substitution (3) in(4)

$$u = 2 \times \frac{4}{3} \pi \left(\frac{a\sqrt{3}}{4}\right)^3$$

$$u = \frac{\pi a^3 \sqrt{3}}{8} \text{-----(5)}$$

Volume of the unit cell for a cubic system is

$$v = a^3 \text{-----(6)}$$

Substitute equation (5) and (6) in equation (1) we get,

$$\text{Atomic packing factor (APF)} = \frac{\frac{\pi a^3 \sqrt{3}}{8}}{a^3} = \frac{\pi \sqrt{3}}{8}$$

$$\text{APF} = 0.68 \text{-----(7)}$$

Therefore, we can say that 68% volume of the unit cell of BCC is occupied by atoms and remaining 32% volume is vacant. Thus the packing density is 68%. Since the packing density is greater than simple cubic, it has tightly packed structure, when compared to SC.

5.2 Unit Cell

The unit cell is a smallest geometric volume containing one or more atoms arranged in three dimension. And also, it is called fundamental building block of a crystal structure.

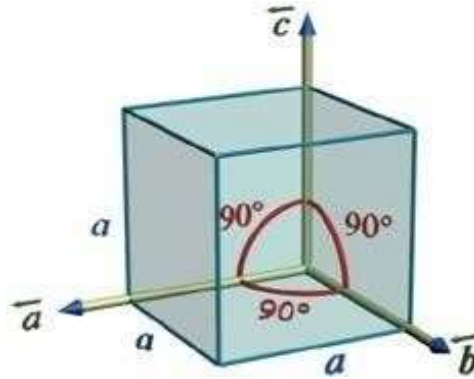


Fig 5.2.1- Unit Cell

Primitive cell

Primitive cell is the smallest volume unit cell which contains the lattice points at the corner only.

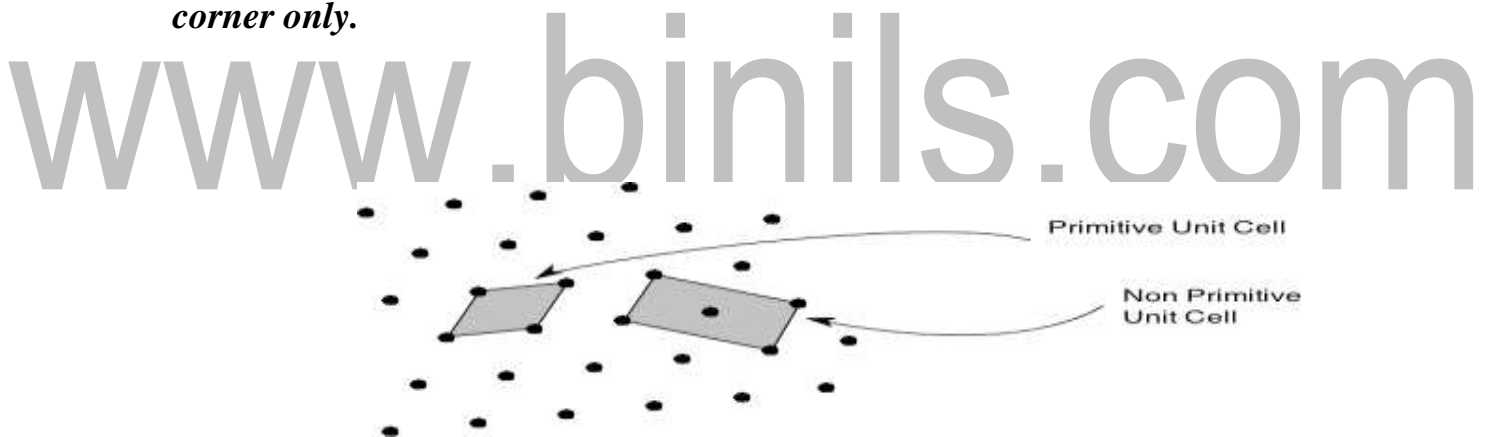


Fig 5.2.2- Primitive cell

Lattice Constant

The distance between any two successive lattice points along any three dimensional directions is called lattice constant.

Parameters determining the Crystal structure of Materials

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

Number of atoms per unit cell or Effective number

The total number of atoms present in or shared by a unit cell is known as number of atoms per unit cell.

Atomic radius

Atomic radius is defined as half of the distance between any two nearest neighbour atoms which have direct contact with each other, in a crystal of a pure element. It is usually expressed in terms of cube edge a .

Co-ordination number

Co-ordination number is the number of nearest neighbouring atoms to a particular atom. Or Co- ordination number is the number of nearest neighbours directly surrounding a given atom.

Atomic packing factor or packing density or density of packing

Atomic packing factor is defined as the ratio between the volumes occupied by the total number of atoms per unit cell (u) to the total volume of the unit cell (v).

$$\text{APF} = \frac{U}{V}$$

Where,

u - Total number of atoms per unit cell X volume of one atom

v - Total volume of the unit cell

Seven Crystal Systems

Based on the fundamental translation vector and interfacial angle, the crystal classified in to seven types. They are,

1. *Cubic*
2. *Triclinic*
3. *Monoclinic*
4. *Orthorhombic*
5. *Tetragonal*
6. *Rhombohedral*

7. Hexagonal.

Sr. No.	Crystal System	Axial length of Unit Cell	Inter axial angles	Number of Lattice in the system
1	Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$	3
2	Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	2
3	Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	4
4	Monodinic	$a \neq b \neq c$	$\alpha = \beta = 90^\circ \neq \gamma$	2
5	Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$	1
6	Trigonal	$a = b = c$	$\alpha = \beta = \gamma < 120^\circ, \neq 90^\circ$	1
7	Hexagonal	$a = b \neq c$	$\alpha = \beta = 90^\circ, \text{ and } \gamma = 120^\circ$	1

Bravais Space Lattice

A three dimensional space lattice is generated by repeated translation of three non-coplanar vectors a , b and c . There are only fourteen distinguishable ways of arranging points in three dimensional spaces. These fourteen space lattices are known as Bravais space lattices. The different Bravais space lattices and their crystal systems are listed in given table.

Crystal System	Bravais Space Lattices	Symbols	
Cubic	Simple	P	3
	Body Centred	I	

	Face Centred	F	
Triclinic	Simple	P	1
Monoclinic	Simple	P	2
	Base Centred	C	
Orthorhombic	Simple	P	4
	Base Centred	C	
	Body Centred	I	
	Face Centred	F	
Tetragonal	Simple	P	2
	Body Centred	I	
Rhombohedral	Simple	P	1
Hexagonal	Simple	P	1