

## Lecture -1

# Structure of Matter

# Classification of solids

Solid is a state of matter in which the particles of a substance are not free to move but have fixed positions about which they can vibrate. In a solid atoms or molecules are attached to one another with strong force of attraction that's why it has particular volume and shape.

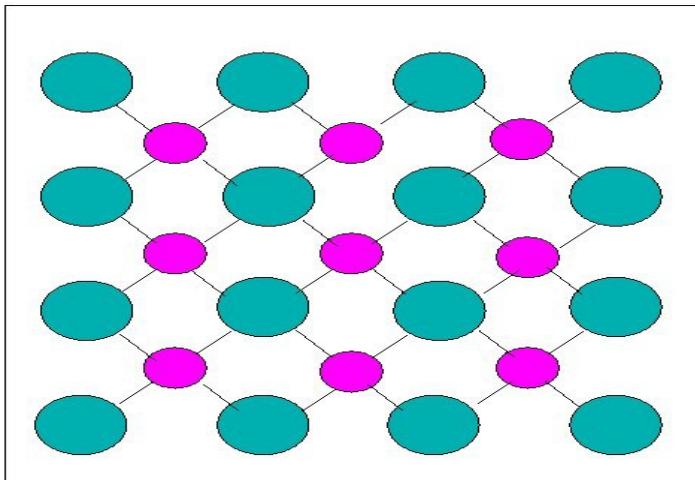
In general solids can be classified into **two** categories such as:

- i) Crystalline
- ii) Amorphous or Non-crystalline

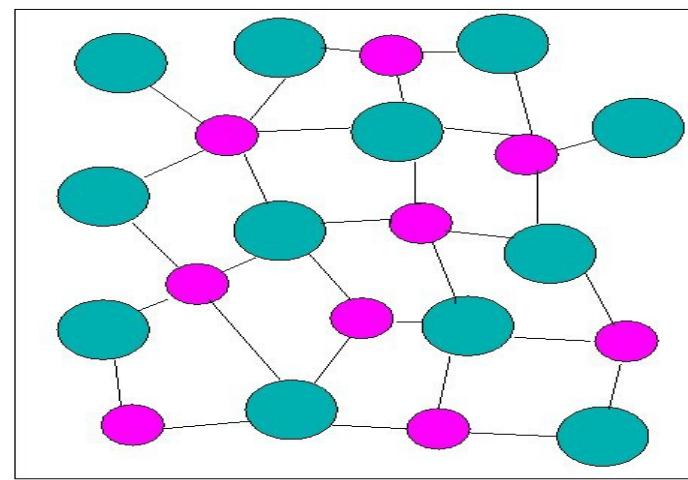
**Crystalline solid:** In crystalline solid the atoms or molecules are arranged in a definite, repeating pattern. Constituent atoms or molecules are arranged in a regular manner and produced by the repetition of pattern unit.  
*Examples:* Salt and sugar.

**Amorphous or Non-crystalline solid:** In Non-crystalline solid the atoms or molecules do not repeat periodically.  
*Examples:* Plastic, rubber and glass.

**Crystalline solid**



**Amorphous solid**



# Differences between Crystalline & Amorphous solids

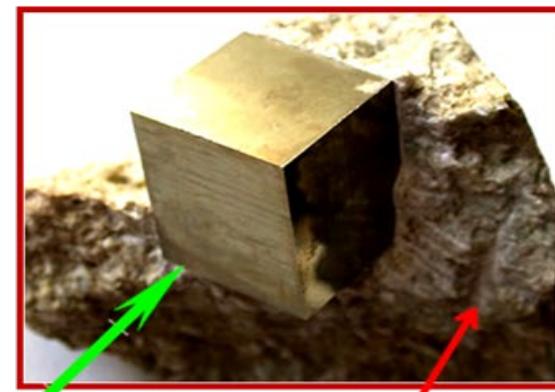
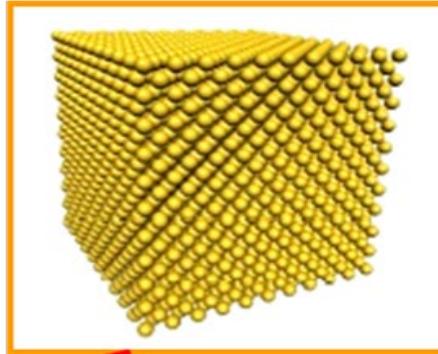
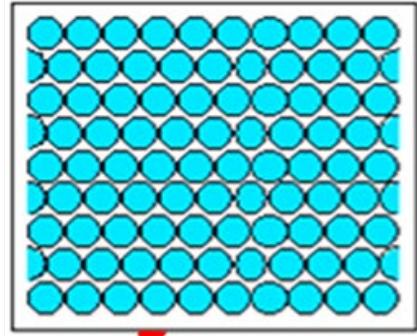
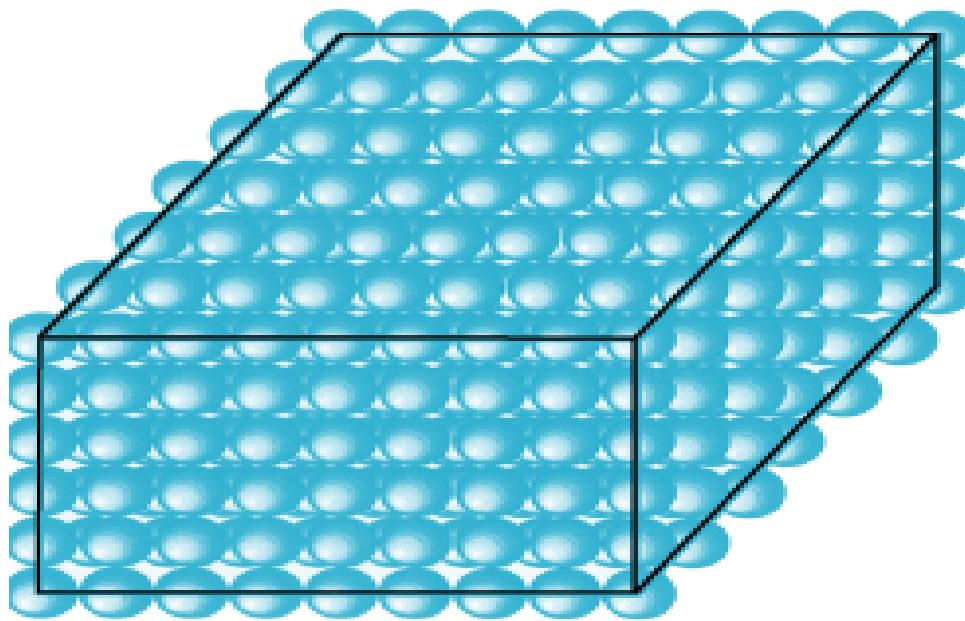
Property	Crystalline solids	Amorphous Solids
Shape	Definite characteristic geometrical shape.	Irregular Shape.
Melting point	Melt at a sharp and characteristic temperature.	Gradually soften over a range of temperature
Cleavage property	When cut with a sharp edged tool, they split into two pieces and the newly generated surfaces are plain and smooth.	When cut with a sharp edged tool, they cut into two pieces with irregular surfaces.
Heat of fusion	They have a definite and characteristic heat of fusion.	They don't have definite heat of transition
Anisotropy	Anisotropic in nature	Isotropic in nature
Order in arrangement	Long range order	Only short range order

## Types of Crystalline Materials

There are two types of crystalline materials

- Single Crystalline materials
- Polycrystalline materials

**Single Crystal:** A single crystal or mono-crystalline solid is a material in which the crystal lattice of the entire sample is continuous and unbroken to the edges of the sample, with no grain boundaries. When periodicity of the pattern stretch out to many cubic cm in volume is called single crystal. In the case of single crystal the periodicities of atoms extend throughout the material, here is no grain boundary. A homogenous solid formed by a repeating, three-dimensional pattern of atoms, ions, or molecules are having fixed distances between constituent parts. The unit cell is of such a pattern. *Example:* Diamond.



**Single Crystals**

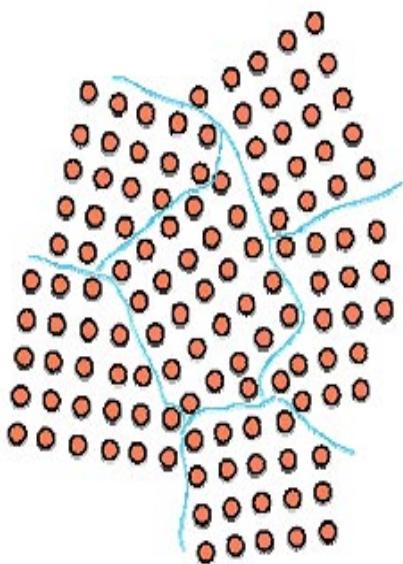
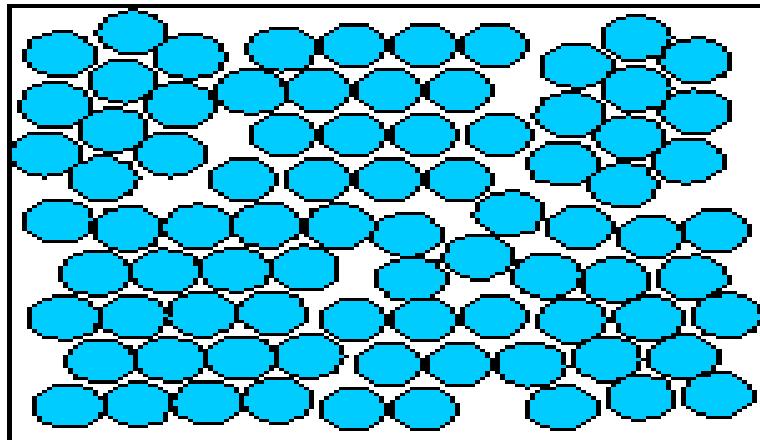
**Single Pyrite  
Crystal**

**Amorphous  
Solid**

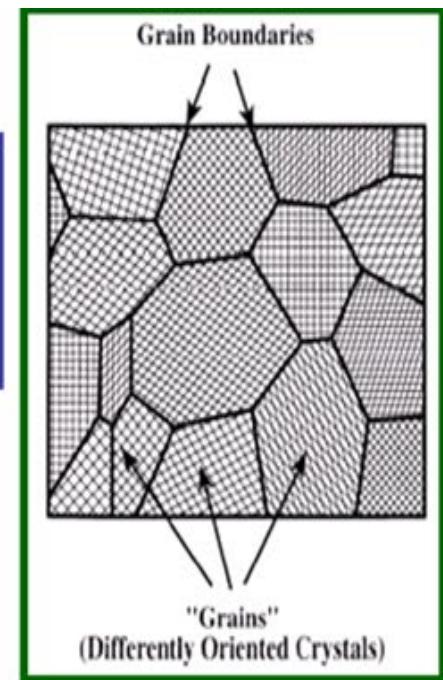
**Polycrystalline materials:** Polycrystalline materials are composed of a number of smaller crystals. Most of the crystalline solids are made up of millions of tiny crystals called grains and are called to be polycrystalline.

In polycrystalline crystals the periodicity does not extend throughout the crystal but is interrupted at grain boundaries. Polycrystalline materials are solids that are composed of many crystals of varying size and orientation.

Polycrystalline is the structure of a solid material that, when cooled, forms crystallite grains at different points within it. The areas where these crystallite grains meet are known as **grain boundaries**. A **grain boundary** is the interface between two grains, or crystallites, in a polycrystalline material.

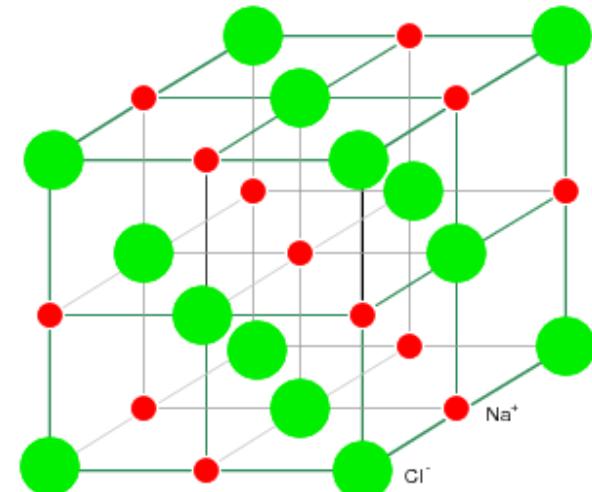
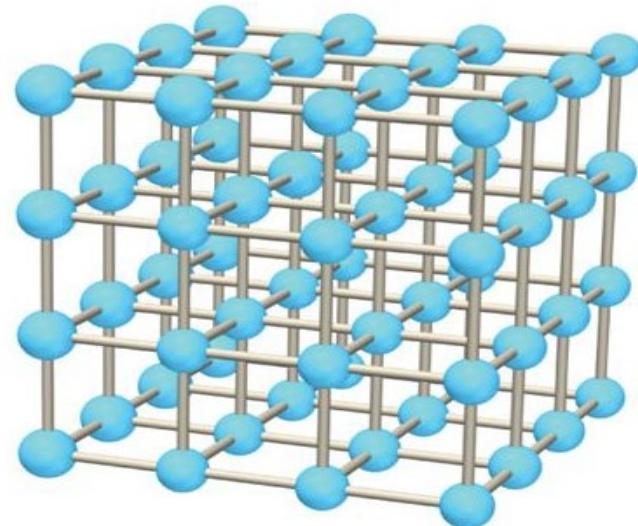


Polycrystalline  
Pyrite Grain



## Some Definitions

**Crystal:** A crystal is a three dimensional regular and periodic arrangement of atoms. An ideal crystal is formed by the infinite regular repetition of identical structural units in space in the form of parallelepiped shaped. NaCl, ZnS are the examples of crystal.



**Lattice:** A lattice is a regular and periodic arrangement of points in space. It may be one, two or three dimensional. In other words the resulting collection of periodic points in space is called crystal lattice.

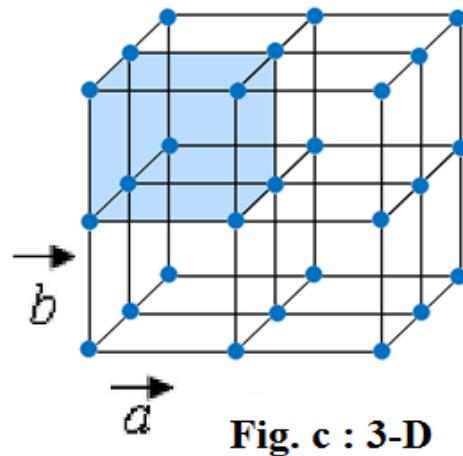
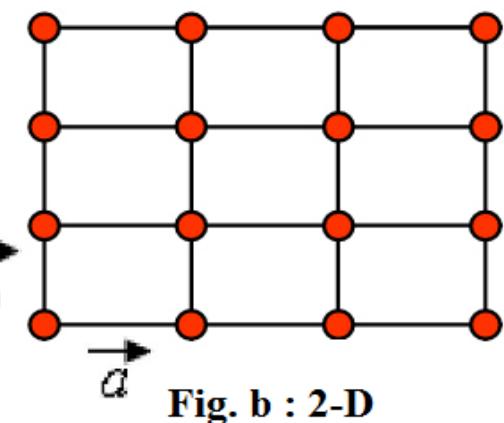
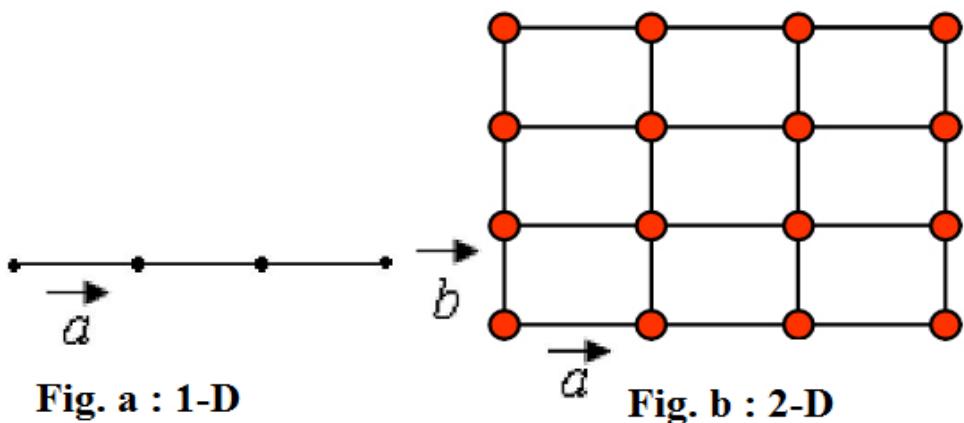


Fig. : Lattice arrangement a) in 1-D is the **line of lattice**, b) in 2-D is the **lattice plane** and c) in 3-D is the **space lattice**.

**Plane lattice:** If all the atoms are arranged in a plane, then it would be visible like in Fig. (b). In this way in two dimension plane all points will have same atomic surroundings. This arrangement of atoms is called **plane lattice**.

**Space lattice:** If all the atoms are having similar surroundings in three dimensional spaces like in Fig. (c), then such type of atomic arrangement is called **space lattice**.

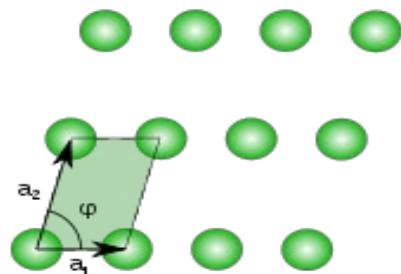
- 2-D non-collinear **translation** define a **plane lattice**
- 3-D non-coplanar **translation** defined a **space lattice**

There are two types of lattice

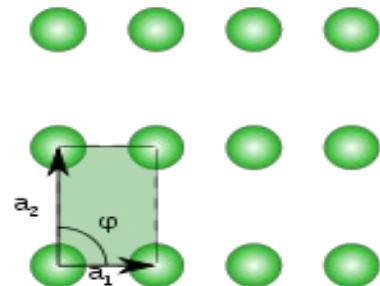
1. Bravais lattice and 2. Non-Bravais lattice

**Bravais lattice:** There are various ways of positioning points (lattice) in space such that all points have same identical surroundings, *i.e.* all points are of same kind and equivalent.

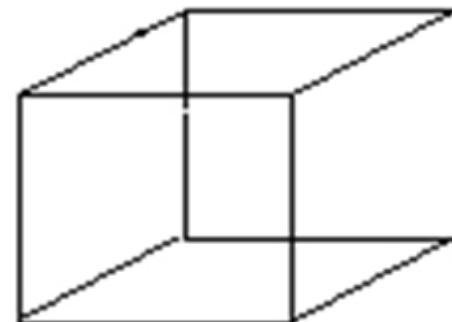
These lattices are known as **Bravais lattices.**



Oblique Lattice



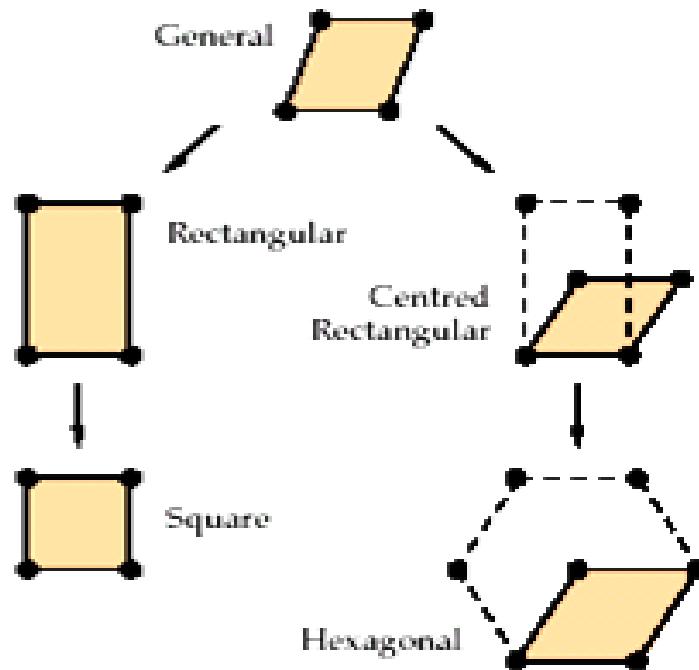
Square Lattice



Cubic Space Lattice

In a **Bravais Lattice**, not only the atomic *arrangement* but also the *orientations* must appear exactly the same from every lattice point.

It can be shown that, in 2 Dimensions, there are Five (5) & ONLY Five Bravais Lattices.



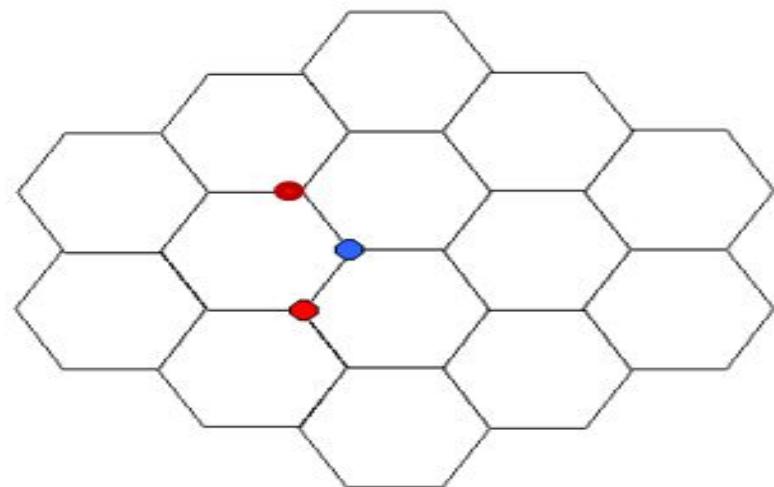
Bravais showed that, there exist no more than 14 space lattices in three dimensions. In order to specify the arrangements of points in a space lattice, he introduced 7-system of axes or crystal system.

**Non-Bravais lattice:** All points are not identical compared to each other known as non-Bravais lattices.

The red side has a neighbour to its immediate left, the blue one instead has a neighbour to its right.

Red (and blue) sides are equivalent and have the same appearance

Red and blue sides are not equivalent. Same appearance can be obtained rotating blue side  $180^\circ$ .



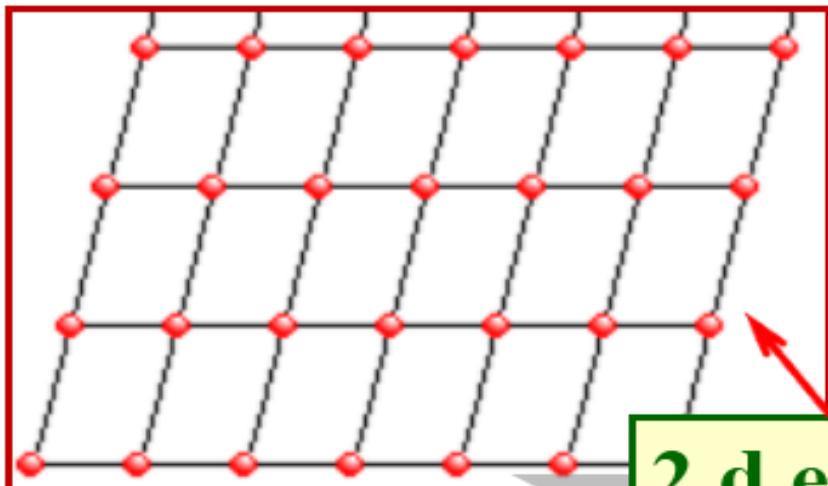
**Honeycomb**

# Crystal Lattices

## Bravais Lattices

(BL)

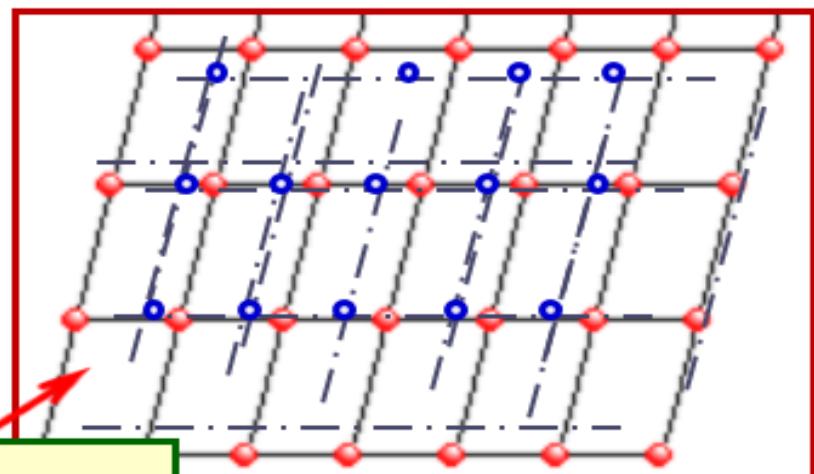
All atoms are the same kind  
All lattice points are equivalent



## Non-Bravais Lattices

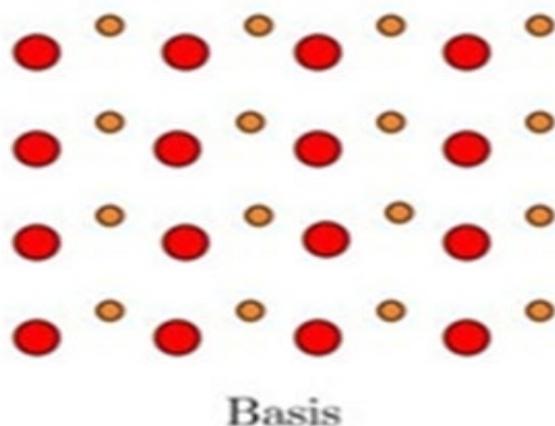
(non-BL)

Atoms are of different kinds.  
Some lattice points aren't equivalent.  
A combination of 2 or more BL



2 d examples

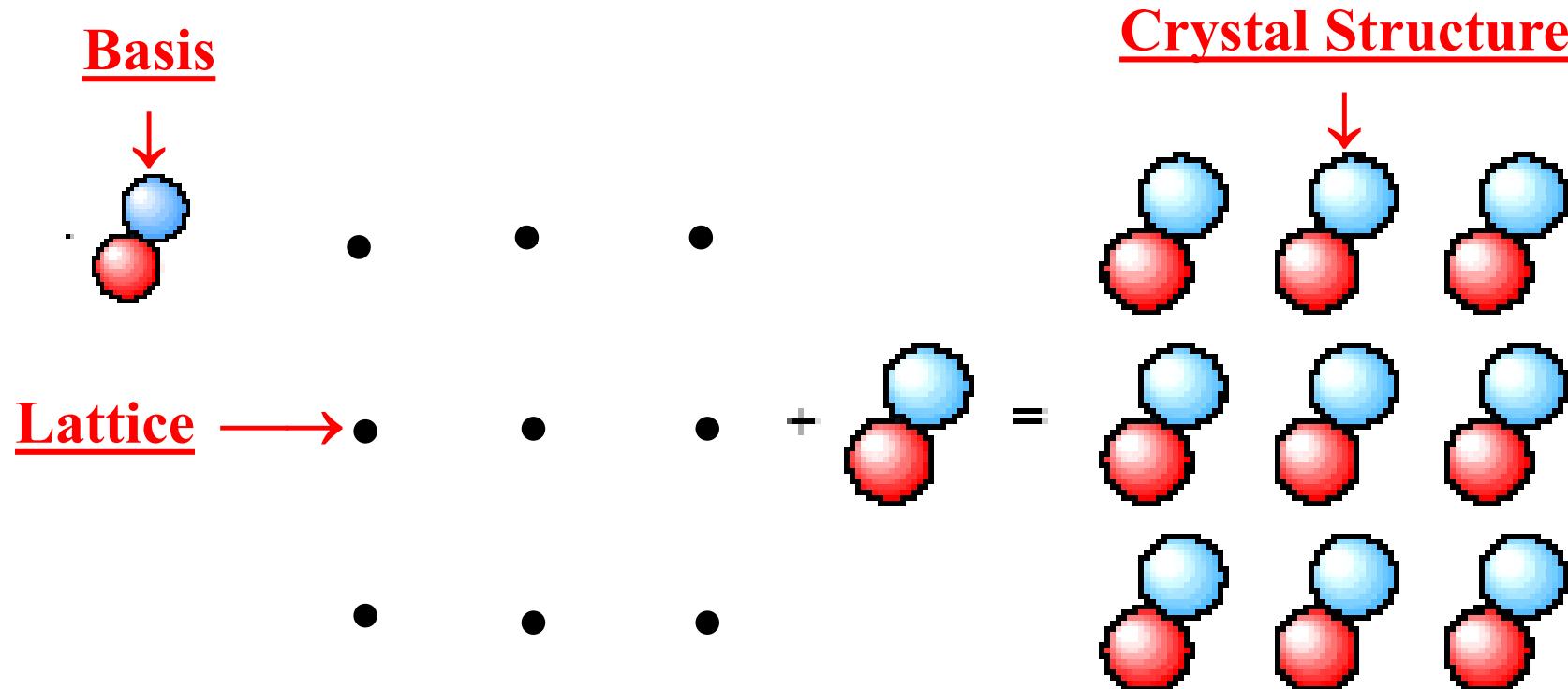
**Basis or Motif:** The structure of all crystal is described in terms of a lattice with a group of atoms attached to each lattice point. The number of atoms or molecules present at the lattice is called basis. It is repeated in space to form the crystal structure. A basis is an assembly of atoms identical in composition, arrangement.

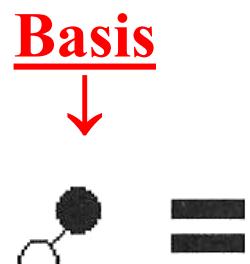
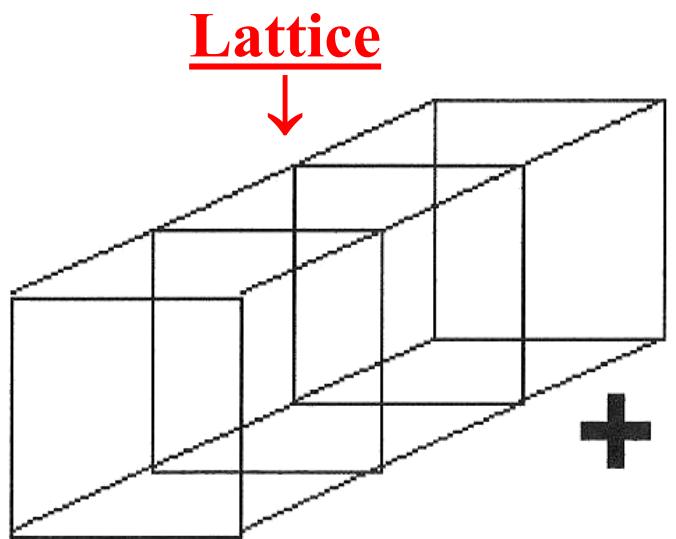


**Crystal structure:** A crystal structure is formed when a basis of atoms is attached identically to every lattice point.

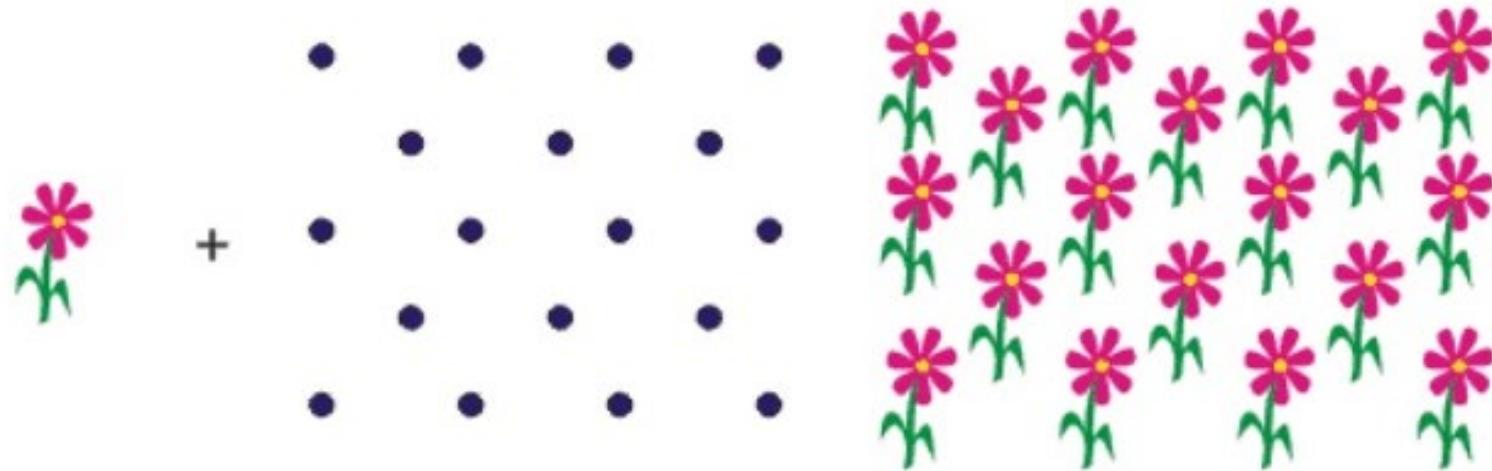
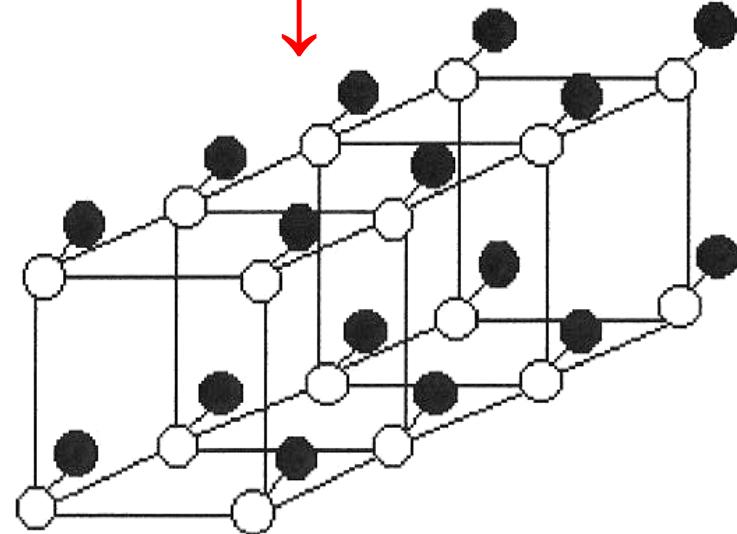
The logical relation is,

**Crystal Structure = Space (Crystal) Lattice + Basis or Motif**





Crystal Structure



Basis

Lattice

=

Crystal

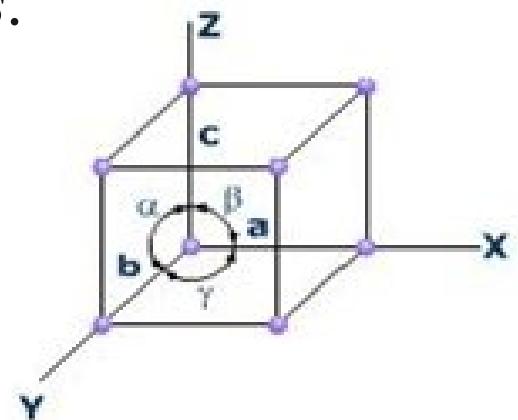
# Lecture-2

## Unit cell, Bravais Lattice

- Primitive & Non-primitive Unit cells
- Different Lattice symbols
- Total no. of atoms in different unit cells
- Bravais lattice in three-dimensions

**Lattice parameters** : Arbitrary arrangements of crystallographic axes, marked  $X$ ,  $Y$  and  $Z$ , defining a unit cell shown in the fig. The three sides of a unit cell which are called the *crystallographic axes*. The angles between the three axes  $\alpha$ ,  $\beta$  and  $\gamma$  are called *interfacial angles*.

The intercepts  $a$ ,  $b$  and  $c$  define the dimensions of a unit cell and are known *lattice parameters of the unit cell*. These are also called the *geometrical constants* of a given crystal.



Representation of dimensions of a unit cell

**Unit Cell** : A crystal lattice is made up of infinite repetitions of a small group of ions in three-dimensional pattern. It is built up by the combination of a regular array of ions in which each ion is surrounded by a definite number of ions of opposite charges.

The small group of ions which is repeated in a crystal lattice in three-dimensional pattern is known as a **unit cell**. The unit cell is thus the smallest portion of the **crystal** lattice which has all the various kind of symmetry which characterise the crystal.

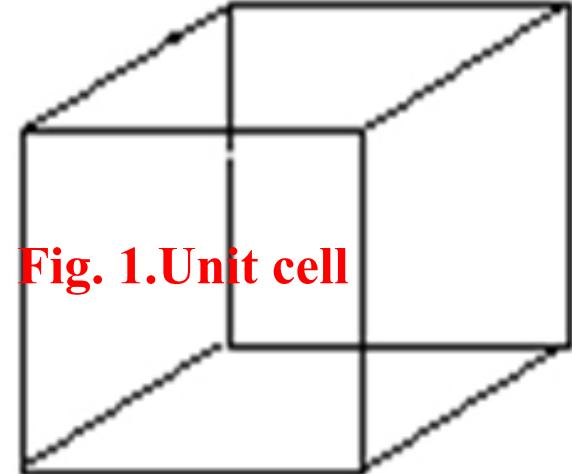
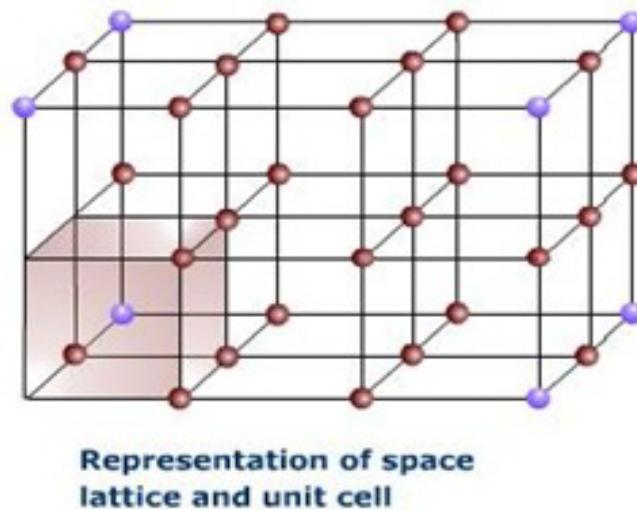
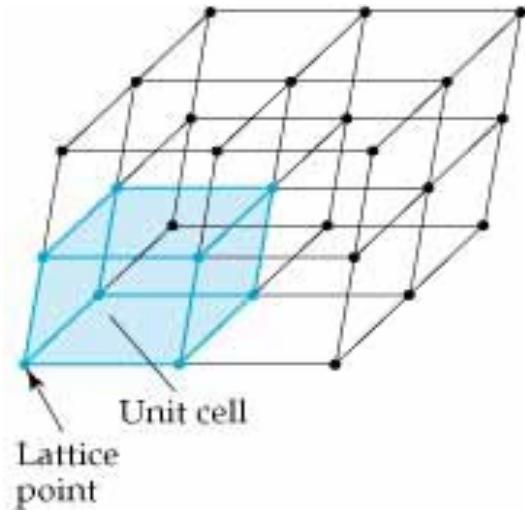
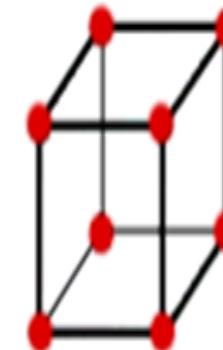
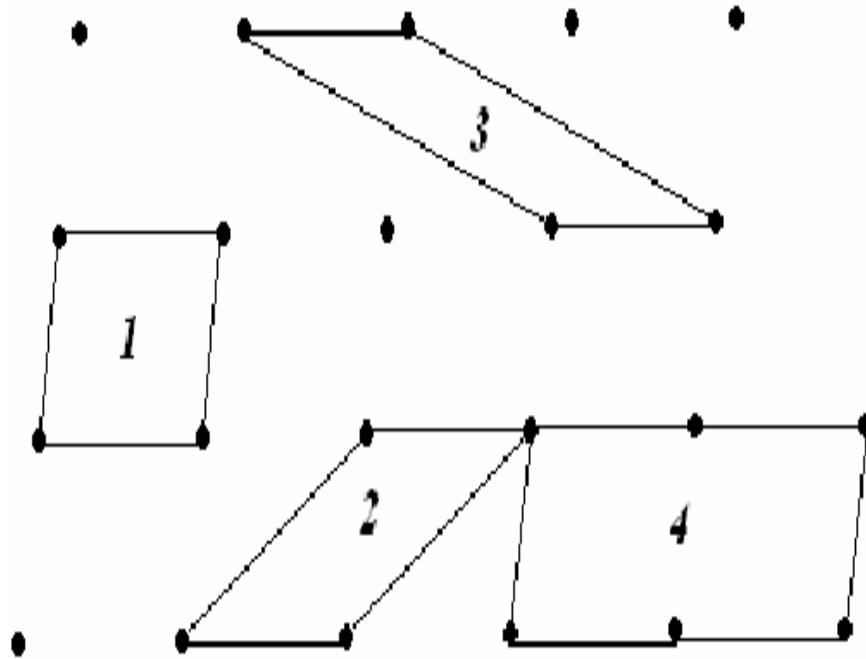


Fig. 1. Unit cell

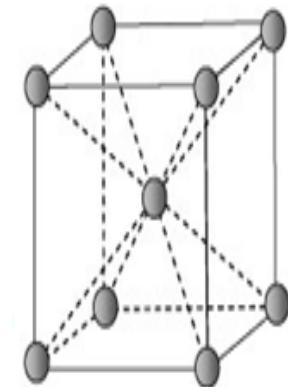
- A parallelepiped shaped volume which reproduced by close packing in three dimension gives the whole crystal, is called the **unit cell**. There are two types of unit cell:
  - Primitive unit cell
  - Non-primitive unit cell

**Primitive unit cell:** The unit cell occupying the smallest volume in a given lattice is called the primitive unit cell. It contains only **one lattice point**.

**Non-Primitive unit cell:** The unit cell which is larger than the minimum volume unit cell is defined as a non-primitive unit cell. A non-primitive unit cell contains **more than one lattice point**. The volume of a non-primitive unit cell is an integral multiple of a primitive cell.



Simple cubic  
Primitive



Body centered cubic  
Non Primitive

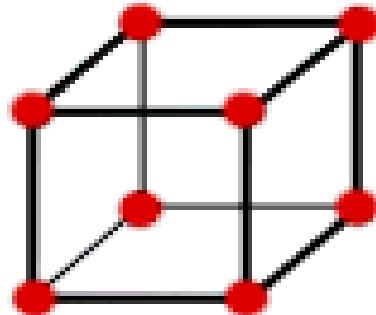
Here parallelogram 1, 2, 3 are equal in area and any one of them could be taken as the **primitive cell**.

The parallelogram 4 has twice the area of a primitive cell and thus a compound cell. The compound cell is also a **non-primitive cell**.

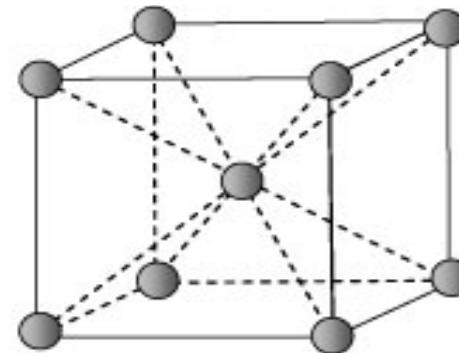
## **Distinguish between primitive unit cell & unit cell:**

<b>Primitive Cell</b>	<b>Unit Cell</b>
1. The unit cell occupying the smallest volume in a given lattice is called the primitive unit cell.	1. A parallelepiped shaped volume, which reproduced by close packing in three dimensions gives the whole crystal is called the unit cell.
2. It always contains only one lattice point.	2. It may contain more than one lattice point.
3. A primitive cell is the smallest cell in crystal. A cell smaller than it is never possible.	3. A unit cell may be smallest or not.
4. It is always a unit cell.	4. But a unit cell is not always a primitive cell.

**Lattice symbol ‘P’:** The lattice symbol ‘P’ means the primitive cell where lattice points are at the corners of the cell. A primitive cell is always a unit cell.



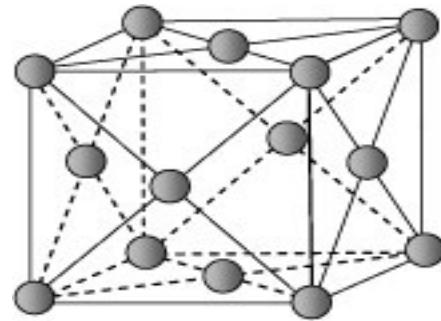
Simple cubic (sc)



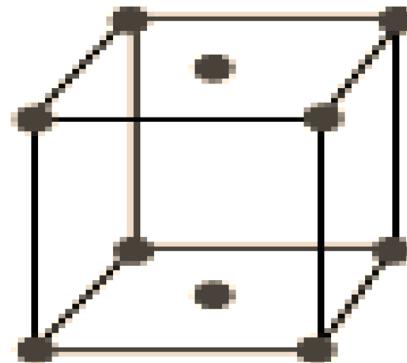
Body centered cubic (bcc)

**Lattice symbol ‘I’:** The lattice symbol ‘I’ means the body centered lattice. In the body centered lattice, the lattice points are at the corners and inside the cell.

**Lattice symbol ‘F’:** The lattice symbol ‘F’ means the face-centered lattice. In the face centered lattice, the lattice points are at the corners and all the faces centered.



Face centered cubic (fcc)



(base centered lattice)

**Lattice symbol ‘C’:** The lattice symbol ‘C’ means the lattice is base centered or the side centered or C-face centered. In the base centered lattice, the lattice points are at the corners and at the face centered of opposite sides.

### Total Number of atoms in different unit cells

The formula for the total number of atoms in a unit cell is

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{8}$$

Where,  $N_i$  = Points inside the cell

$N_f$  = Points on the faces

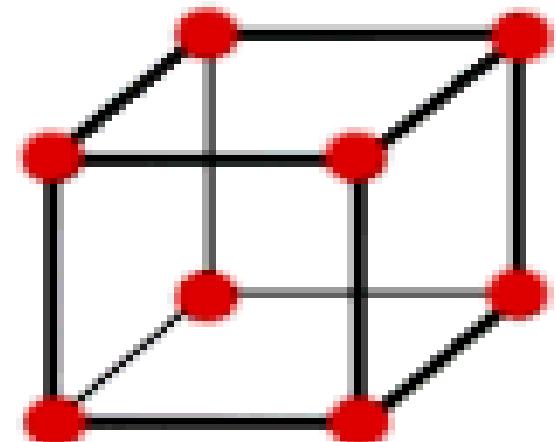
$N_c$  = Points at the corners

Primitive cell: For a primitive cell, the lattice points are at the eight corners of the cell. So for primitive cell  $N_i = 0$ ,  $N_f = 0$  and  $N_c = 8$ .

Thus the total number of atoms in a primitive cell is

$$N = 0 + \frac{0}{2} + \frac{8}{8} = 1$$

So, the primitive cell has only one lattice point.



### Total Number of atoms in different unit cells

The formula for the total number of atoms in a unit cell is

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{8}$$

Where,  $N_i$  = Points inside the cell

$N_f$  = Points on the faces

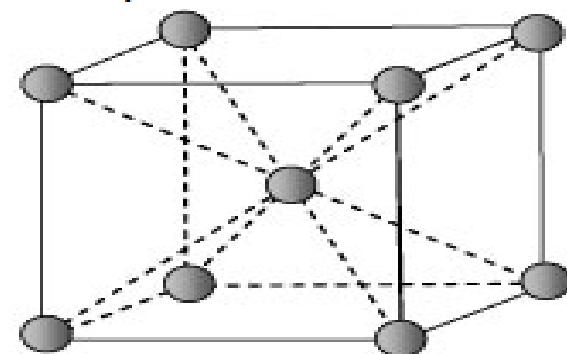
$N_c$  = Points at the corners

**Body centered cubic:** For a body centered cubic lattice, the lattice points are at the eight corners and inside the cell. So, for body centered cubic lattice  $N_i = 1$ ,  $N_f = 0$  and  $N_c = 8$ .

Thus the total number of atoms in body centered cubic lattice is

$$N = 1 + \frac{0}{2} + \frac{8}{8} = 2$$

So, the body centered cubic lattice has only two lattice points.



Body centered cubic (bcc)

### Total Number of atoms in different unit cells

The formula for the total number of atoms in a unit cell is

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{8}$$

Where,  $N_i$  = Points inside the cell

$N_f$  = Points on the faces

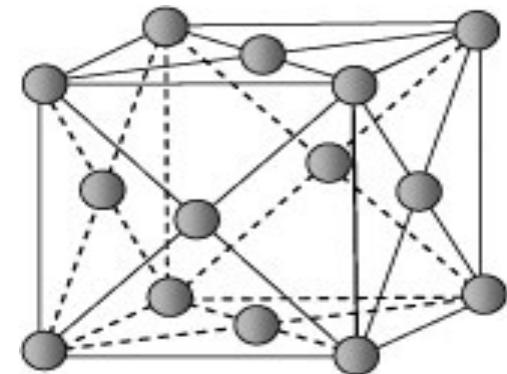
$N_c$  = Points at the corners

Face-centered cubic: For a face centered cubic lattice, the lattice points are at the eight corners and all (six) the faces centered. So, for face centered cubic lattice  $N_i = 0$ ,  $N_f = 6$  and  $N_c = 8$ .

Thus the total number of atoms in a face centered cubic lattice is

$$N = 0 + \frac{6}{2} + \frac{8}{8} = 4$$

So, the face centered cubic lattice has only four lattice points.



Face centered cubic (fcc)

### Total Number of atoms in different unit cells

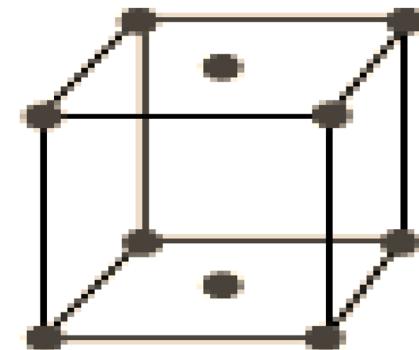
The formula for the total number of atoms in a unit cell is

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{8}$$

Where,  $N_i$  = Points inside the cell

$N_f$  = Points on the faces

$N_c$  = Points at the corners



**Base centered cubic:** For a base centered cubic lattice, the lattice points are at the eight corners and two opposite faces centered. So for base centered cubic lattice  $N_i = 0$ ,  $N_f = 2$  and  $N_c = 8$ .

Thus the total number of atoms in a base centered cubic lattice is

$$N = 0 + \frac{2}{2} + \frac{8}{8} = 2$$

So, the base centered cubic lattice has only two lattice points.

## **Seven crystal system**

The names of seven crystal system are: Triclinic, Monoclinic, Orthorhombic, Tetragonal, Cubic, Trigonal and Hexagonal.

### **Restrictions on conventional cell axes and angles:**

System	No. of lattice in the system	Lattice Symbol	Restrictions on	
			Conventional cell axes	Conventional axial angles
Triclinic	1	P	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma$
Monoclinic	2	P, C	$a \neq b \neq c$	$\alpha = \gamma = \frac{\pi}{2} \neq \beta$
Orthorhombic	4	P, C, I, F	$a \neq b \neq c$	$\alpha = \beta = \gamma = \frac{\pi}{2}$
Tetragonal	2	P, I	$a = b \neq c$	$\alpha = \beta = \gamma = \frac{\pi}{2}$
Cubic	3	P, I, F	$a = b = c$	$\alpha = \beta = \gamma = \frac{\pi}{2}$
Trigonal	1	R	$a = b = c$	$\alpha = \beta = \gamma < \frac{2\pi}{3} \neq \frac{\pi}{2}$
Hexagonal	1	P	$a = b \neq c$	$\alpha = \beta = \frac{\pi}{2}, \gamma < \frac{2\pi}{3}$

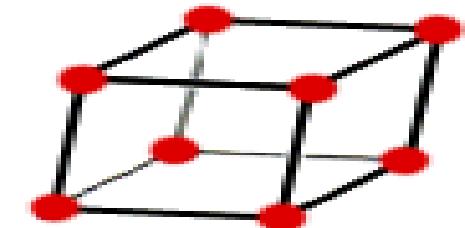
Table - 1. The seven crystal systems, divided into 14 Bravais lattices

System	Bravais lattice	Unit cell characteristics		Characteristic symmetry elements	Examples
Cubic	Simple	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$	Four 3-fold rotation axes (along cube diagonal)	NaCl, CaF <sub>2</sub> , NaClO <sub>2</sub>
	Body - centred				
	Face - centred				
Monoclinic	Simple Base - centred	$a \neq b \neq c$	$\alpha = \beta = 90^\circ \neq \gamma$	One 2-fold rotation axis	Na <sub>2</sub> SO <sub>4</sub> , FeSO <sub>4</sub>
Triclinic	Simple	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$	None	Cu SO <sub>4</sub> , K <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub>
Tetragonal	Simple Body - centred	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	One 4-fold rotation axis	Ni SO <sub>4</sub> , SnO <sub>2</sub>
Orthorhombic	Simple	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	Three mutually orthogonal 2-fold rotation axes	KNO <sub>3</sub> , BaSO <sub>4</sub> , MgSO <sub>4</sub>
	Base - centred				
	Body - centred				
	Face - centred				
Rhombohedral (Trigonal)	Simple	$a = b = c$	$\alpha = \beta = \gamma \neq 90^\circ$	One 3-fold rotation axis	Ca SO <sub>4</sub>
Hexagonal	Simple	$a = b \neq c$	$\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$	One 3-fold rotation axis	SiO <sub>2</sub> , AgI

**Triclinic:** In the triclinic system, the single lattice type has a primitive unit cell (P) with three crystallographic axes of unequal lengths and unequal angles between them. *i.e.*

$$a \neq b \neq c$$

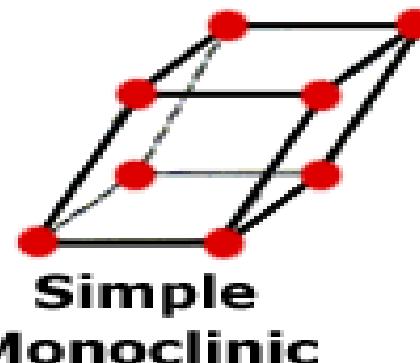
$$\alpha \neq \beta \neq \gamma \neq 90^\circ$$



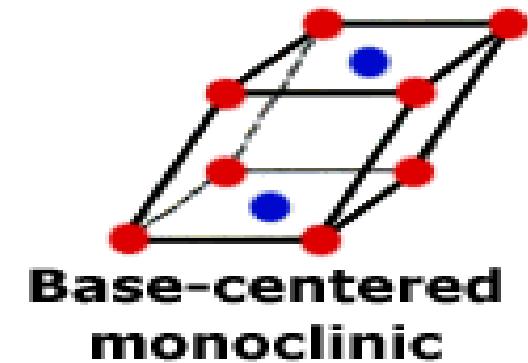
**Triclinic**

**Monoclinic:** In the monoclinic system, there are two lattice types: one with a primitive unit cell (P) and other with a non-primitive conventional cell which may be base centred (C) with the lattice point at the centre of the rectangular cell faces. Where

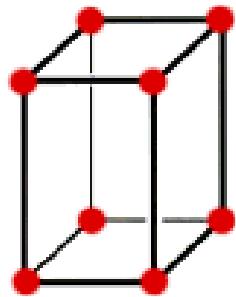
$$a \neq b \neq c$$



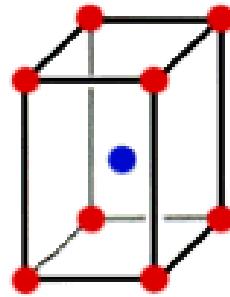
$$\alpha = \beta = 90^\circ \neq \gamma$$



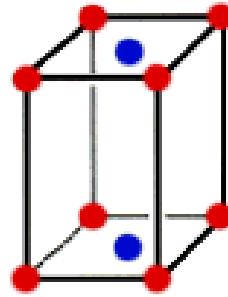
**Orthorhombic:** In the orthorhombic system, there are four lattice types: one lattice has a primitive unit cell (P), one lattice is base centered (C), one lattice is body centered (I), and one lattice is face centered (F). Here,  $a \neq b \neq c$        $\alpha = \beta = \gamma = 90^\circ$



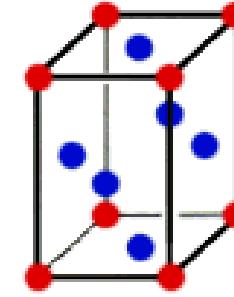
Simple  
orthorhombic



Body-centered  
orthorhombic

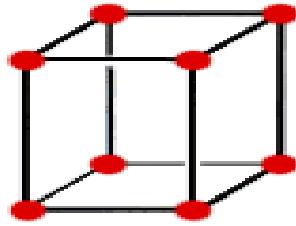


Base-centered  
orthorhombic

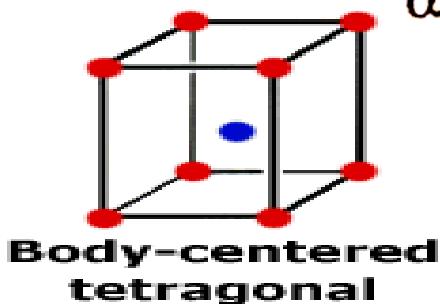


Face-centered  
orthorhombic

**Tetragonal:** In the tetragonal system, there are two lattice types: one is primitive unit cell (*P*) and another is body centered (*I*). In this case  $a = b \neq c$



Simple  
tetragonal

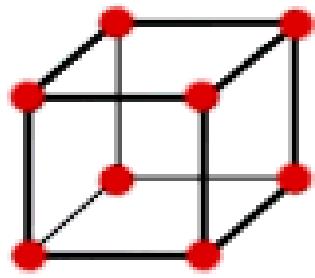


Body-centered  
tetragonal

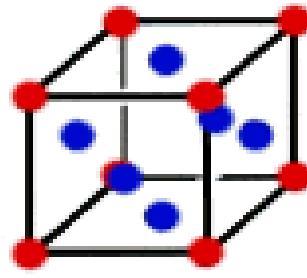
$$\alpha = \beta = \gamma = 90^\circ$$

**Cubic:** In the cubic system, there are three lattice types: the simple-cubic lattice (sc), the body centered cubic (bcc), and the face centered cubic (fcc). Here,

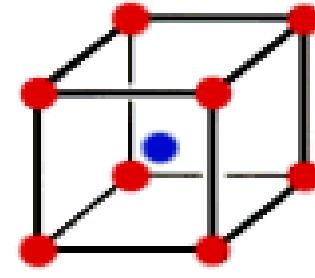
$$a = b = c \quad \alpha = \beta = \gamma = 90^\circ$$



**Simple  
cubic**



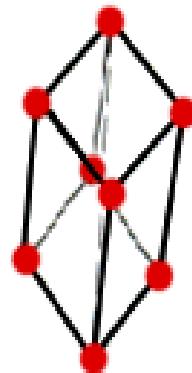
**Face-centered  
cubic**



**Body-centered  
cubic**

**Trigonal/ Rhombohedral:** In the Trigonal system, is usually chosen as the primitive cell. In this case

$$a = b = c$$

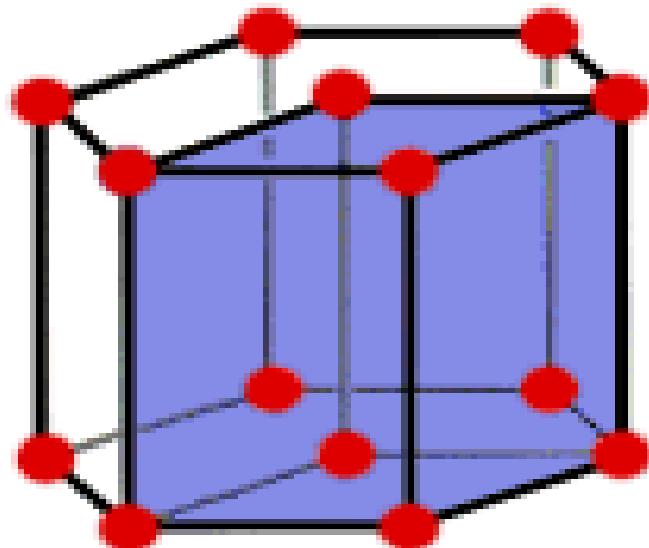


$$\alpha = \beta = \gamma \neq 90^\circ$$

**Rhombohedral**

**Hexagonal:** In the Hexagonal system, the lattice is primitive and for this  $a = b \neq c$

$$\alpha = \beta = 90^\circ$$
$$\gamma = 120^\circ$$



**Hexagonal**

# Lecture-4

## Packing Factor

- Atomic Radius
- Packing factor
- Coordination number

# Atomic Radius

It is defined as half the distance between nearest neighbors in a crystal of a pure element. Usually, it is expressed in terms of the cube edge  $a$ . It must be remembered that any two nearest neighboring atoms touch each other.

## Atomic Radius for different structures

**Simple Cubic Structure:** In fig.1. (a) and (b),  $AB$  represents the atomic radius. It is obvious from fig.1. (a) and (b) that  $r = \frac{a}{2}$ .

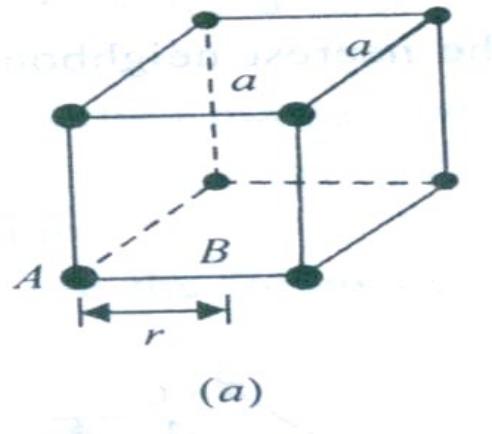
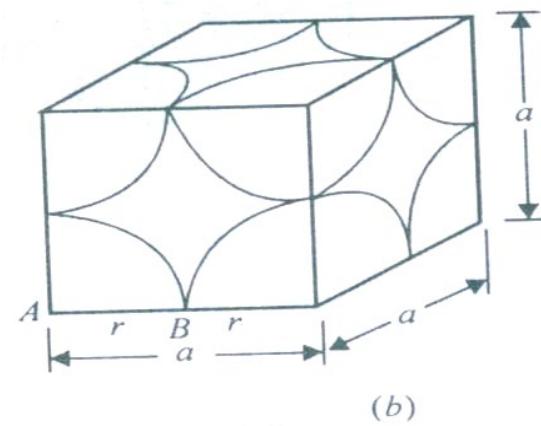
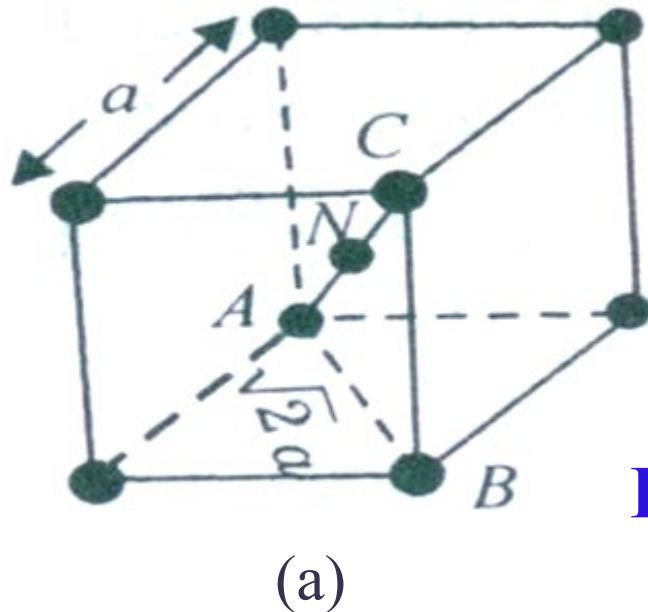


Fig. 1.



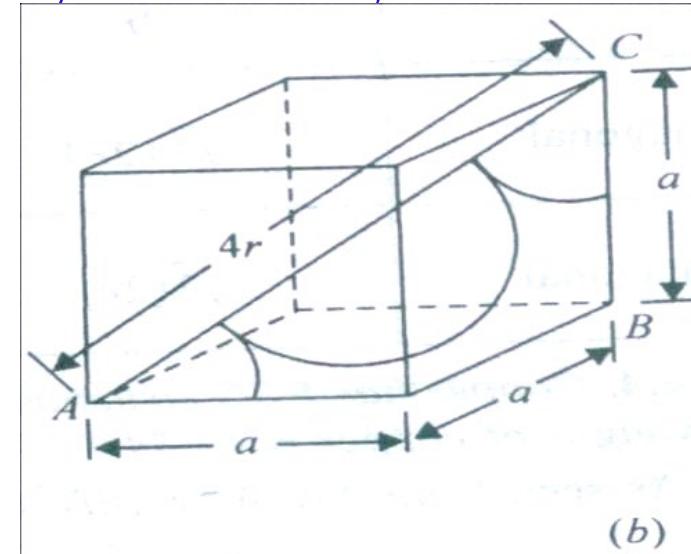
**Body Centered Cubic Structure** As seen from fig. 2 (a), atoms C and N are the nearest neighbours. By definition,  $r = CN/2$ .



$$\text{Now, } AC = \sqrt{AB^2 + BC^2} = \sqrt{(\sqrt{2}a)^2 + a^2} = \sqrt{3}a$$

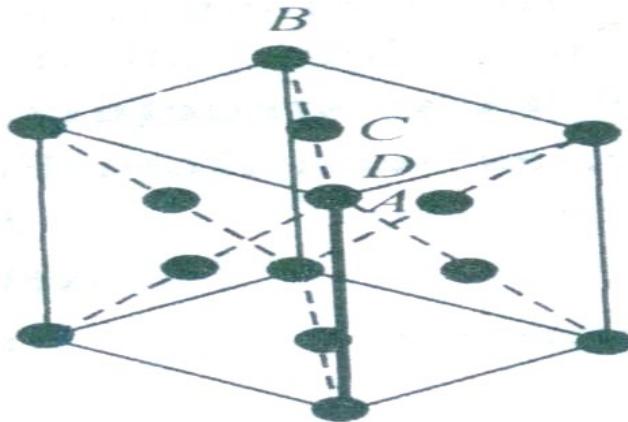
$$\text{But } r = \frac{CN}{2} = \frac{AC}{4} = \frac{\sqrt{3}a}{4}$$

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



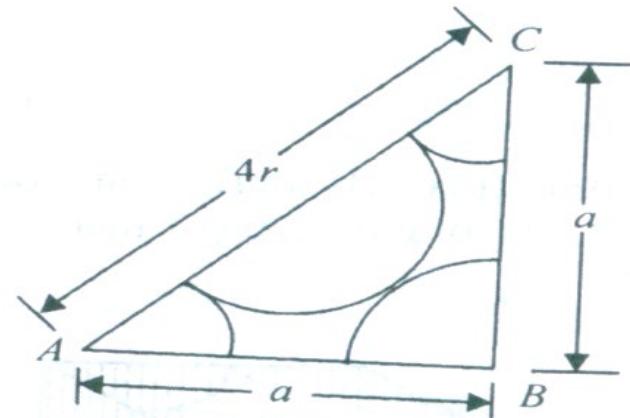
A more detailed view is shown in fig. 2 (b), where solid diagonal AC equals four times the radius of a single atom.

**Face Centered Cubic Structure** Here, as seen from fig. 3 (a), atoms A and C are the nearest neighbours.



(a)

Fig. 3.



(b)

Hence,  $r = AD = \frac{AC}{2} = \frac{AB}{4}$

Now,  $AB = \sqrt{2}a \quad \therefore r = \frac{\sqrt{2}a}{4}$

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

Fig. 3 (b) shows more detailed view of the same. Here surface diagonal AC equals four times the atomic radii.

## Packing factor

The fraction of the space occupied by the atoms in the unit cell is known as atomic packing factor or simply packing factor. It is the ratio of the volume of the atoms occupying the unit cell to the volume of the unit cell relating to that structure.

$$\therefore \text{Packing factor} = \frac{\text{Volume of all the atoms}}{\text{Volume of the unit cell}}$$

## Packing factor for different structures

**Simple Cubic Structure** In simple cubic structure, eight atoms are at the eight corners of the cell and each atom is common for eight cubes.

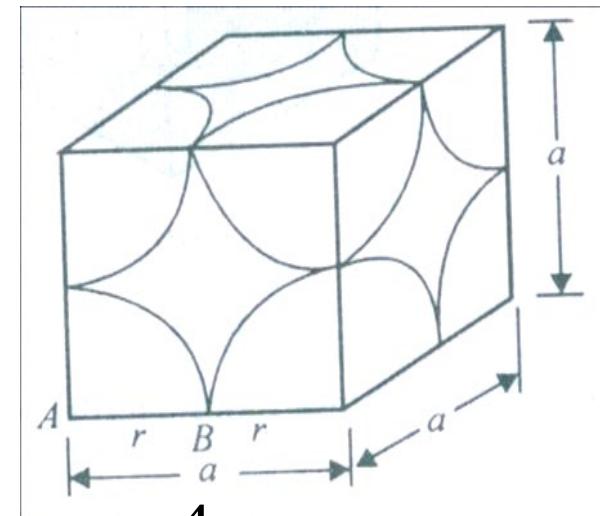
Thus the total number of atoms in a unit cell of simple cubic

$$\text{lattice is } = 0 + \frac{0}{2} + \frac{8}{8} = 1$$

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

$$\text{From the figure, atomic radius, } r = \frac{a}{2}$$

$$\text{Volume of the unit cell} = a^3 = (2r)^3 = 8r^3$$



$$\therefore \text{Packing factor} = \frac{\text{Volume of all the atoms}}{\text{Volume of the unit cell}} = \frac{\frac{4}{3} \pi r^3}{8r^3} = \frac{\pi}{6} = 0.52$$

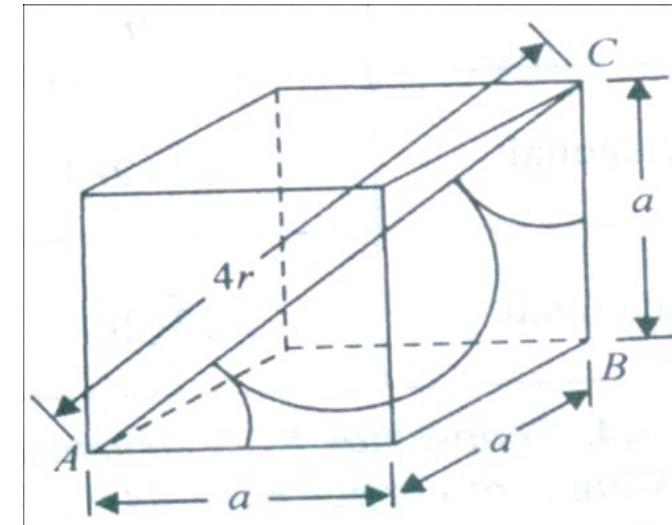
Thus, the packing factor of simple cubic structure is 0.52 means that, 52% of the total volume of the simple cubic unit cell is filled with the atoms.

# Body Centered Cubic Structure

**Body Centered Cubic Structure** In body centered cubic structure, eight atoms are at the eight corners and one atom is inside the cell. Thus the total number of atoms in a unit cell of body centered cubic lattice is  $= 1 + \frac{0}{2} + \frac{8}{8} = 2$

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

$$\therefore \text{Volume of all the atoms} = 2 \times \frac{4}{3}\pi r^3 = \frac{8}{3}\pi r^3$$



$$\text{From the figure, } AC = \sqrt{AB^2 + BC^2} = \sqrt{(\sqrt{2}a)^2 + a^2} = \sqrt{3}a$$

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

## Body Centered Cubic Structure:

$$\text{volume of the unit cell} = a^3 = \left( \frac{4r}{\sqrt{3}} \right)^3 = \frac{64r^3}{3\sqrt{3}}$$

$$\therefore \text{Packing factor} = \frac{\text{Volume of all the atoms}}{\text{Volume of the unit cell}}$$

$$= \frac{\frac{8}{3}\pi r^3}{\frac{64r^3}{3\sqrt{3}}} = \frac{\pi\sqrt{3}}{8} = 0.68$$

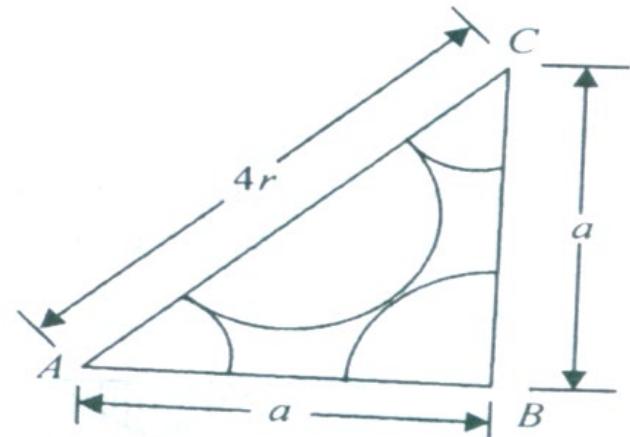
Thus, the packing factor of body centered cubic structure is 0.68 means that, 68% of the total volume of the body centered cubic unit cell is filled with the atoms.

## Face Centered Cubic Structure

**Face Centered Cubic Structure** In face centered cubic structure, eight atoms are at the eight corners and all (six) the faces centered. Thus the total number of atoms in a unit cell of face centered cubic lattice is  $= 0 + \frac{6}{2} + \frac{8}{8} = 4$

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

$$\therefore \text{Volume of all the atoms} = 4 \times \frac{4}{3} \pi r^3 = \frac{16}{3} \pi r^3$$



$$\text{From the figure, } AC = \sqrt{AB^2 + BC^2} = \sqrt{a^2 + a^2} = \sqrt{2}a$$

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

## Face Centered Cubic Structure

$$\text{volume of the unit cell} = a^3 = (2\sqrt{2}r)^3 = 16\sqrt{2}r^3$$

$$\therefore \text{Packing factor} = \frac{\text{Volume of all the atoms}}{\text{Volume of the unit cell}}$$

$$= \frac{\frac{16}{3}\pi r^3}{16\sqrt{2}r^3} = \frac{\pi}{2\sqrt{3}} = 0.74$$

Thus, the packing factor of face centered cubic structure is 0.74 means that, 74% of the total volume of the face centered cubic unit cell is filled with the atoms.

# **Coordination Number**

The number of oppositely charged ions surrounding any particular ion in an unit cell is called the coordination number of that particular ion.

By coordination number, it is meant the number of nearest neighbors which an atom has in the unit cell of any crystal structure.

## **Coordination Number for different structures**

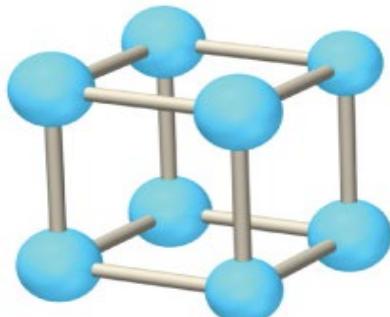
### **Simple Cubic Structure**

In this case, the coordination number is six. It is so because each corner atom is linked with seven other unit cells that can be imagined to be built around the unit cell containing the atom.

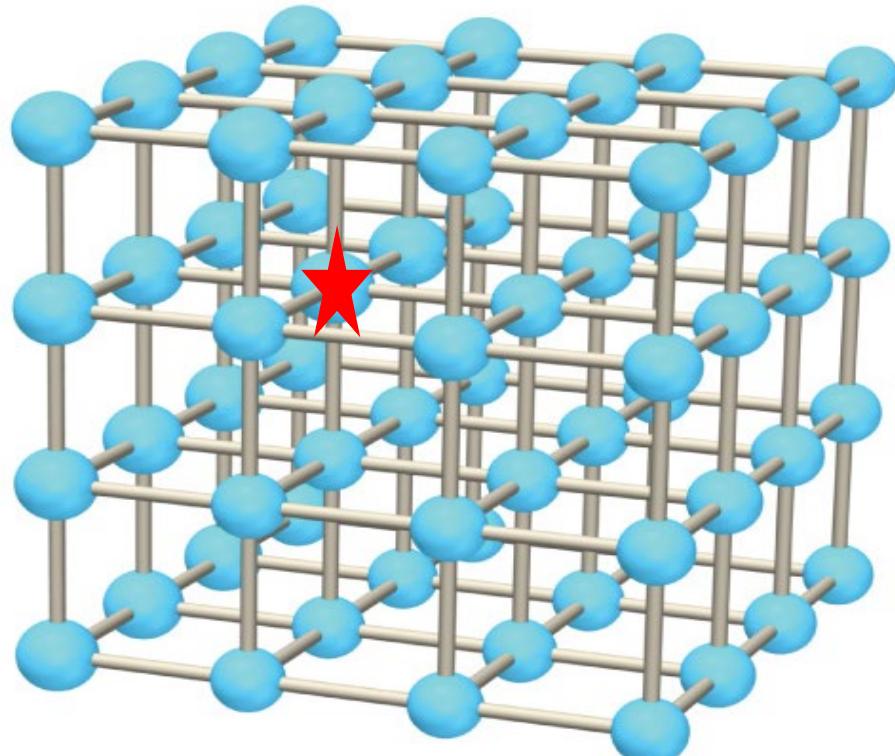
## Simple Cubic Structure

In this case, each corner atom has four neighbors in the same plane, one vertically above and one immediately below, giving a total of six nearest neighboring atoms.

- Coordination # = 6  
(# nearest neighbors)



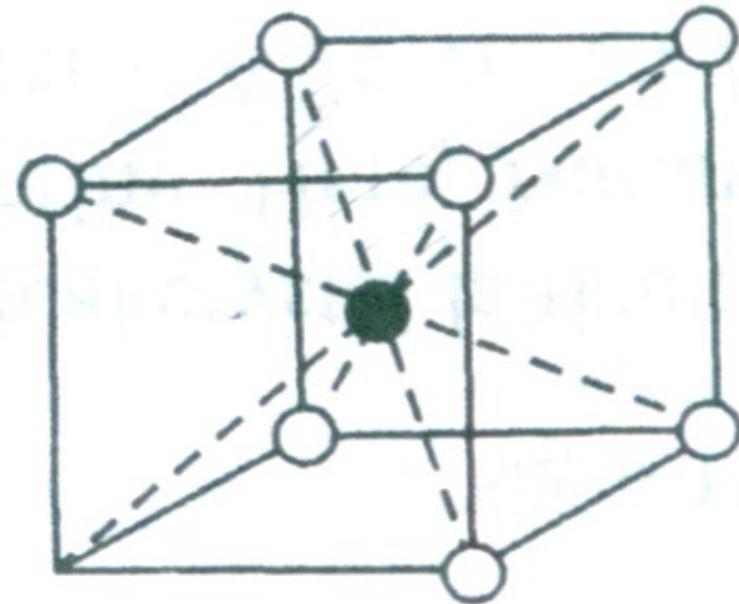
(a)



(b)

## Body Centered Cubic Structure

It should be noted that in this case, the nearest neighbors of any corner atom are the body-centered atoms. Since, there are eight surrounding unit cells for any corner atom, their eight-centered atoms from the nearest neighbors for any corner atom.

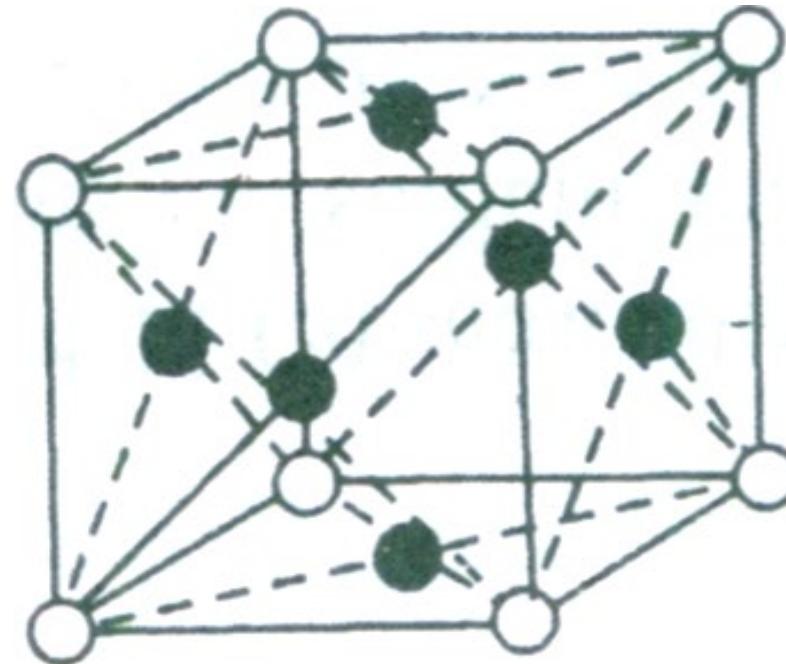


- Coordination # = 8  
(# nearest neighbors)

## Face Centered Cubic Structure

The coordination number is twelve. In this case, 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 a plane above it and four in a plane below it.

- Coordination # = 12  
(# nearest neighbors)



# WELCOME

PHY-103

## Structure of Matter

Lecture-3

# Lecture-3

## Miller Indices

- Relation between the lattice constant and the density of crystal material.
- Mathematical Problems.
- Miller indices.
- Determination of Miller Indices.
- Direction of plane.

## Relation between lattice constant & density of crystal material

Consider a unit cell with volume  $V$  (cm<sup>3</sup>). Let  $\rho$  (gm/cm<sup>3</sup>) be the density of the crystal. The weight of the matter in the unit cell is  $V \times \rho$

If  $n$  is the number of atoms or molecules per unit cell and  $M$  being the atomic (molecular) weight of one atom or molecule. Then the weight of matter in the unit cell is given by  $n \frac{M}{N}$ ,  $N$  is the Avogadro's no.

$$\text{Thus, } n \frac{M}{N} = V \times \rho; \quad \therefore n = \frac{V \times \rho \times N}{M}$$

$$\text{For a cubic crystal, } V = a^3. \text{ Thus } n = \frac{a^3 \times \rho \times N}{M}$$

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

$$r = ?$$

## Mathematical Problems

**Problem-1:** The atomic weight of silver is 108. It has lattice constant 4.077 Å. Calculate the density of silver if it has the fcc structure.

**Problem-2:** Calculate the number of atoms per unit cell for a face centered cubic (fcc) lattice of copper crystal. Given  $a = 3.60 \text{ \AA}$ , Atomic weight of copper = 63.6 and density of copper = 8.86.

**Problem-3:** NaCl has fcc structure. The density of sodium chloride is  $2180 \text{ kg/m}^3$ . Calculate the distance between two adjacent atoms. Given the atomic weight of sodium=23 and the Chlorine=35.5. Take  $N = 6.023 \times 10^{26}$  per kg-mole.

**Problem-4:** Iron has bcc structure. Its density is  $7.86 \text{ kg/m}^3$ . Atomic weight of Iron is 55.85. Calculate the dimension of the unit cell.

## Miller indices

The position and orientation of a crystal plane is determined by three numbers is called **Miller indices**. It is denoted by  $(h k l)$ .

### Determination of Miller Indices of a plane

- Taking any atom in the crystal as the origin and erect coordinate axes from this atom.
  - Taking intercepts on the axis  $a, b, c$  in terms of the lattice constants.
  - Taking the reciprocal of these intercepts.
  - Taking the lowest common multiple of the denominator.
  - Multiplying each reciprocal by the lowest common multiple of the denominator, thus obtained into smallest set of integers.
- These integers are denoted by  $h, k, l$ .

➤ The result is conventionally enclosed in first parenthesis  $(hkl)$  which is Miller indices of the plane. The meaning of these indices is that a set of parallel planes  $(hkl)$  cuts the  $a$ -axis into  $h$  parts, the  $b$ -axis into  $k$  parts and the  $c$ -axis into  $l$  parts.

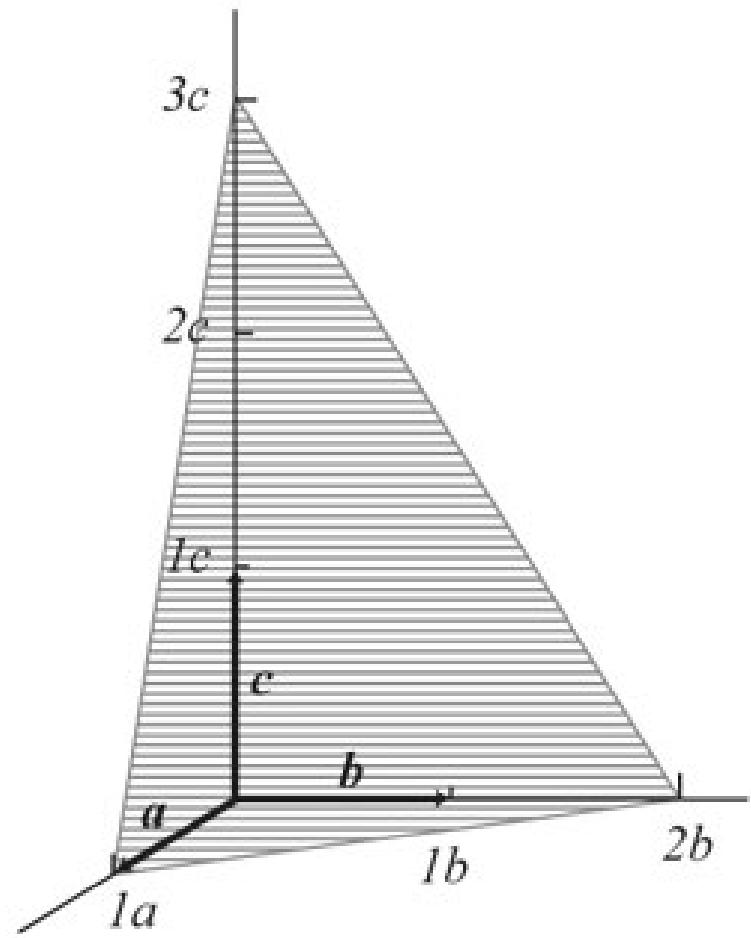
**While finding MI of a plane, following points should be kept in mind:**

- When the plane is parallel to one of the coordinate axes, it is said to meet that axis at infinity. Since  $\frac{1}{\infty} = 0$  the miller index for that axis is zero.
- If a plane cuts on axis on the negative side of the origin, the corresponding index is negative and is indicated by a bar sign, above the index  $(\overline{h}\overline{k}\overline{l})$ .

# Importance or Uses of Miller Indices

- In Materials Science it is important to have a notation system for atomic planes since these planes influence
  - Optical properties
  - Reactivity
  - Surface tension
  - Dislocations

**Example:** The figure shows a plane whose intercepts are  $1a$ ,  $2b$ ,  $3c$ . The Miller indices of the family to which this plane belongs are obtained by taking the reciprocals of these numbers :  $1, \frac{1}{2}, \frac{1}{3}$  and reducing these fractions to the smallest set of integers. This can be done by multiplying each of the fractions by the lowest common multiple of the denominator 6. In this case we get  $6, 3, 2$ .



**Thus the Miller indices of this plane are  $(632)$**

## Miller indices for planes in each of the following sets of intercepts:

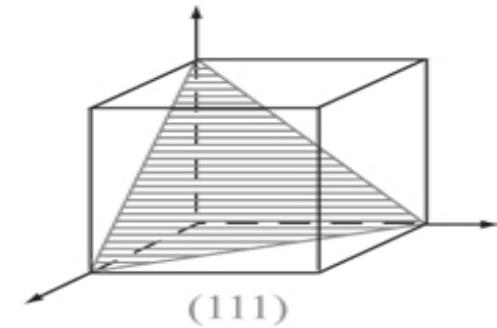
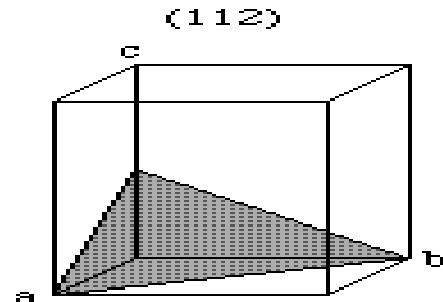
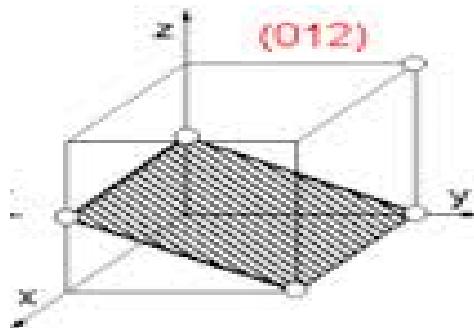
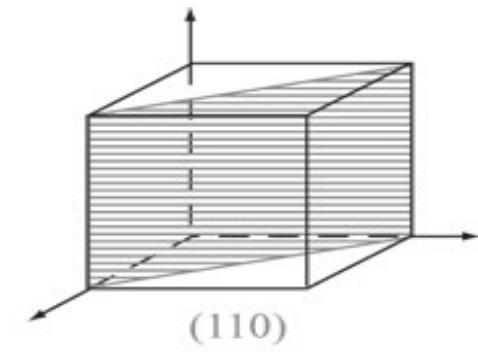
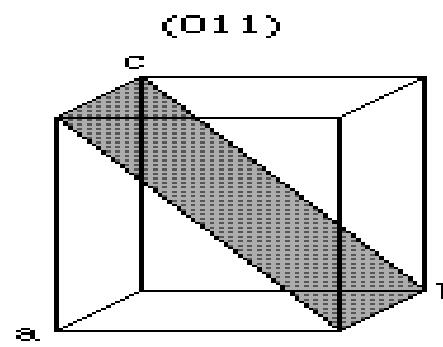
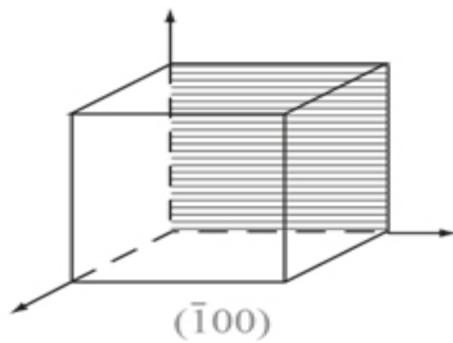
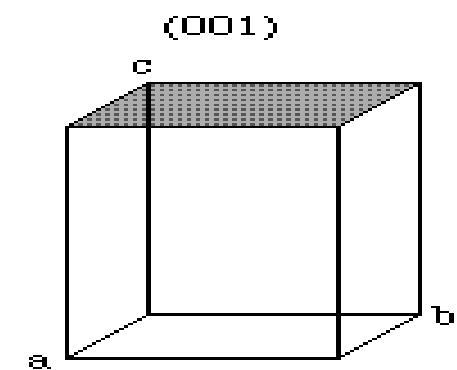
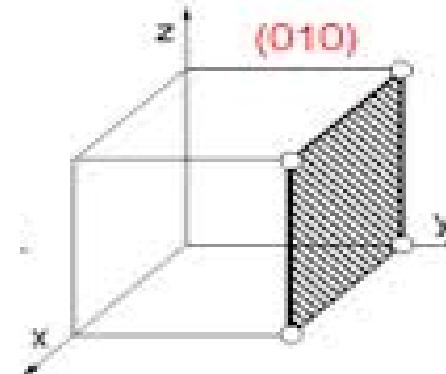
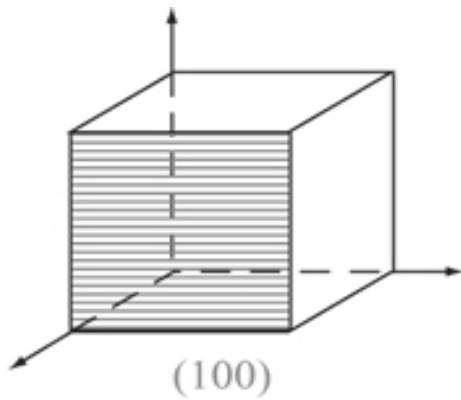
$$i) a, 2b, \infty; \quad ii) a, \frac{b}{2}, c; \quad iii) 3a, 3b, 3c$$

i. It indicates a plane whose intercepts are  $a, 2b, \infty$ . For  $c$ -axis the intercept is at  $\infty$ . The Miller indices of the family to which this plane belongs are obtained by taking the reciprocals of these numbers:  $1, \frac{1}{2}, \frac{1}{\infty}$ . From this we can write :  $1, \frac{1}{2}, 0$ . For reducing these fractions to the smallest set of integers, multiply each of the fractions by the lowest common multiple of the denominator 2. In this case we get the Miller indices  $(2, 1, 0)$ .

**ii.** It indicates a plane whose intercepts are  $a$ ,  $b/2$ ,  $c$ . The Miller indices of the family to which this plane belongs are obtaining by taking the reciprocals of these numbers: 1, 2, 1 and reducing these fractions to the smallest set of integers. This can be done by multiplying each of the fractions by the lowest common multiple of the denominator 1. In this case we get the Miller indices (1, 2, 1).

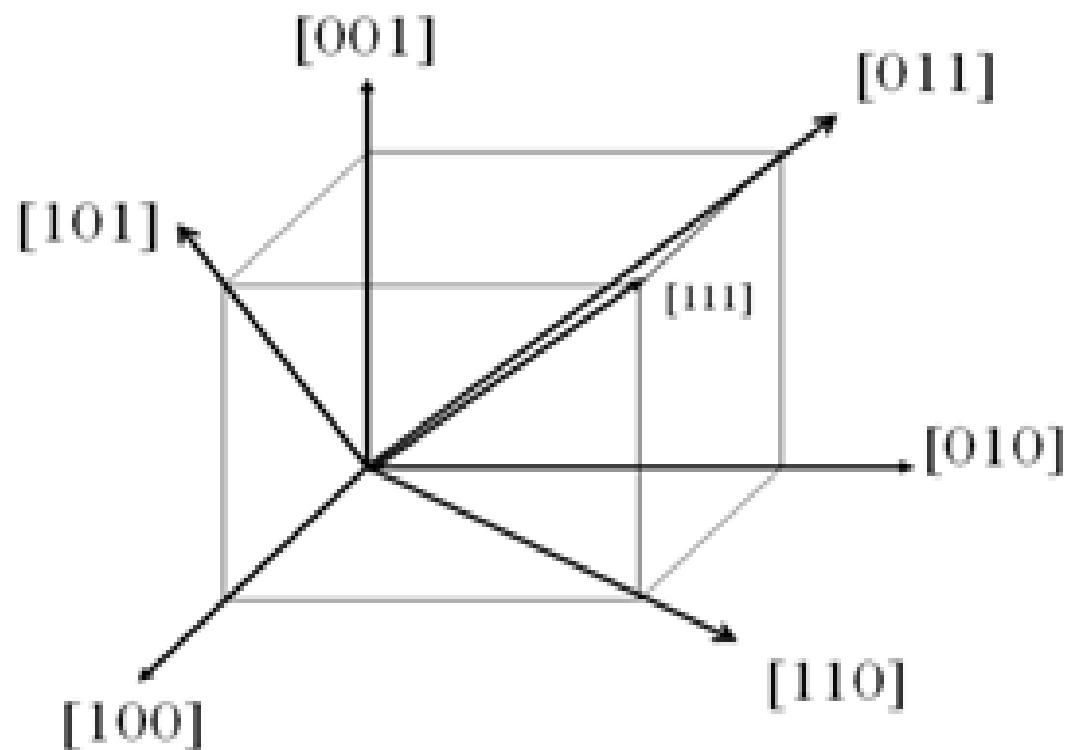
**iii.** It indicates a plane whose intercepts are  $3a$ ,  $3b$ ,  $3c$ . The Miller indices of the family to which this plane belongs are obtaining by taking the reciprocals of these numbers:  $1/3$ ,  $1/3$ ,  $1/3$ . and reducing these fractions to the smallest set of integers. This can be done by multiplying each of the fractions by the lowest common multiple of the denominator 3. In this case we get the Miller indices (1, 1, 1).

# Drawing planes from Miller indices



## Direction of plane

Any vector drawn from the origin to a lattice point is defined as **direction**. It is denoted by  $[hkl]$ . For example, in a cubic unit cell, if the origin is at the corner and axes are parallel to the edges, the body diagonal would be represented as  $[111]$ .



## Direction of plane

$[hkl]$ : The direction specified by this symbol is obtained as follows: Move from the origin over a distance  $ha$  along the  $a$ -axis,  $kb$  along the  $b$ -axis and  $lc$  along the  $c$ -axis. The vector connecting the origin with the point so obtained is then the direction specified by the symbol  $[hkl]$ .

Thus in a cubic crystal, the direction of the X-axis is indicated by  $[100]$ , the Y-axis by  $[010]$  and the Z-axis by  $[001]$ . Similarly, the direction of the negative X-axis is indicated by  $[\bar{1}00]$ , the negative Y-axis by  $[0\bar{1}0]$  and the negative Z-axis by  $[00\bar{1}]$ .

### In cubic crystal [hkl] direction is normal to the (hkl) plane:

Let OP be the direction of [hkl] and ABC be the (hkl) plane. Again, let  $x_0$ ,  $y_0$  and  $z_0$  are the intercepts of the plane (hkl) along X, Y and Z directions.

Miller indices are  $\frac{1}{x_0}, \frac{1}{y_0}, \frac{1}{z_0}$ .

and the reduced indices becomes  $\frac{g}{x_0}, \frac{g}{y_0}, \frac{g}{z_0}$

Where  $g$  is an integer.

For cubic lattice  $h = k = l = 1$ .

Or  $x_0 = y_0 = z_0 = a$ .

And the direction  $\overrightarrow{OP} = \left( i\frac{g}{a} + j\frac{g}{a} + k\frac{g}{a} \right)$

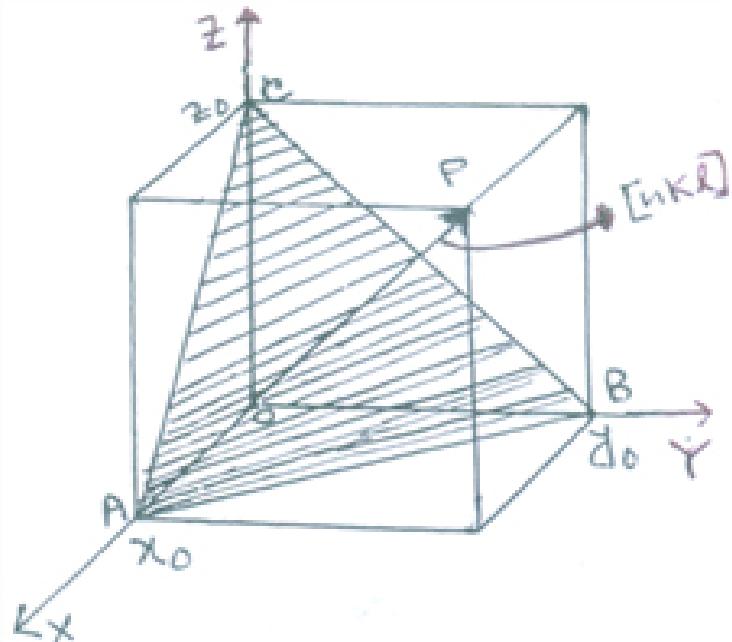
But  $\overrightarrow{AB} = \overrightarrow{OB} - \overrightarrow{OA} = j\frac{g}{a} - i\frac{g}{a}$

$$\text{Now } \overrightarrow{OP} \cdot \overrightarrow{AB} = \left( i\frac{g}{a} + j\frac{g}{a} + k\frac{g}{a} \right) \cdot \left( j\frac{g}{a} - i\frac{g}{a} \right) = -\frac{g^2}{a^2} + \frac{g^2}{a^2} = 0$$

Similarly we can write  $\overrightarrow{OP} \cdot \overrightarrow{BC} = 0$ ,  $\overrightarrow{OP} \cdot \overrightarrow{CA} = 0$ .

Hence the dot product of  $\overrightarrow{OP}$  with  $\overrightarrow{AB}$ ,  $\overrightarrow{BC}$  and  $\overrightarrow{CA}$  is zero. So,  $\overrightarrow{OP}$  is normal to  $\overrightarrow{AB}$ ,  $\overrightarrow{BC}$  or  $\overrightarrow{CA}$ .

Hence [hkl] direction is normal to the (hkl) plane.



## What is meant by {100}?

A family of planes of a particular type is represented by enclosing the Miller Indices of any one of that family into curly brackets (braces). Thus  $\{100\}$  represents the family of planes which has the planes  $(100)$ ,  $(010)$ ,  $(001)$ ,  $(\bar{1}00)$ ,  $(0\bar{1}0)$ ,  $(00\bar{1})$  as its members. The six planes represent the faces of the cube.

# Lecture-5

- Interplaner spacing
- Bragg's law

# Interplaner spacing

The perpendicular distance between successive planes of lattice point is called **interplaner spacing**. For a plane  $(hkl)$  it is denoted by  $d_{hkl}$ . It is also known as ***d*-spacing**.

## Expression for the interplaner spacing between the adjacent (hkl) planes

Consider a family of parallel planes  $(hkl)$ . The spacing  $d_{hkl}$  between the adjacent planes of this family can be calculated by taking any lattice point as origin and erecting the coordinate axes in  $OA$ -,  $OB$ -,  $OC$ -directions and finding the perpendicular distance between this origin and the planes which is nearest to the origin. This plane would obviously have  $a/h$ ,  $b/k$ ,  $c/l$  intercepts on the axes at  $A$ ,  $B$ ,  $C$  respectively.

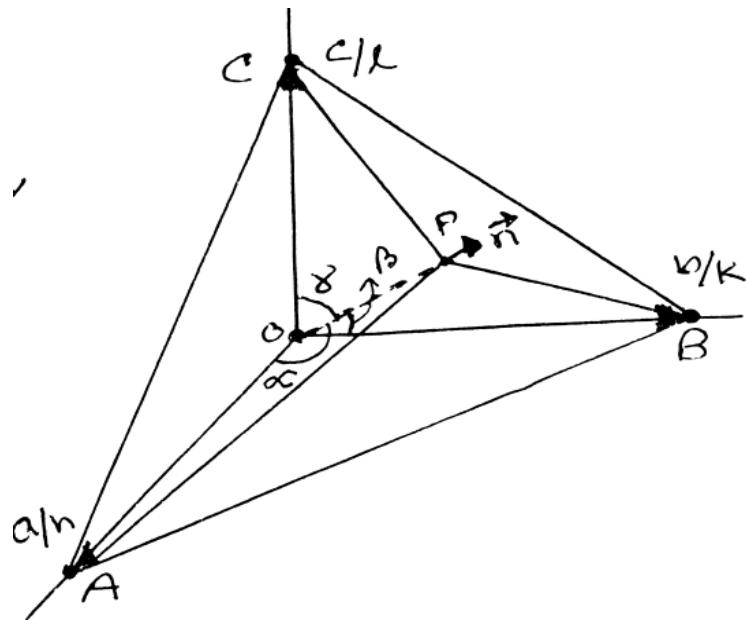


Fig. 1.

Further,  $OP = d_{hkl}$ , be the normal to the plane drawn from the origin and makes angle  $\alpha, \beta, \gamma$  with the three axes respectively. Therefore

$$OA = \frac{a}{h}, OB = \frac{b}{k} \text{ and } OC = \frac{c}{l}$$

From the triangle  $\Delta OPA$

$$\cos \alpha = \frac{OP}{OA} = \frac{d_{hkl}}{\frac{a}{h}} \quad (1)$$

Similarly, from the triangle  $\Delta OPB$  &  $\Delta OPC$

$$\cos \beta = \frac{OP}{OB} = \frac{d_{hkl}}{\frac{b}{k}} \quad (2)$$

$$\cos \gamma = \frac{OP}{OC} = \frac{d_{hkl}}{\frac{c}{l}} \quad (3)$$

According to the direction of properties of Cosine, we get

$$\cos^2 \alpha + \cos^2 \beta + \cos^2 \gamma = d_{hkl}^2 \left[ \frac{1}{\left(\frac{a}{h}\right)^2} + \frac{1}{\left(\frac{b}{k}\right)^2} + \frac{1}{\left(\frac{c}{l}\right)^2} \right]$$

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

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

This is the expression for the interplaner spacing.

What is the value of interplaner spacing for cubic crystal?

## X-ray diffraction

When a beam of monochromatic X-rays falls on a crystal, it is scattered by the individual atoms which are arranged in set of parallel layers. Each atom becomes a source of scattered radiations. The combined scattering of X-rays from these planes can be looked upon as *reflections* from these *planes*. Because of this Bragg scattering is usually referred to as Bragg reflection and these planes are known as *Bragg planes*.

For certain glancing angles, reflections from these sets of parallel planes are in phase with each other. Hence, different reflected X-rays reinforce each other so that the resulting reflection is exceptionally strong.

For some other values of glancing angle, the X-rays reflections from different planes are anti phase with other so that the resulting reflection is either zero or extremely feeble. Obviously, as the glancing angle is change by rotating, a series of alternate maxima and minima of intensity is obtained.

# Bragg's law

**Fig. 2.**

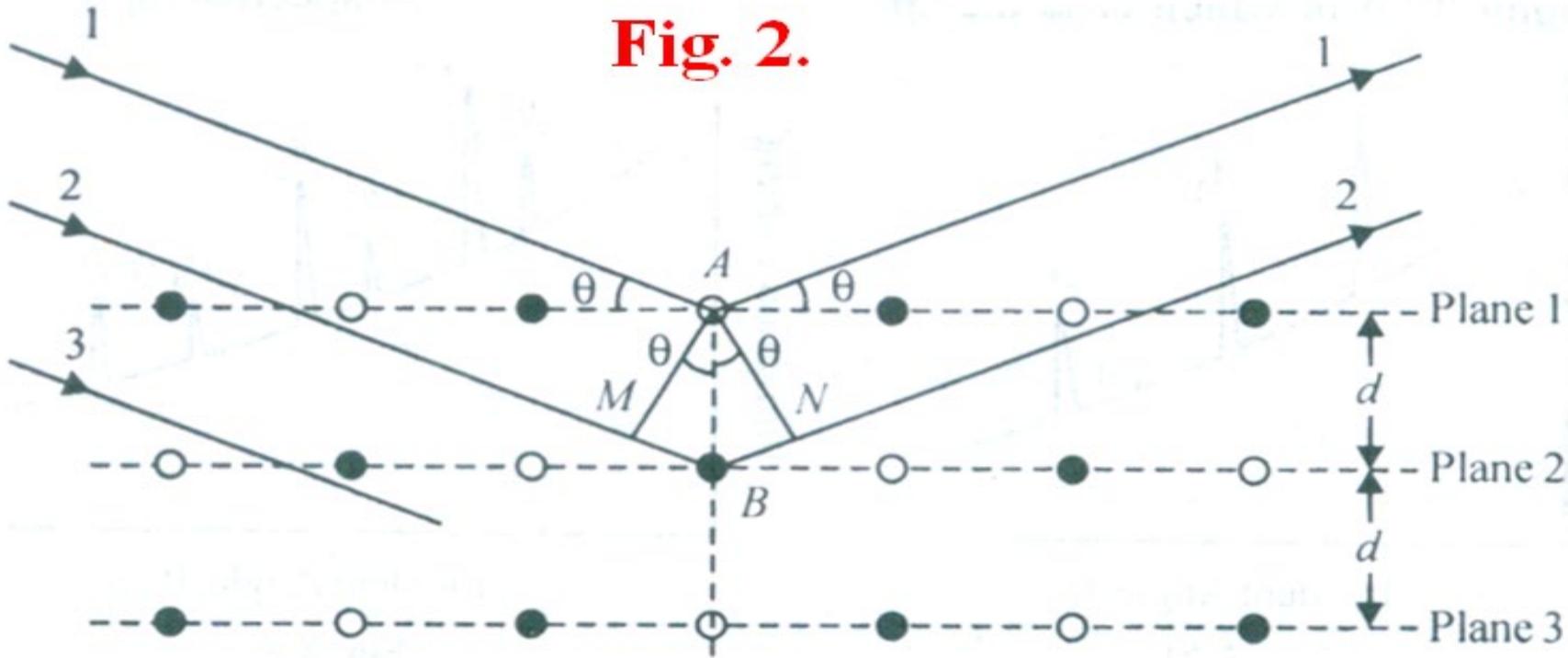


Fig. 2. Shows a beam of monochromatic X-rays incident at a glancing angle on a set of parallel planes. The beam is partially reflected at the successive layers rich in atoms. Ray no. 1 is reflected from atom  $A$  in plane 1 whereas ray no. 2 is reflected from atom  $B$  lying in plane 2 immediately below atom  $A$ .

## Bragg's law

Whether two reflected rays will be in phase or ant phase with other will depend on their path difference. This path difference can be found by drawing perpendiculars  $AM$  and  $AN$  on ray no. 2. Since the two rays travel the same distance from points  $A$  and  $N$  onwards, it is obvious that ray no. 2 travels an extra distance =  $MB + BN$ .

Hence, the path difference between the two reflected beams

$$= MB + BN = d \sin \theta + d \sin \theta = 2d \sin \theta$$

Where  $d$  is the interplaner spacing i.e. vertical distance between two adjacent planes belonging to the same set.

The two reflected beams will be in phase with each other if this path difference equals an integral multiple of  $\lambda$  and will be anti phase if it equals an odd multiple of  $\lambda/2$ .

Hence, the condition for producing maxima becomes

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

Where  $n = 1, 2, 3, \dots$  etc for the first-order, second-order and third order maxima respectively. This relation is known as **Bragg's law**.

If we substitute the value of  $d$  in terms of the Miller indices of the planes for a cubic system, we get

$$2 \frac{a}{\sqrt{h^2 + k^2 + l^2}} \sin \theta = n\lambda$$

From this we can calculate the wavelength of X-rays ( $\lambda$ ), if the Miller indices of a certain plane are given as  $(h, k, l)$ .

# Lecture-6

- Atomic arrangement in solid
- Characteristics of Ionic solids

## **Atomic arrangement in solid**

As compared to gaseous and liquid state, the atoms and molecules in solid state are more closely-packed and are held together by strong mutual forces of attraction. These interatomic forces are basically electrostatic in nature and are a direct consequence of the electronic structure of matter. When atoms come close and finally unite to form molecules, their electrons *rearrange themselves in such a way as to achieve a stable configuration*. This rearrangement of electrons gives rise to different types of bonds which hold the atoms together in a solid state. The principle types of bonds in solids are:

1. Ionic or electrovalent bonds
2. Covalent or homopolar bonds
3. Metallic bonds *and*
4. Molecular bonds (Van der Waal's forces)

## Atomic arrangement in solid

These bonds are electrostatic in origin and, in many cases, determine the characteristic physical properties of a solid.

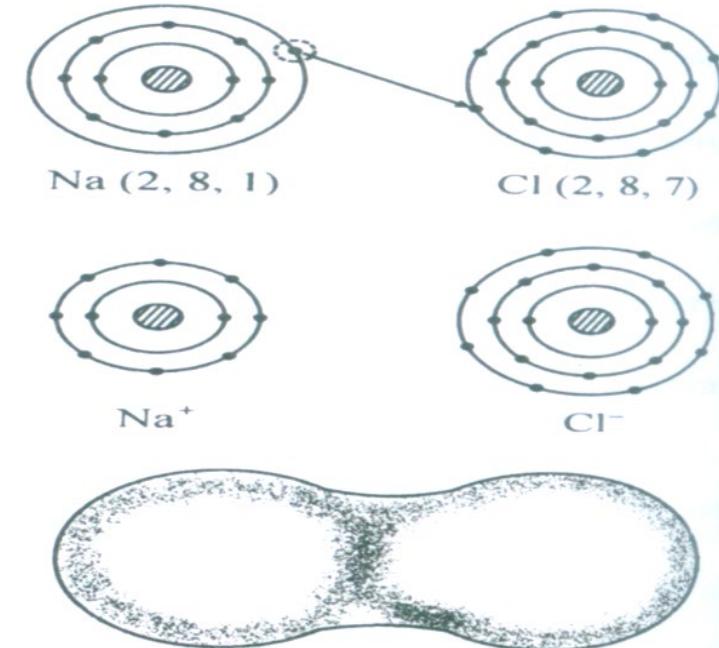
Depending on the **type of bonding force**, the different solids may be categorized as follows:

1. Ionic or electrovalent solids: NaCl, MgO, CaF<sub>2</sub>.
2. Covalent or homopolar solids: C, Si, Ge.
3. Metallic solids: Na, Al, Cu, Ag.
4. Molecular solids: Solid Ar, solid Kr and solid Xe.

## Ionic bonds

Ionic bonding is the electrostatic force of attraction between positively and negatively charged ions (between non-metals and metals). These ions have been produced as a result of a transfer of electrons between two atoms with a large difference in electro negativities. The metallic elements have only up to the valence electrons in their outer shell will lose their electrons and become positive ions, whereas electronegative elements tend to acquire additional electrons to complete their octet and become negative ions. NaCl is a typical example of ionic bonding.

Consider the formation of ionic bond in NaCl. Notice that when sodium loses its one valence electron it gets smaller in size, while chlorine grows larger. After the reaction takes place, the charged  $\text{Na}^+$  and  $\text{Cl}^-$  ions are held together by electrostatic forces, thus forming an ionic bond.



**Fig. 1. Ionic bond**

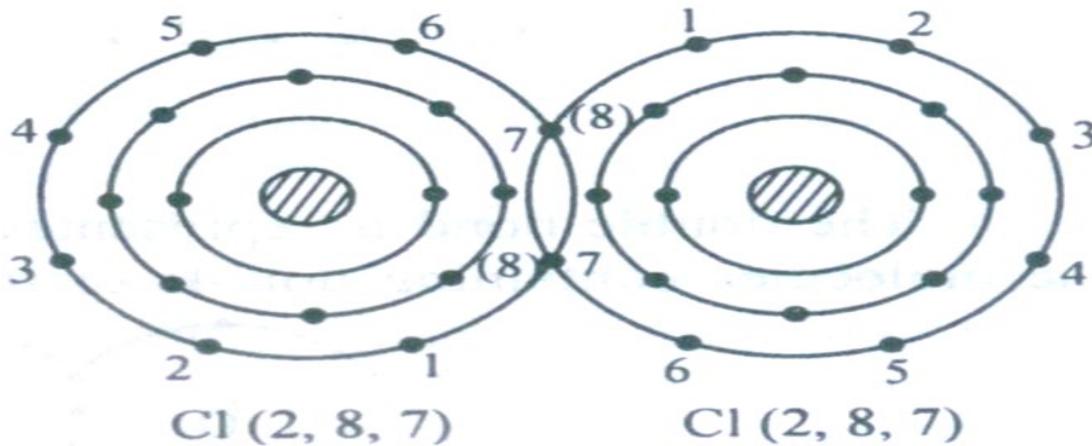
When the  $\text{Na}^+$  and  $\text{Cl}^-$  ions approach each other closely enough so that the orbits of the electron in the ions begin to overlap each other, then the electron begins to repel each other by virtue of the repulsive force. But the repulsive forces are of shorter range than the attractive one.

## Covalent bonds

A covalent bond is formed when two similar or dissimilar atoms (*between non-metals and non-metals*) achieve stability by sharing valence electrons (*i.e., s and p electrons*) between themselves. By sharing electrons, the two atoms, acquire the noble gas electronic configuration. The compound so formed is known as *covalent* compound. Each electron in a shared pair is attracted to both nuclei involved in the bond.

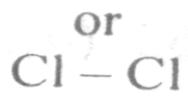
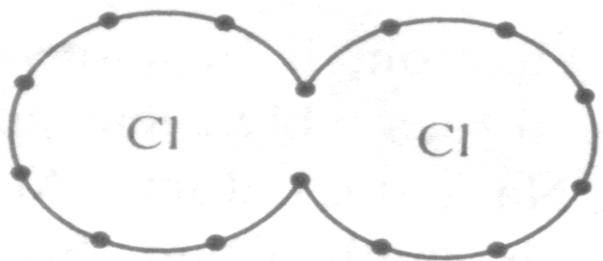
Consider the case of Cl atoms. As shown in fig. 2, each Cl atom has 7 valence electrons. Covalent bond is established between the two atoms because each contributes one electron and the electron *pair* is shared by the two atoms so that each has 8 electrons in its valence shell thereby achieving stability, *i.e.*, each chlorine atom achieves argon structure.

## Covalent bonds

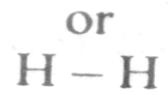
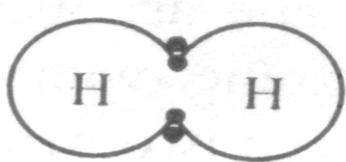


**Fig. 2. Covalent bond**

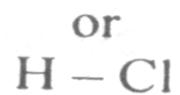
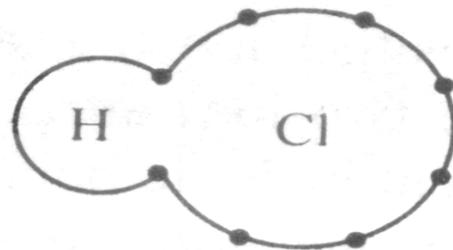
For clarity sake, the two electrons have been shown by dots and crosses in fig. 3(a). Similarly, covalent bond between hydrogen atoms is created due to their sharing their  $1s$  electrons [Fig. 3(b)]. The two hydrogen atoms acquire helium structure. Fig. 3(c) shows covalent bond between hydrogen and chlorine atoms. In this case, hydrogen achieves helium structure whereas chlorine achieves the argon structure.



(a)



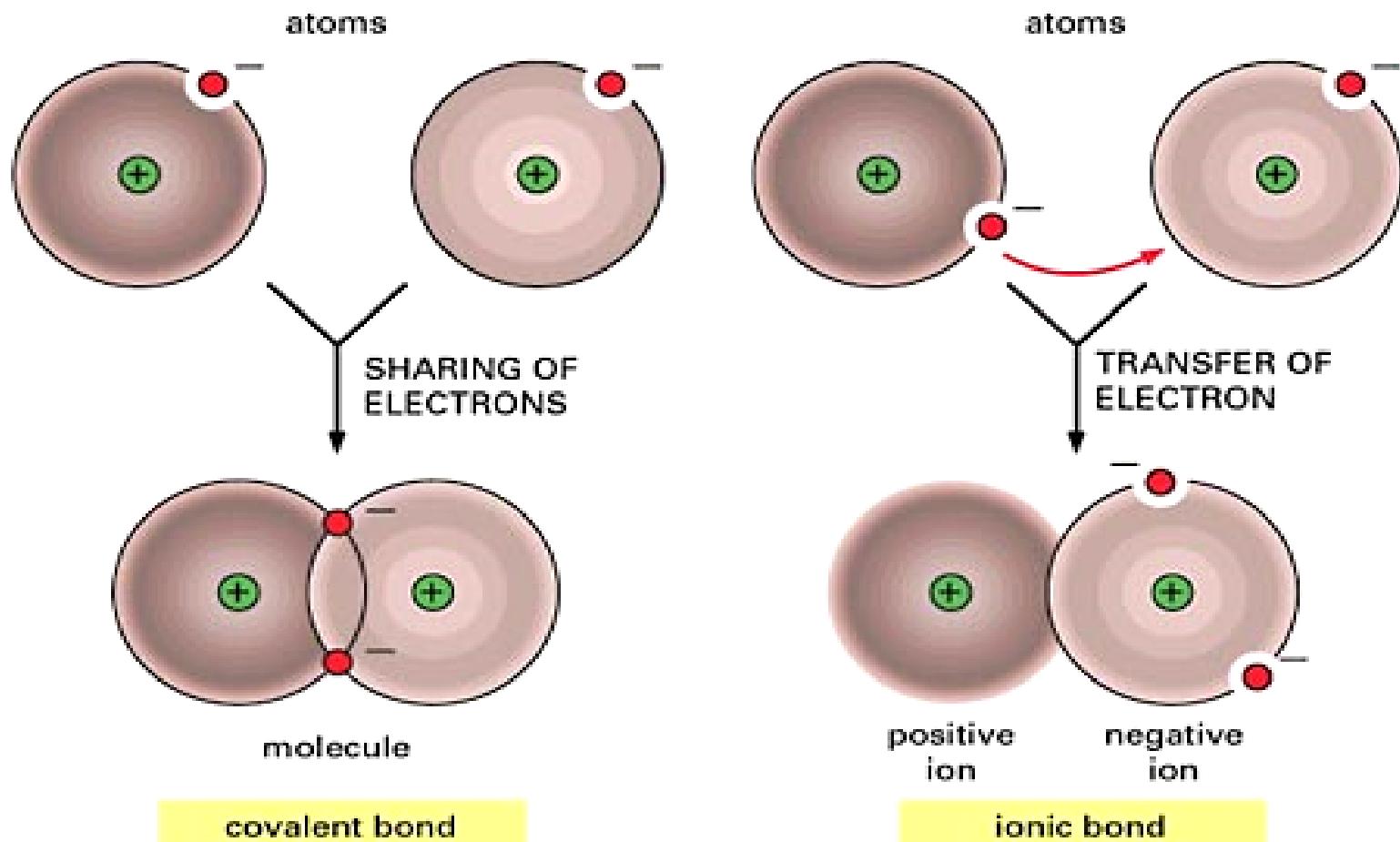
(b)



(c)

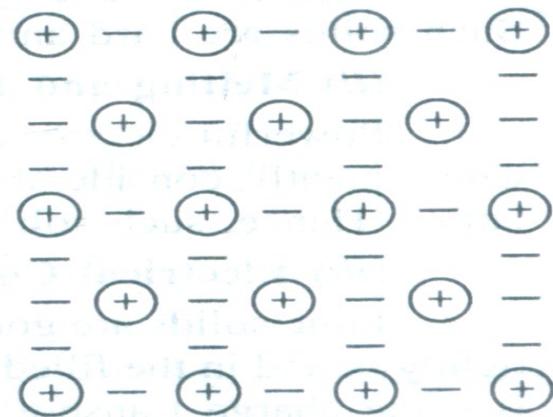
Fig. 3. Covalent bond

# Comparison-Ionic and Covalent Bond

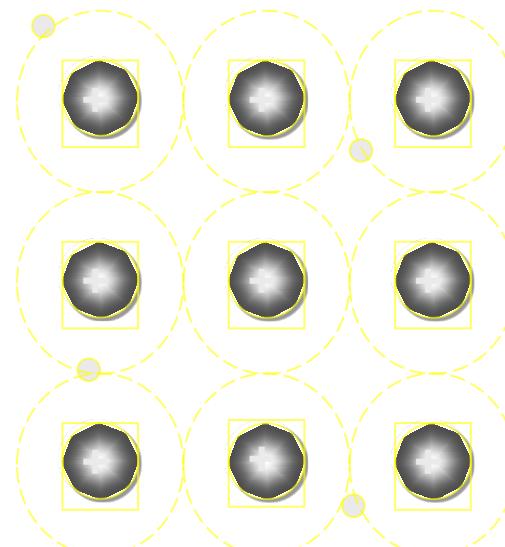


## Metallic bonds

Metallic bonding is the type of bonding found in metal elements. This is the electrostatic force of attraction between positively charged ions and delocalized outer electrons. A metallic bond results from the sharing of a *variable* number of electrons by a *variable* number of atoms. In metals, each atom loses all its valence electrons and becomes positively-charged ion. All valence electrons in a metal combine to form *cloud of electrons* that move freely between the atom cores. The positively charged cores are held together by these negatively charged electrons. The metallic bond is weaker than the ionic and the covalent bonds.



**Fig. 4. Metallic bonds**



## **Molecular bonds or Vander Waals' forces**

It occurs for those elements or compounds whose electronic configuration is such that little electron transfer between their atoms. The explanation of these weak forces of attraction is that there are natural fluctuation in the electron density of all molecules and these cause small temporary dipoles within the molecules. It is these temporary dipoles that attract one molecule to another by a force called Vander Waals' forces.

Therefore atoms or molecules containing dipoles are attracted to each other by electrostatic forces. These forces are due to the electrostatic attraction between the nucleus of one atom and the electrons of the other. Van der waals interaction occurs generally between atoms which have noble gas configuration.

# INTERPLANAR SPACING

Let us consider a plane ABC nearest to origin having miller indices (hkl) which intersect with the axes at A, B, C as shown in the Fig.-1. The perpendicular OP from the origin to the plane represents the interplanar spacing d of this family of planes.

Let us now take any lattice point P on the plane. Intercept of the ABC planes on the axes are

$$OA = a/h, OB = b/k, OC = c/l$$

Let the direction cosine of OP be  $\cos \alpha, \cos \beta, \cos \gamma$

In triangle  $\Delta OPA$   $\cos \alpha = d_{hkl} / OA = d_{hkl} h/a$  [ $OA = a/h$ ]

$d_{hkl}$  is the interplanar distance between the planes

Similarly for  $\Delta OPB$  and  $\Delta OPC$

$$\cos \beta = d_{hkl} k/b \text{ and } \cos \gamma = d_{hkl} l/c$$

**We know**

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

$$(dh/a)^2 + (dk/b)^2 + (dl/c)^2 = 1$$

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

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

**Which is the interplanar distance between two planes having same Miller indices (hkl)**

## **DIRECTION AND PLANE**

Let OP be the direction of [hkl] and ABC be the (hkl) plane. Again, let  $x_0$ ,  $y_0$  and  $z_0$  are the intercepts of the plane (hkl) along X, Y and Z directions.

Hence, Miller indices are:

$$1/x_0, 1/y_0, 1/z_0$$

and reduced indices becomes

$$\xi/x_0, \xi/y_0, \xi/z_0 \text{ where, } \xi \text{ is an integer}$$

For cubic lattice,  $h = k = l$  or  $x_0 = y_0 = z_0 = a$

and the direction,  $OP = i \frac{\xi}{a} + j \frac{\xi}{a} + k \frac{\xi}{a}$

From Fig-1, we can write

$$OB = OA + AB$$

$$AB = OB - OA = j \frac{\xi}{a} - i \frac{\xi}{a}$$

$$\begin{aligned} \text{Now, } OP \cdot AB &= \left( i \frac{\xi}{a} + j \frac{\xi}{a} + k \frac{\xi}{a} \right) \cdot \left( j \frac{\xi}{a} - i \frac{\xi}{a} \right) \\ &= -i \frac{\xi^2}{a^2} + j \frac{\xi^2}{a^2} = 0 \end{aligned}$$

**Similarly, we can prove that**

$$\mathbf{OP} \cdot \mathbf{BC} = 0$$

and  $\mathbf{OP} \cdot \mathbf{CA} = 0$

Hence, the dot product of  $\mathbf{OP}$  with  $\mathbf{AB}$ ,  $\mathbf{BC}$  and  $\mathbf{CA}$  is zero. So,  $\mathbf{OP}$  is normal to  $\mathbf{AB}$ ,  $\mathbf{BC}$  and  $\mathbf{CA}$ .

Thus, the  $[hkl]$  direction is normal to the plane  $(hkl)$ .

## ORIGIN OF BONDS

**Atom and molecules in a solid state are more closely packed and are held together by strong mutual forces of attraction. These inter atomic forces are basically electrostatic in nature and direct consequence of the electronic structure of matter. When atoms come closer and finally unite to form molecules, their electrons rearrange themselves in such a way as to achieve a stable configuration.**

**This stable configuration is achieved when the outermost shell or valence shell of atoms filled with 8 in number electrons whatever be the principal number of the valence shell. This rearrangement of electrons gives rise to different types of bonds, which hold the atoms together, in a solid state.**

**Hence the bonds in solids are the following principal types:**

- (i) **Ionic bonds**, as in NaCl (transfer of valence electrons)
- (ii) **Covalent bonds**, as in Chlorine atom (sharing of valence electrons)
- (iii) **Metallic Bonds**, as in Ag, Cu (free nature of valence electrons)
- (iv) **Vander Waals bonds**, as in solid nitrogen (electrons remain associated with original molecules)

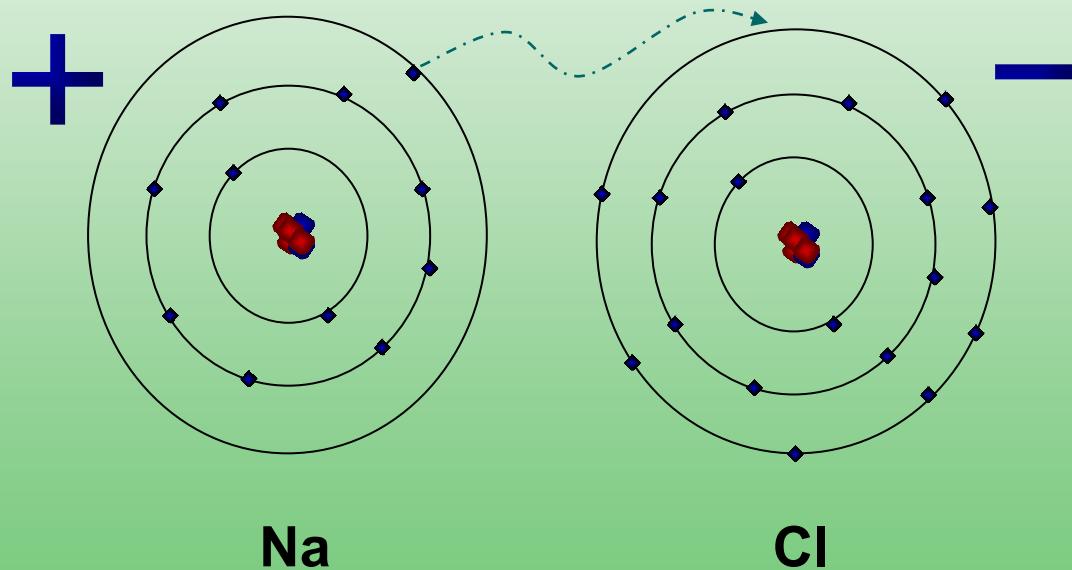
## IONIC BOND

**Ionic bonds are mainly formed in inorganic compounds like NaCl, KOH etc and never in elements. They are very strong bonds and develop between those two atoms one of which has low ionization energy and the other has high electron affinity.**

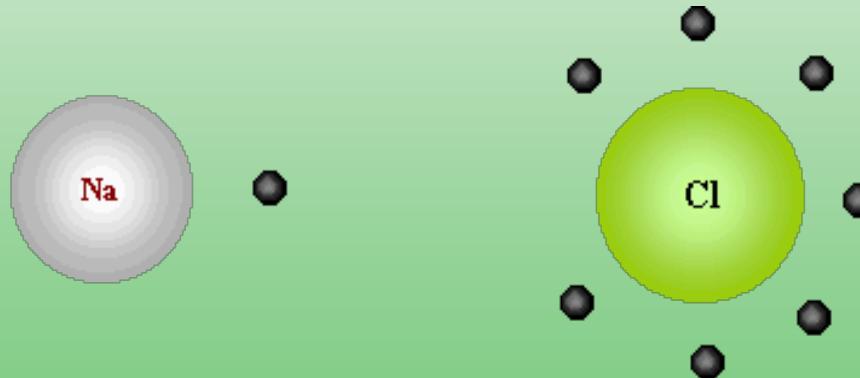
**These bonds are formed due to the electrostatic attraction between two stable ions, which are themselves produced due to complete transfer of electrons from one atom to another.**

**NaCl is a typical example of ionic bonding.**

The metallic elements have only up to the valence electrons in their outer shell will lose their electrons and become positive ions, whereas electronegative elements tend to acquire additional electrons to complete their octet and become negative ions, or anions.



**When the  $\text{Na}^+$  and  $\text{Cl}^-$  ions approach each other closely enough so that the orbits of the electron in the ions begin to overlap each other, then the electron begins to repel each other by virtue of the repulsive electrostatic coulomb force. Of course the closer together the ions are, the greater the **repulsive force**.**



1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	
<b>H</b> Hydrogen 1.00794																	<b>He</b> Helium 4.002602	
<b>Li</b> Lithium 6.941	<b>Be</b> Beryllium 9.012182																<b>Ne</b> Neon 20.1797	
<b>Na</b> Sodium 22.98976928	<b>Mg</b> Magnesium 24.3050																<b>Ar</b> Argon 39.948	
<b>K</b> Potassium 39.0983	<b>Ca</b> Calcium 40.078	<b>Sc</b> Scandium 44.955912	<b>Ti</b> Titanium 47.867	<b>V</b> Vanadium 50.9415	<b>Cr</b> Chromium 51.9961	<b>Mn</b> Manganese 54.938045	<b>Fe</b> Iron 55.845	<b>Co</b> Cobalt 58.933195	<b>Ni</b> Nickel 58.6934	<b>Cu</b> Copper 63.546	<b>Zn</b> Zinc 65.38	<b>Ga</b> Gallium 69.723	<b>Ge</b> Germanium 72.64	<b>As</b> Arsenic 74.92160	<b>Se</b> Selenium 78.96	<b>Br</b> Bromine 79.904	<b>Kr</b> Krypton 83.798	
<b>Rb</b> Rubidium 85.4678	<b>Sr</b> Strontium 87.62	<b>Y</b> Yttrium 88.90585	<b>Zr</b> Zirconium 91.224	<b>Nb</b> Niobium 92.90638	<b>Mo</b> Molybdenum 95.96	<b>Tc</b> Technetium (97.9072)	<b>Ru</b> Ruthenium 101.07	<b>Rh</b> Rhodium 102.90550	<b>Pd</b> Palladium 106.42	<b>Ag</b> Silver 107.8682	<b>Cd</b> Cadmium 112.411	<b>In</b> Indium 114.818	<b>Sn</b> Tin 118.710	<b>Sb</b> Antimony 121.760	<b>Te</b> Tellurium 127.60	<b>I</b> Iodine 126.90447	<b>Xe</b> Xenon 131.293	
<b>Cs</b> Caesium 132.9054519	<b>Ba</b> Barium 137.327	<b>La-Lu</b> <b>La-Lu</b>	<b>Hf</b> Hafnium 178.49	<b>Ta</b> Tantalum 180.94788	<b>W</b> Tungsten 183.84	<b>Re</b> Rhenium 186.207	<b>Os</b> Osmium 190.23	<b>Ir</b> Iridium 192.217	<b>Pt</b> Platinum 195.084	<b>Au</b> Gold 196.966569	<b>Hg</b> Mercury 200.59	<b>Tl</b> Thallium 204.3833	<b>Pb</b> Lead 207.2	<b>Bi</b> Bismuth 208.98040	<b>Po</b> Polonium (208.9824)	<b>At</b> Astatine (209.9871)	<b>Rn</b> Radon (222.0176)	
<b>Fr</b> Francium (223)	<b>Ra</b> Radium (226)	<b>Ac-Lr</b> <b>Ac-Lr</b>	<b>Rf</b> Rutherfordium (261)	<b>Db</b> Dubnium (262)	<b>Sg</b> Seaborgium (266)	<b>Bh</b> Bohrium (264)	<b>Hs</b> Hassium (277)	<b>Mt</b> Meitnerium (268)	<b>Ds</b> Darmstadtium (271)	<b>Rg</b> Roentgenium (272)	<b>Cn</b> Copernicium (285)	<b>Uut</b> Ununtrium (284)	<b>Fl</b> Flerovium (289)	<b>Uup</b> Ununpentium (288)	<b>Lv</b> Livermorium (292)	<b>Uus</b> Ununseptium (294)	<b>Uuo</b> Ununoctium (294)	
For elements with no stable isotopes, the mass number of the isotope with the longest half-life is in parentheses.																		
<b>La</b> Lanthanum 138.90547	<b>Ce</b> Cerium 140.116	<b>Pr</b> Praseodymium 140.90765	<b>Nd</b> Neodymium 144.242	<b>Pm</b> Promethium (145)	<b>Sm</b> Samarium 150.36	<b>Eu</b> Europium 151.964	<b>Gd</b> Gadolinium 157.25	<b>Tb</b> Terbium 158.92535	<b>Dy</b> Dysprosium 162.5	<b>Ho</b> Holmium 164.93032	<b>Er</b> Erbium 167.259	<b>Tm</b> Thulium 168.93421	<b>Yb</b> Ytterbium 173.054	<b>Lu</b> Lutetium 174.9668				
<b>Ac</b> Actinium (227)	<b>Th</b> Thorium 232.03806	<b>Pa</b> Protactinium 231.03588	<b>U</b> Uranium 238.02891	<b>Np</b> Neptunium (237)	<b>Pu</b> Plutonium (244)	<b>Am</b> Americium (243)	<b>Cm</b> Curium (247)	<b>Bk</b> Berkelium (247)	<b>Cf</b> Californium (251)	<b>Es</b> Einsteinium (252)	<b>Fm</b> Fermium (257)	<b>Md</b> Mendelevium (258)	<b>No</b> Nobelium (259)	<b>Lr</b> Lawrencium (262)				

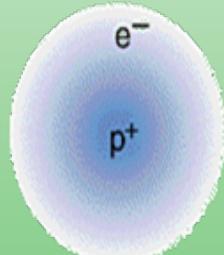
## COVALENT BOND

**The covalent bonding is formed by sharing of outer shell electrons between atoms rather than by electron transfer.**

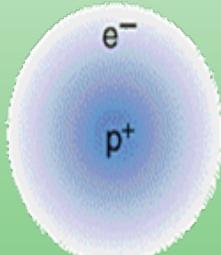
**This bonding can be attained if the two atoms each share one of the other's electrons.**

**So the noble gas electron configuration can be attained.**

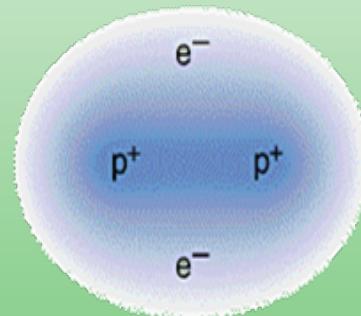
**Each electron in a shared pair is attracted to both nuclei involved in the bond. The approach, electron overlap, and attraction can be visualized as shown in the following figure representing the nuclei and electrons in a hydrogen molecule.**



A No interaction



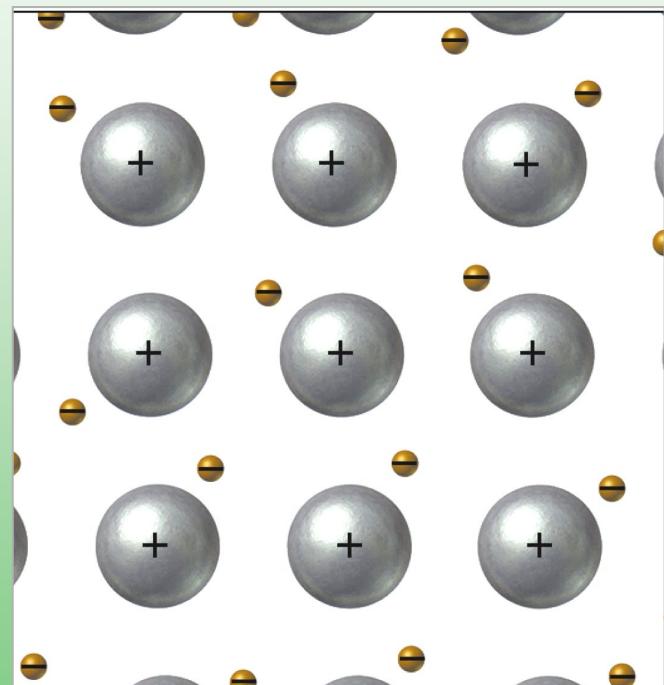
B Attraction



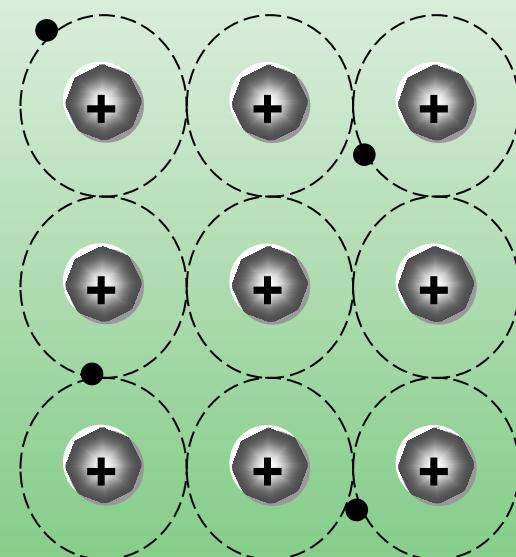
C Covalent bond

# METALLIC BOND

- Metallic bonding is the type of bonding found in metal elements. This is the electrostatic force of attraction between positively charged ions and delocalized outer electrons.
- The metallic bond is weaker than the ionic and the covalent bonds.



- ❑ Valence electrons are relatively bound to the nucleus and therefore they move freely through the metal and they are spread out among the atoms in the form of a low-density electron cloud.
- ❑ A metallic bond result from the sharing of a variable number of electrons by a variable number of atoms. A metal may be described as a cloud of free electrons.
- ❑ Therefore, metals have high electrical and thermal conductivity.



- All valence electrons in a metal combine to form a “sea” of electrons that move freely between the atom cores. The more electrons, the stronger the attraction. This means the melting and boiling points are higher, and the metal is stronger and harder.
- The positively charged cores are held together by these negatively charged electrons.
- The free electrons act as the bond (or as a “glue”) between the positively charged ions.

## ○Molecular bonds or Vander Waals' forces

- It occurs for those elements or compounds whose electronic configuration is such that little electron transfer between their atoms. The explanation of these weak forces of attraction is that there are natural fluctuation in the electron density of all molecules and these cause small temporary dipoles within the molecules. It is these temporary dipoles that attract one molecule to another by a force called Vander Waals' forces.
- Therefore atoms or molecules containing dipoles are attracted to each other by electrostatic forces. These forces are due to the electrostatic attraction between the nucleus of one atom and the electrons of the other. Van der waals interaction occurs generally between atoms which have noble gas configuration.

# CRYSTAL DEFECTS

It can be three types

- (i) Point defect
- (ii) Line defect
- (iii) Plane defect

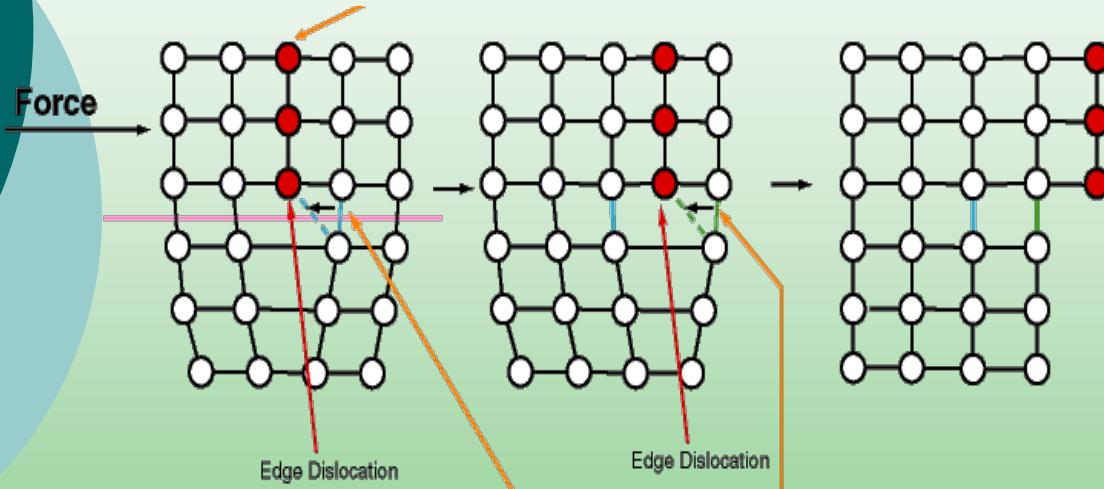
## POINT DEFECT

- (i) Interstitial atom
- (ii) Schottky defect or vacancy
- (iii) Frenkle defect
- (iv) Substitutional impurity atom

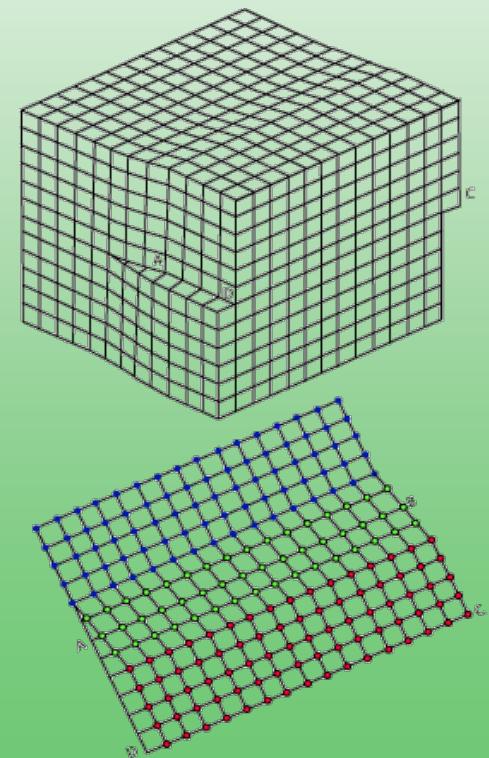
# LINE DEFECT

It can be two types

(i) Edge dislocation

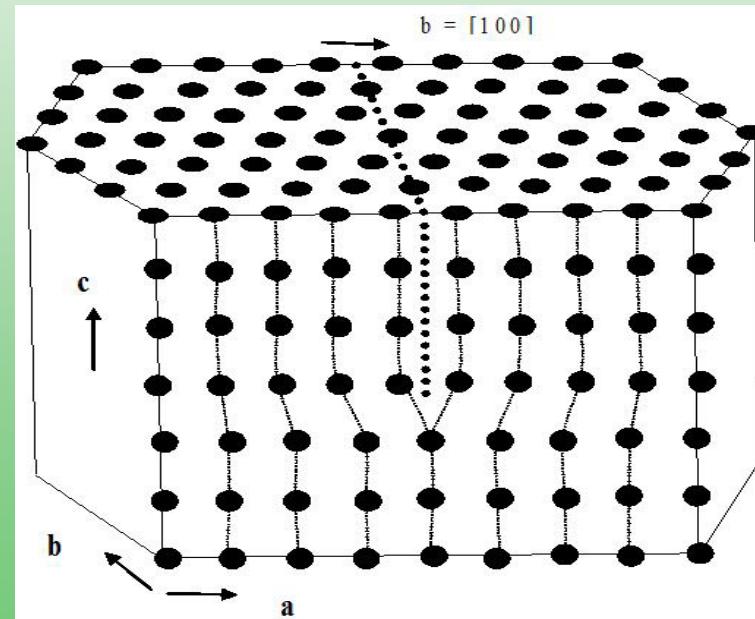


(ii) Screw dislocation



## PLANE DEFECT

- (i) Lineage boundary
- (ii) Grain boundary
- (iii) Stacking fault



## ○ **Band Theory of Solids**

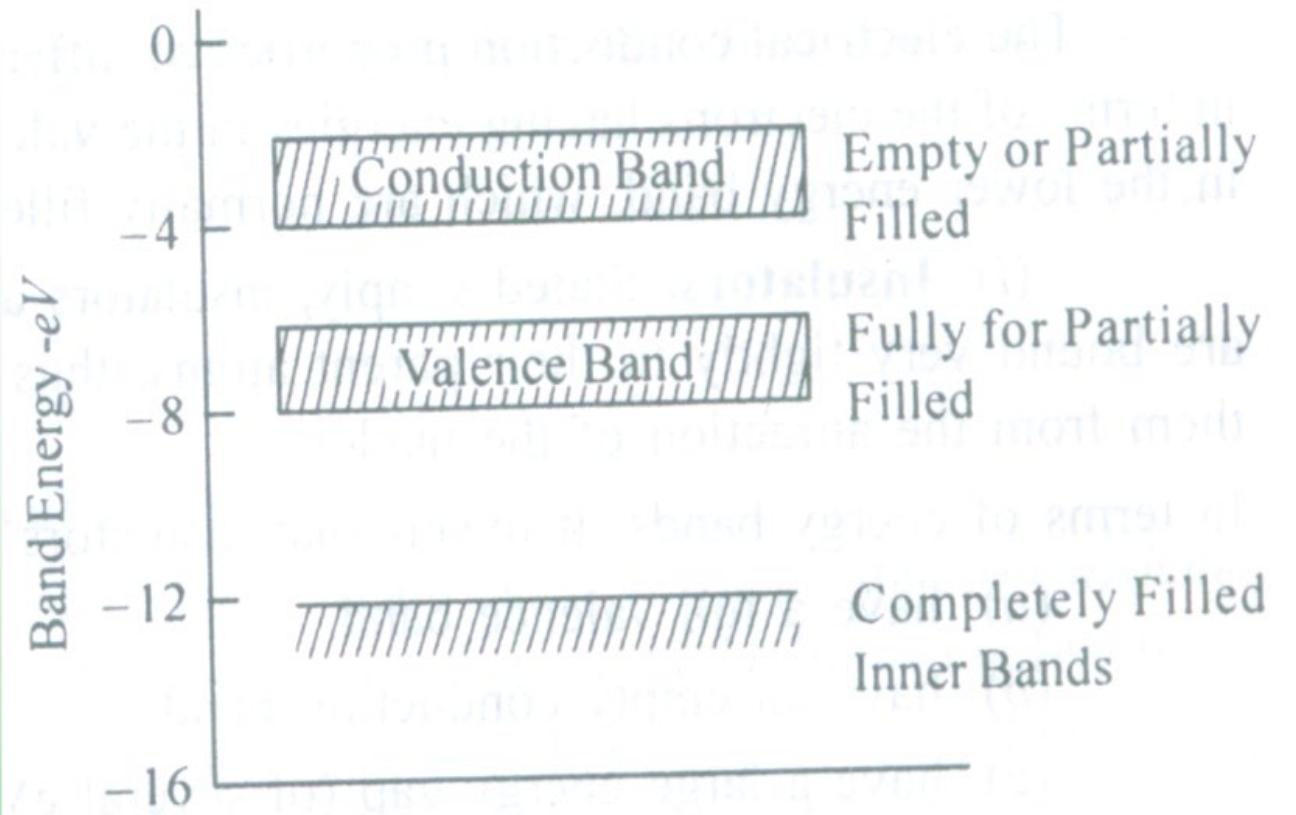
- **Band:** It describes those ranges of energy that an electron in the solid may have (valence band/conduction band) and that may not have (forbidden gap).
- **Valence band:** The outermost electrons of an atom *i.e.* those in the shell furthermost from the nucleus are called *valence* electrons and have the *highest energy*. It is these electrons which are most affected when number of atoms are brought very close together as during the formation of a solid.
- The states of lower energy electrons orbiting in shells nearer to the nucleus are little, if at all affected by this atomic proximity.
- The band of energy occupied by the valence electrons is called the *valence band* and is obviously the *highest occupied band*. It may be completely filled and partially filled with electrons.

## ○ **Band Theory of Solids**

○ **Conduction band:** The next higher permitted energy band is called the conduction band and may either be empty or partially filled with electrons. In fact, it may be defined as the lowest unfilled energy bands. In conduction band electrons can move freely and hence known as conduction electrons.

○ **Forbidden energy gap:** The gap between the valence band and the conduction band is called the forbidden energy gap.

○ It is noted the covalent forces of the crystal lattice have their source in the valence band. If a valence electron happens to absorb enough energy, it jumps across the forbidden energy gap and enters the conduction band.

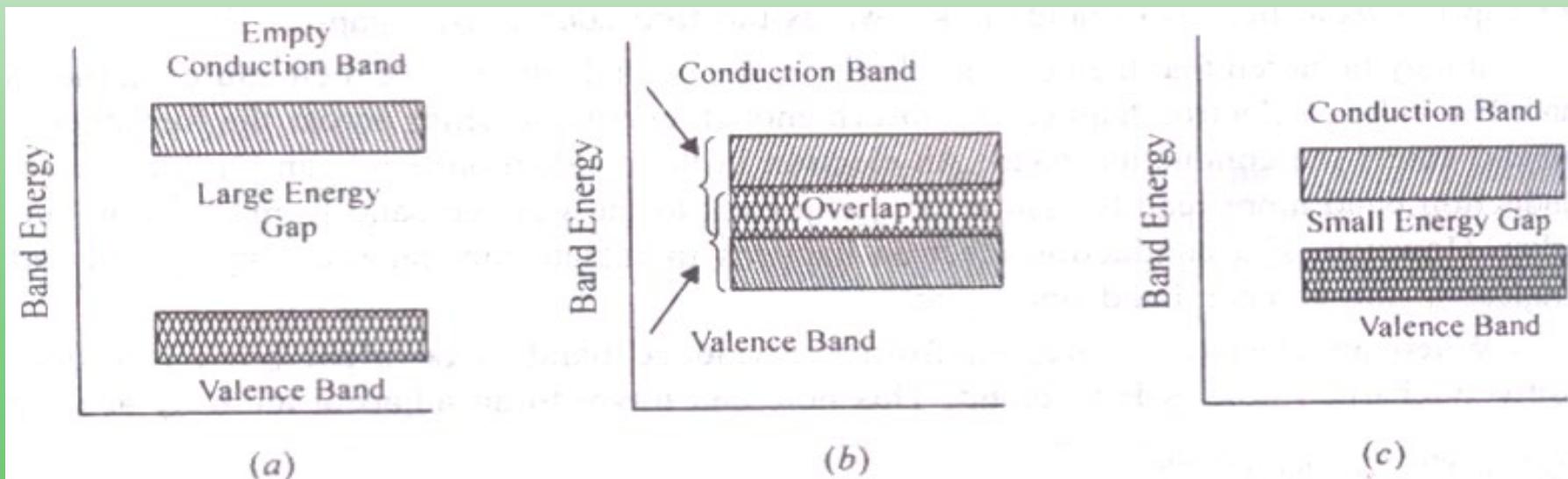


## Conductors, Semiconductors and Insulators

The electrical conduction properties of different elements and compounds can be explained in terms of the electrons having energies in the valence and conduction bands. The electrons lying in the lower energy band, which are normally filled, play no part in the conduction process.

- **Insulators:** Insulators are those materials in which the valence electrons are bound very tightly to their parent atoms, thus requiring very large electric fields to remove them from the attraction of the nuclei.
- In terms of energy bands, it means that insulators
  - a. Have a full valence band
  - b. Have an empty conduction band
  - c. Have a large energy gap
  - d. At all ordinary temperatures, the probability of electrons from full valence band gaining sufficient energy so as to surmount the energy gap and becoming available for conduction in the conduction band.
- This is shown in fig (a). For conduction to take place, electrons must be given sufficient energy to jump from the valence band to the conduction band. Increase in temperature enables some electrons to go to the conduction band.

○ **Conductors:** Conductors are those in which plenty of free electrons are available for electric conduction. In terms of energy bands, it means that electrical conductors are those which have overlapping *valence and conduction bands* as shown in fig (b). In fact there is no physical distinction *between the two bands*. Hence, the availability of a large number of conduction electrons. There is absence of *forbidden energy gap* in good conductors.



**Semiconductors:** A semiconductor material is one whose electrical properties lie in between those of insulators and good conductors. In terms of energy bands, semiconductors can be defined as those materials which have *almost an empty conduction band* and *almost filled valence band* with a very narrow energy gap (of the order of 1 eV) separating the two.

At  $0^0$  K, there are no electrons in the conduction band and the valence band is completely filled. However, with the increase in temperature, width of the forbidden energy band is decreased so that some of the electrons are liberated into the conduction band. In other words, conductivity of semiconductors increases with temperature.

## Structure of Matter

**1. Explain the terms:**

**Crystalline Solids, Amorphous or Non-crystalline/solids, Single Crystalline materials, Polycrystalline materials/solids, Lattice, Space lattice, Bravais lattice and Non-Bravais lattice, Basis or Motif, Unit Cell, Coordination number, Cohesive energy, Polymer, Ceramic, Plasticity, Elasticity, Forbidden energy gap, Conduction band, Valance band, Plasma states of matter**

**Or, Distinguish between primitive unit cell and Non-Primitive unit cell.**

**Or, What are the differences between crystalline and amorphous solids?**

**2. What are the symbols ‘P’, ‘I’. ‘F’, ‘C’ stand for?**

**3. Calculate the total number of atoms in a body in different unit cell (S.C., F.C.C. and B.C.C.)**

**4. Write down the name of seven crystal system in appropriate condition and examples.**

**5. What are the Miller Indices? With example write the procedure for finding the Miller Indices. Write the importance or Uses of Miller Indices.**

**Or, Explain the suitable diagram, how in a crystal planes are denoted the Miller Indices (hkl).**

**6. Draw the direction of Plane [100], [010], [001], [111], [101], [110], [011], [020], [212],**

**[0 $\bar{1}$ 0], [01 $\bar{0}$ ], [0 $\bar{1}$ 0], [ $\bar{2}$ 12], [ $\bar{1}$ 10], [1 $\bar{1}$ 1], [1 $\bar{2}$ 1], [ $\bar{1}$ 22], [11 $\bar{1}$ ], [111]**

**7. Drawing planes from Miller indices (121), (212), (124), (012), (101), (100), (010), (001), (011), (110), (112), (013), (110), (100)**

**8(a). Define packing factor/fraction. Show that the packing factor/fraction for simple cubic structure is 0.52**

**8(b). Define packing factor/fraction. Show that the packing factor/fraction for body centered cubic (bcc) structure is 0.68**

**Or, Show that the packing factor for body centered cubic (bcc) structure/crystal is  $\frac{\sqrt{3}\pi}{8}$ .**

**Or, Find out the packing factor for body centered cubic (bcc) structure/crystal.**

**8(c). Define packing factor/fraction. Show that the packing factor/fraction for face centered cubic (fcc) structure is 0.74**

**9. What is meant by interplanar spacing? Derive/Find an expression for the interplanar spacing ‘d’ between the adjacent (hkl) planes.**

**Or, Show that, interplanar spacing for crystal is**

$$d_{hkl} = \frac{1}{\sqrt{\left(\frac{h}{a}\right)^2 + \left(\frac{k}{b}\right)^2 + \left(\frac{l}{c}\right)^2}}, \text{ where the symbols have their usual meanings.}$$

**Or, What is interplanar spacing? Calculate the interplanar spacing for a cubic crystal system.**

**10. What do you mean by X-ray diffraction? Describe Bragg’s law for the diffraction of X-rays in crystal.**

**11. Describe/Explain different (Various) types of bonds in solid.**

**Or, Describe how the ionic and covalent bonds are formed in solid.**

**12. What do you mean by crystal defect? Discuss in details on various types of crystal defect with necessary diagram.**

**13. What is energy band? Distinguish between metal/Conductors, Semiconductors and Insulators using the band theory of solids.**

**Or, With the help of energy band, explain the differences between metal/Conductors, Semiconductors and Insulators using the band theory of solids.**

**14. Prove that in a cubic crystal, the [hkl] direction is normal to the plane (hkl) plane.**

**15. Deduce the total potential energy/cohesive energy at the equilibrium separation of an ionic crystal.**

## **Structure of Matter**

### **Phy-109**

1. The spacing between successive **(100)** planes in NaCl is **2.82 Å**. X-ray incident upon the surface of this crystal is found to give rise to the first order Bragg's reflection at a glancing angle of **8°35'**. Calculate the wavelength of X-ray and find the angle at which the second orders Bragg's reflection would occur.
2. Calculate the longest wavelength that can be analyzed by a rock salt crystal of spacing, **d= 2.82 Å** for (i) in the first order and (ii) in the second order.
3. In Bragg's reflection of X-rays a reflection was found at **30°** glancing angle with lattice planes of spacing **1.87 Å** if this a second order reflection. Calculate the wavelength of X-rays.
4. The first order reflection from the plane of NaCl is obtained at an angle **2θ= 20°** with the incident beam. If **d = 2.82 Å**, Calculate the wavelength of X-ray used.
5. An X-ray beam of wavelength **0.97 Å** is obtained in the third order reflection at **60°** from the crystal plane. Another beam is obtained in the first order after reflection at **30°** from the same crystal plane. Find the wavelength of second X-ray beam.
6. From the following data calculate wavelength of the neutron beam and the speed of neutrons **θ= 30°**, **d= 3.84 Å**, **n=1**.
7. Electrons are accelerated by **344 volt** and are reflected from a crystal. The first reflection maximum occurs when glancing angle is **30°**. Determine the spacing of the crystal.  
**(h=6.63×10<sup>-34</sup> JS, e=1.6×10<sup>-19</sup>C, m=9.1×10<sup>-31</sup>Kg).**
8. The Bragg's angle for the first order reflection from **(111)** plane in a crystal is **60° (30°)**. Calculate the interatomic spacing if X-rays of wavelength **1.8×10<sup>-10</sup> m (1.75 Å)** are used.
9. Determine the glancing angle on the cube face **(100)** of a NaCl crystal corresponding to second order reflection. (**a= 2.814 Å and λ= 0.710 Å**).
10. Calculate the angle between **[100]** and **[111]** direction of cubic unit cell.
11. Calculate the angles which **[111]** direction of cubic unit cell makes with **[100]** and **[110]** direction.

**Professor Dr. H. M. A. R. Maruf, Department of Physics, CUET**

**E-mail: hasnatmaruf@gmail.com**

**Structure of Matter****Phy-109**

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7. Electrons are accelerated by **344 volt** and are reflected from a crystal. The first reflection maximum occurs when glancing angle is **30°**. Determine the spacing of the crystal.  
( $h = 6.63 \times 10^{-34} \text{ JS}$ ,  $e = 1.6 \times 10^{-19} \text{ C}$ ,  $m = 9.1 \times 10^{-31} \text{ Kg}$ ).

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Miller indices are the reciprocals of the intercepts, made by the plane on the crystallographic axes, when reduced to smallest integers.

Miller indices are used to designate the planes in a crystal lattice.

Intercepts on x, y and z axes :- 1, 2, infinity

The reciprocals of intercepts :- 1/1, 1/2, 1/infinity

i.e. 1/1, 1/2, 0

Reciprocals are reduced to smallest set of integers by taking LCM :- 2, 1, 0

So, miller indices :- (2,1,0)

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### FOR BCC

i) Number of atoms per unit cell :-  $(8 \times 1/8) + 1 = 2$ .

ii) The co-ordination number :- 8, because there are eight unit cells surrounding a corner atom in BCC unit cell. Atom at the centre of the unit cell is nearest to the corner atom in unit cell.

iii) The packing fraction :-  $2 \times (4/3) \pi R^3 / a^3$

i.e.  $2/1 \times 4/3 \times \pi/1 \times [(\text{square root of } 3) \times a/4]^3 \times 1/(a)^3$

i.e.  $(\text{square root of } 3) \times (\pi / 8)$

i.e. 0.68

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### GIVEN :-

Lamda = 1.54 Angstrom =  $1.54 \times 10^{-10}$  m.

Theta = 22.4 degrees.

Spacing of (2,0,0) planes in Aluminium =  $d = [a / \sqrt{2^2 + 0 + 0}]$  i.e  $a / 2$ .

$a = ?$

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

$$\text{i.e. } 2 \times (a/2) \times \sin(22.4) = 1 \times 1.54 \times 10^{-10}$$

i.e.  $a = (1.54 \times 10^{-10}) / (0.3811)$   
i.e.  $a = 4.04 \text{ \AA}^0$

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The packing fraction in FCC :-

$$4 \times (4/3) \pi (R)^3 / (a)^3$$

i.e.  $4/1 \times 4/3 \times \pi/1 \times [(\text{square root of } 2) \times a/4]^3 \times 1/(a)^3$   
i.e.  $\pi / (3 \times \text{square root of } 2)$   
i.e. 0.74.

The packing fraction in BCC :-

$$2 \times (4/3) \pi (R)^3 / (a)^3$$

i.e.  $2/1 \times 4/3 \times \pi/1 \times [(\text{square root of } 3) \times a/4]^3 \times 1/(a)^3$   
i.e.  $(\text{square root of } 3) \times (\pi / 8)$   
i.e. 0.68.

i.e. packing fraction in FCC is more than in the BCC structure.

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For the given crystal, it is possible to obtain experimentally the glancing angles for the maxima of reflected X-rays respectively using three different reflecting planes.

For example, In case of KCL crystal, Bragg obtained the first order of maximum of reflected X-rays at glancing angles 5.22 degrees, 7.30 degrees and 9.05 degrees respectively using three different reflecting planes.

From Bragg's equation  $2d \sin(\theta) = n \lambda$   
So, for first order spectrum  $2d \sin(\theta) = \lambda$   
i.e.  $1/d = 2 \sin(\theta) / \lambda$

Thus, knowing the values of theta for reflections from different reflecting planes in given crystal and lambda, it is possible to find the ratio  $1/d_{100} : 1/d_{110} : 1/d_{111}$  and from this ratio, it is possible to analyse the given crystal structure.

For example for KCL crystal,

$$1/d_1 : 1/d_2 : 1/d_3 :: \sin 5.22 : \sin 7.30 : \sin 9.05$$

i.e.  $1/d_1 : 1/d_2 : 1/d_3 :: 0.091 : 0.127 : 0.157$   
i.e.  $1/d_1 : 1/d_2 : 1/d_3 :: 1 : 1.4 : 1.73$

This result shows that KCL is simple cubic crystal.

In this way Bragg's law is useful in the analysis of the crystal structures.

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The packing fraction in SC :-

$$1 \times (4/3) \pi (R)^3 / (a)^3$$

$$\text{i.e. } 1/1 \times 4/3 \times \pi/1 \times [a/2]^3 \times 1/(a)^3$$

$$\text{i.e. } \pi/6$$

$$\text{i.e. } 0.52$$

The packing fraction in BCC :-

$$2 \times (4/3) \pi (R)^3 / (a)^3$$

$$\text{i.e. } 2/1 \times 4/3 \times \pi/1 \times [(square\ root\ of\ 3) \times a/4]^3 \times 1/(a)^3$$

$$\text{i.e. } (square\ root\ of\ 3) \times (\pi/8)$$

$$\text{i.e. } 0.68.$$

The packing fraction in FCC :-

$$4 \times (4/3) \pi (R)^3 / (a)^3$$

$$\text{i.e. } 4/1 \times 4/3 \times \pi/1 \times [(square\ root\ of\ 2) \times a/4]^3 \times 1/(a)^3$$

$$\text{i.e. } \pi/(\sqrt{2} \times 3)$$

$$\text{i.e. } 0.74.$$

Hence the FCC structure possesses maximum packing density among the three crystal structures SC, BCC and FCC.

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GIVEN :-

$$r = 1.68 \text{ \AA}^0 = 1.68 \times 10^{-10} \text{ m.}$$

Lattice system = SC

M = 209 kg / k. mol

N =  $6.02 \times 10^{26}$  atoms / k. mol.

For SC,  $r = a/2$

$$\text{So } a = 2r = 2 \times 1.68 \times 10^{-10} \text{ m} = 3.36 \times 10^{-10} \text{ m}$$

and n = 1

$$\begin{aligned}\text{So Density} &= nM / N (a)^3 \\ &= [(1 \text{ atom}) (209 \text{ kg / k. mol})] / [(6.02 \times 10^{26} \text{ atoms / k. mol}) (3.36 \times 10^{-10} \text{ m})^3] \\ &= [(209 / 228.34)] \times 10^4 \text{ kg / m}^3 \\ &= 9150 \text{ kg / m}^3\end{aligned}$$

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Space lattice is defined as an array of points arranged in regular periodic fashion in three dimensional space such that each point in the lattice has exactly identical surrounding. The points are called lattice points or lattice sites.

A crystal structure is a space lattice in which the lattice sites are occupied by atoms or clusters of atoms. Each lattice point is associated with the same unit of groups of atoms, called the basis. The basis must be identical in composition, arrangement and orientation such that the crystal appears exactly the same at one point as it does at other equivalent points. When the basis is associated with each lattice site, the crystal structure is obtained.

Thus Space lattice + Basis = Crystal structure.

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### FOR BCC

- i) Number of atoms per unit cell :-  $(8 \times 1/8) + 1 = 2$ .
  - ii) The co-ordination number :- 8, because there are eight unit cells surrounding a corner atom in BCC unit cell. Atom at the centre of the unit cell is nearest to the corner atom in unit cell.
  - iii) The packing fraction :-  $2 \times (4/3) \pi (R)^3 / (a)^3$   
i.e.  $2/1 \times 4/3 \times \pi/1 \times [(\text{square root of } 3) \times a/4]^3 \times 1/(a)^3$   
i.e.  $(\text{square root of } 3) \times (\pi / 8)$   
i.e. 0.68
- 
- 

### GIVEN :-

Lattice system = FCC

Edge of unit cell,  $a = 3.52 \text{ \AA}^0 = 3.52 \times 10^{-10} \text{ m}$

$M = 58.71 \text{ kg / k. mol}$

$N = 6.02 \times 10^{26} \text{ atoms / k. mol.}$

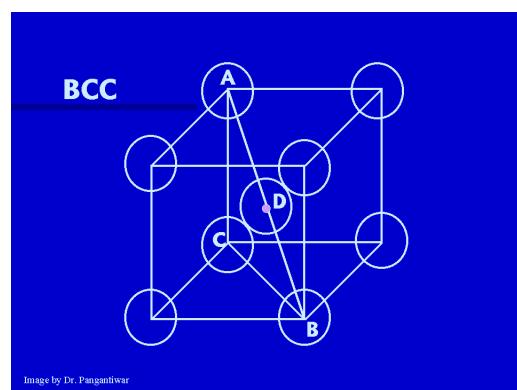
and For FCC,  $n = 4$

Density =  $nM / N (a)^3$

$$= [(4 \text{ atoms}) (58.71 \text{ kg / k. mol})] / [6.02 \times 10^{26} \text{ atoms / k. mol}] (3.52 \times 10^{-10} \text{ m})^3]$$

$$= [(234.84 / 262.56)] \times 10^4 \text{ kg / m}^3$$

$$= 8944 \text{ kg / m}^3$$



In BCC nearest neighbours are atoms at A and D.

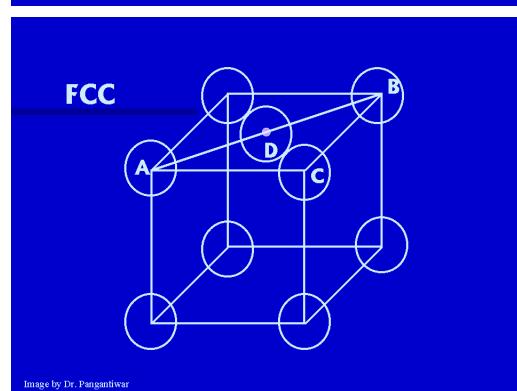
The Distance AB = (square root of 3) a

So AD = Half of AB = [(square root of 3) a] / 2

So radius r = Half of the distance between nearest neighbours

i.e. radius r = [(square root of 3) a] / 4

So lattice constant a = 4r / (square root of 3)



In FCC nearest neighbours are atoms at A and D.

The Distance AB is (square root of 2) a

So AD = Half of AB = [(square root of 2) a] / 2

So radius r = Half of the distance between nearest neighbours

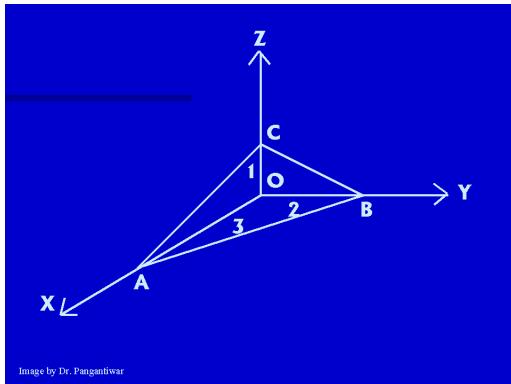
i.e. radius r = [(square root of 2) a] / 4

So lattice constant a = 4r / (square root of 2)

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Miller indices are the reciprocals of the intercepts, made by the plane on the crystallographic axes, when reduced to smallest integers.

Miller indices are used to designate the planes in a crystal lattice.



The intercepts are OA, OB, OC

i.e. 3, 2, 1

The reciprocals of intercepts are  $1/3, 1/2, 1/1$

Taking LCM we get 2, 3, 6

So the miller indices of plane ABC are (2,3,6)

### GIVEN :-

$$r = 1.44 \text{ Å}^0 = 1.44 \times 10^{-10} \text{ m.}$$

For FCC,  $a = 2$  (square root of 2)  $r$

$$\text{i.e. } a = 2 \times 1.414 \times 1.44 \times 10^{-10} \text{ m}$$

$$\text{i.e. } a = 4.07 \times 10^{-10} \text{ m}$$

Spacing of (111) plane =  $d_{111} = [a / \text{square root of } (h^2 + k^2 + l^2)]$

$$\text{i.e. } d_{111} = [4.07 \times 10^{-10} / \text{square root of } (1^2 + 1^2 + 1^2)]$$

$$\text{i.e. } d_{111} = 2.35 \times 10^{-10} \text{ m.}$$

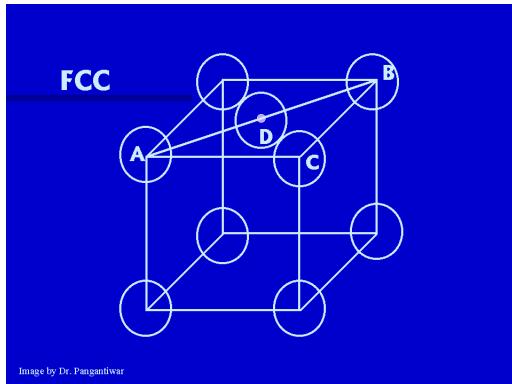
We know that,  $2d \sin(\theta) = n \lambda$

$$\text{i.e. } 2 \times 2.35 \times 10^{-10} \times \sin(32.1) = 1 \text{ lamda}$$

$$\text{So, } \lambda = 2.498 \times 10^{-10} \text{ m}$$

Cubic crystal structure FCC has closest packing of atoms.

An atom in this type of crystal have 12 nearest neighbours.



In FCC nearest neighbours are atoms at A and D.  
 The Distance AB is  $(\text{square root of } 2) a$   
 So AD = Half of AB =  $[(\text{square root of } 2) a] / 2$   
 So radius r = Half of the distance between nearest neighbours  
 i.e. radius r =  $[(\text{square root of } 2) a] / 4$   
 So a (unit cell dimension) =  $4r / (\text{square root of } 2)$

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### GIVEN :-

Lattice constant,  $a = 2.87 \text{ \AA}^0 = 2.87 \times 10^{-10} \text{ m}$ .

Lattice system = BCC

Density =  $7870 \text{ kg/m}^3$

$N = 6.02 \times 10^{26} \text{ atoms/k. mol.}$

For BCC,  $n = 2 \text{ atoms}$

$$\text{Density} = nM / N (a)^3$$

$$\text{So, atomic mass, } M = (\text{Density}) N (a)^3 / n$$

$$\text{i.e. } M = [(7870 \text{ kg/m}^3) (6.02 \times 10^{26} \text{ atoms/k. mol}) (2.87 \times 10^{-10} \text{ m})^3] / 2 \text{ atoms}$$

$$\text{i.e. } M = 56 \text{ kg/k.mol}$$


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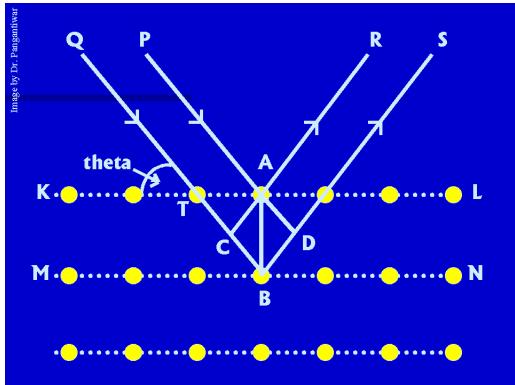


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### $2d \sin(\theta) = n(\lambda)$ ,

where  $d$  is the interplaner distance,  $(\theta)$  is the angle between the Bragg plane and the direction of the incident beam and  $n = 1, 2, 3 \dots \dots \dots$  etc., for first order, second order, third order ..... etc., maxima respectively, is known as Bragg's law.

Let us consider a set of parallel lattice planes of a crystal separated by a distance  $d$  apart, i.e.  $AB = d$ . Suppose a narrow beam of X-rays of wavelength  $(\lambda)$  be incident upon these planes at an angle  $(\theta)$  as shown in figure. The beam will be reflected in all directions by the atoms of various atomic planes. Because the refractive index of the matter of the crystal is very nearly equal to unity, there is practically no bending of the rays entering or leaving the crystal.



Consider a ray PA reflected at atom A in the direction AR from plane KL and another ray QB reflected at another atom B from plane MN in the direction BS. Now from the atom A, draw two perpendiculars AC and AD on the incident ray QB and reflected ray BS respectively. The path difference between these two rays is (CB+BD). The two reflected rays will be in phase or out of phase, will depend upon this path difference. When the path difference (CB+BD) is an integral multiple of the wavelength ( $\lambda$ ), then the

two reflected rays will reinforce each other and produce an intense spot. Thus the condition of reinforcement is  $CB + BD = n \lambda$

From figure,

$$\text{angle } PAT = \text{angle } QTK = \theta$$

$$\text{But angle } PAC = 90^\circ$$

$$\text{So, angle } TAC = 90^\circ - \theta$$

$$\text{Now angle } TAB = 90^\circ$$

$$\text{So, as angle } TAC = 90^\circ - \theta, \text{ angle } CAB = \theta$$

Now in right angled triangle ACB,

$$\sin(\text{angle } CAB) = \sin(\theta) = CB / AB = CB / d$$

$$\text{So, } CB = d \sin(\theta).$$

Similarly, it can be shown that  $BD = d \sin(\theta)$

$$\text{So, } CB + BD = 2d \sin(\theta) = n \lambda$$

where  $n = 1, 2, 3, \dots$  etc., for first order, second order, third order ..... etc., maxima respectively. This relation is known as Bragg's law.

Intercepts on x, y and z axes :-  $a, 2a, 3a$

The reciprocals of intercepts :-  $1/a, 1/2a, 1/3a$

Reciprocals are reduced to smallest set of integers by taking LCM :-  $6, 3, 2$

So, miller indices :-  $(6, 3, 2)$

Now we have to draw  $(1, 2, 0)$  plane. Let intercepts by this plane on x, y and z axes are OA, OB

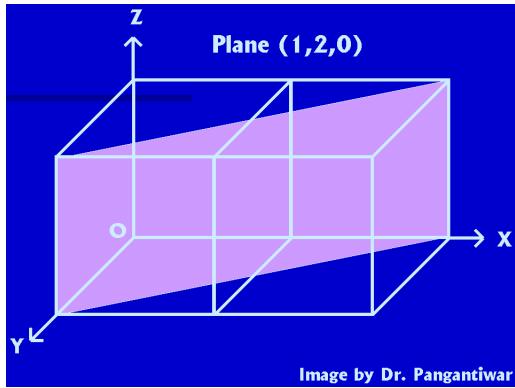


Image by Dr. Pangantiwar

and OC.

The reciprocals of intercepts :-  $1/OA, 1/OB, 1/OC$

Reciprocals are reduced to smallest set of integers by taking LCM :-  $a/OA, a/OB, a/OC$

But, miller indices of this plane are:-  $(1,2,0)$

So,  $1 = a/OA, 2 = a/OB, 0 = a/OC$

So,  $OA = a, OB = a/2$  and  $OC = \infty$  i.e plane is parallel to z axis.

i.e.  $OA = 2a, OB = 1a$  and plane is parallel to z axis.  
or,  $OA = 2, OB = 1$  and plane is parallel to z axis.

The packing density (PD) in SC :-

$$1 \times (4/3) \pi R^3 / a^3$$

i.e.  $1/1 \times 4/3 \pi / 1 \times [a/2]^3 \times 1 / (a)^3$

i.e.  $\pi / 6$

i.e. 0.52

The percentage of void space in SC :-

$$(1 - PD) \times 100$$

i.e.  $(1 - 0.52) \times 100 = 48\%$

The packing density in BCC :-

$$2 \times (4/3) \pi R^3 / a^3$$

i.e.  $2/1 \times 4/3 \pi / 1 \times [( \text{square root of } 3 ) \times a / 4]^3 \times 1 / (a)^3$

i.e.  $( \text{square root of } 3 ) \times (\pi / 8)$

i.e. 0.68.

The percentage of void space in BCC :-

$$(1 - PD) \times 100$$

i.e.  $(1 - 0.68) \times 100 = 32\%$

The packing density in FCC :-

$$4 \times (4/3) \pi R^3 / a^3$$

i.e.  $4/1 \times 4/3 \pi / 1 \times [( \text{square root of } 2 ) \times a / 4]^3 \times 1 / (a)^3$

i.e.  $\pi / (3 \times \text{square root of } 2)$

i.e. 0.74.

The percentage of void space in FCC :-

$$(1 - PD) \times 100$$

i.e.  $(1 - 0.74) \times 100 = 26\%$

Hence the FCC structure possesses maximum packing density and minimum percentage of void space among the three crystal structures SC, BCC and FCC.

$$\text{Density} = n M / N (a)^3$$

So, for SC, where  $n = 1$ ,

$$\text{Density} = M / N (a)^3$$

So, for BCC, where  $n = 2$ ,

$$\text{Density} = 2M / N (a)^3$$

So, for FCC, where  $n = 4$ ,

$$\text{Density} = 4M / N (a)^3$$

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GIVEN :-

Interplaner spacing,  $d = 2.82 \text{ \AA}^0 = 2.82 \times 10^{-10} \text{ m}$ .

Order of spectrum,  $n = 1$

We know that, Bragg's law is  $2d \sin(\theta) = n \lambda$

For  $\lambda$  to be maximum,  $\theta = 90^\circ$

So,  $\lambda = 2d$  for first order longest wavelength

$$\text{So, } \lambda = 2 \times 2.82 \text{ \AA}^0 = 5.64 \text{ \AA}^0$$

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(i) The relation between atomic radius ( $r$ ) and unit cell dimension ( $a$ ) for FCC structure is

$$r = a / [2(\text{square root of 2})].$$

(ii) The coordination number for a typical BCC structure is **8**.

(iii) The atomic packing fraction for a simple cubic structure is  **$\pi/6 = 0.52$** .

(iv) The percent void space for the BCC structure is **32%**.

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GIVEN :-

Lattice system = FCC

Density = 2180 kg / m<sup>3</sup>

Atomic weight of Na, M<sub>1</sub> = 23 kg / k.mol

Atomic weight of Cl, M<sub>2</sub> = 35.5 kg / k.mol

N = 6.02 x 10<sup>26</sup> atoms / k. mol.

For FCC, n = 4 atoms

Density = nM / N (a)<sup>3</sup>

And weight of NaCl molecule = M<sub>1</sub> + M<sub>2</sub>

So, a<sup>3</sup> = n (M<sub>1</sub> + M<sub>2</sub>) / (Density) N

i.e. a<sup>3</sup> = [(4 atoms) (23 + 35.5) kg / k.mol] / [(2180 kg / m<sup>3</sup>) (6.02 x 10<sup>26</sup> atoms / k. mol)]

i.e. a<sup>3</sup> = 234 x 10<sup>-31</sup> m<sup>3</sup> / 1.31

i.e. a<sup>3</sup> = 178.63 x 10<sup>-30</sup> m<sup>3</sup>

So, Lattice constant, a = cube root of [178.63 x 10<sup>-30</sup> m<sup>3</sup>]

i.e. a = 5.63 Å<sup>0</sup>

So the distance between adjacent atoms, sodium and chlorine is, d = a / 2

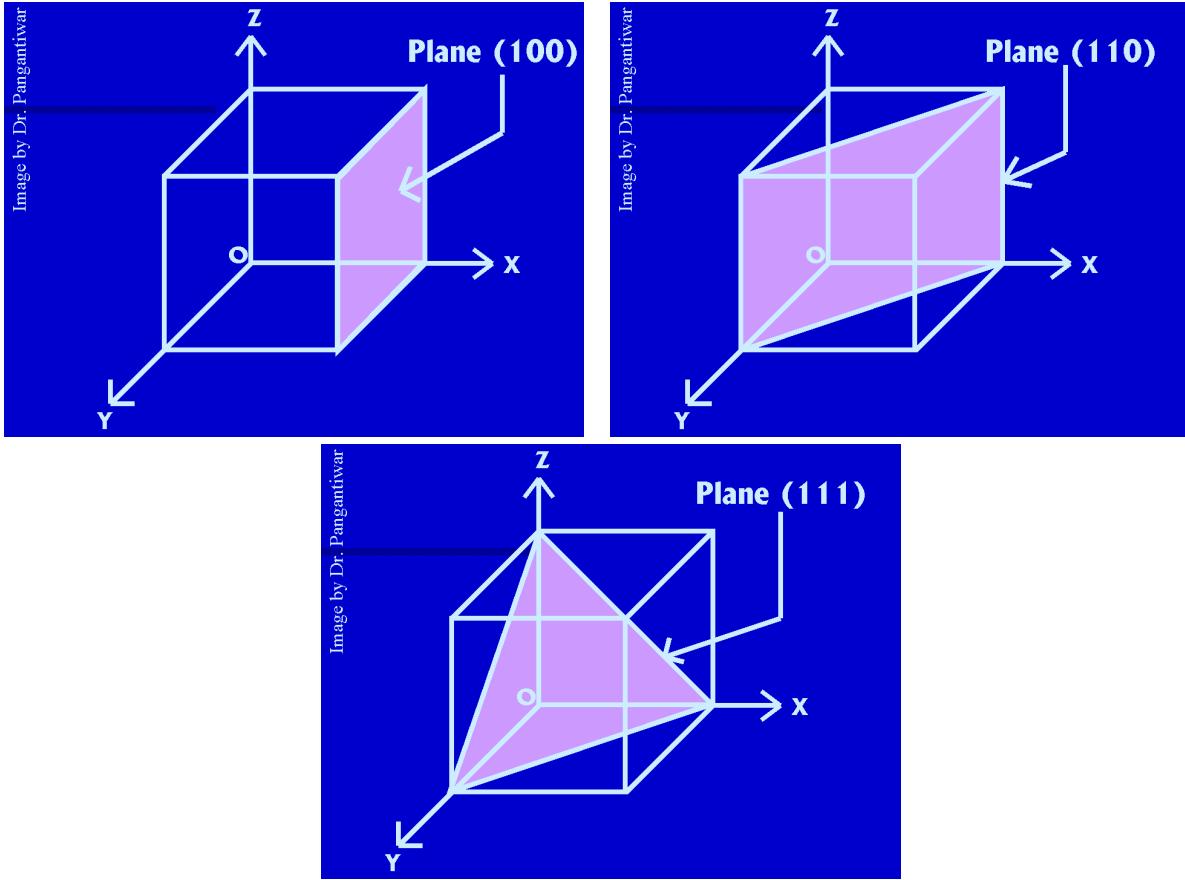
i.e. d = (5.63 / 2) Å<sup>0</sup> = 2.815 Å<sup>0</sup>

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Miller indices are the reciprocals of the intercepts, made by the plane on the crystallographic axes, when reduced to smallest integers.

Miller indices are used to designate the planes in a crystal lattice.



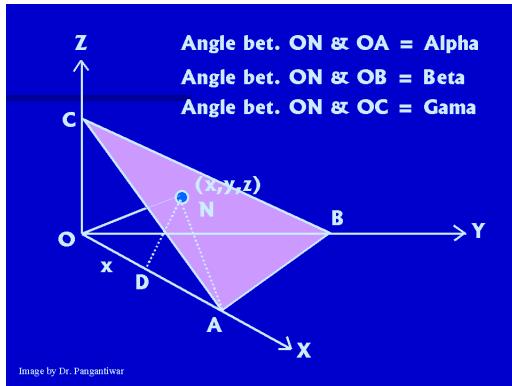
Let  $d_{hkl}$  represent the distance between two adjacent parallel planes having Miller indices  $(hkl)$ . Let the plane ABC be one of the planes. The perpendicular ON in figure from the origin to the plane ABC is equal to  $d_{hkl}$ . Let ON makes angles alpha, beta and gamma with x, y and z axes respectively. The intercepts of the plane ABC on the coordinate axes x, y and z are OA, OB and OC respectively.

Intercepts made by plane ABC on coordinate axes = OA, OB, OC

Reciprocals of these intercepts =  $1/OA, 1/OB, 1/OC$

Taking LCM, we get  $a/OA, a/OB, a/OC$

So Miller indices  $h = a/OA, k = a/OB, l = a/OC$



i.e. intercepts  $OA = a/h$ ,  $OB = a/k$ ,  $OC = a/l$ .  
 Let the coordinates of foot of perpendicular from O (Origin) to plane ABC i.e. point N are  $(x, y, z)$ .  
 Then  $(d_{hkl})^2 = x^2 + y^2 + z^2$

In right angled triangle OND, angle NOD is 90 degrees.

$$\text{So } \cos(\alpha) = x/d$$

$$\text{So } x = d \cos(\alpha)$$

Similarly  $y = d \cos(\beta)$  and  $z = d \cos(\gamma)$ .

$$\text{So } (d_{hkl})^2 = d^2 = d^2 \cos^2(\alpha) + d^2 \cos^2(\beta) + d^2 \cos^2(\gamma)$$

$$\text{i.e. } \cos^2(\alpha) + \cos^2(\beta) + \cos^2(\gamma) = 1 \quad \dots \dots \dots (1)$$

The points N and A lie in the plane ABC and ON is perpendicular to plane ABC. So ON is perpendicular to NA.

Now consider right angled triangle ONA. Here angle ONA is 90 degrees.

$$\text{So, here } \cos(\alpha) = d/NA = dh/a$$

$$\text{Similarly } \cos(\beta) = dk/a \text{ and } \cos(\gamma) = dl/a.$$

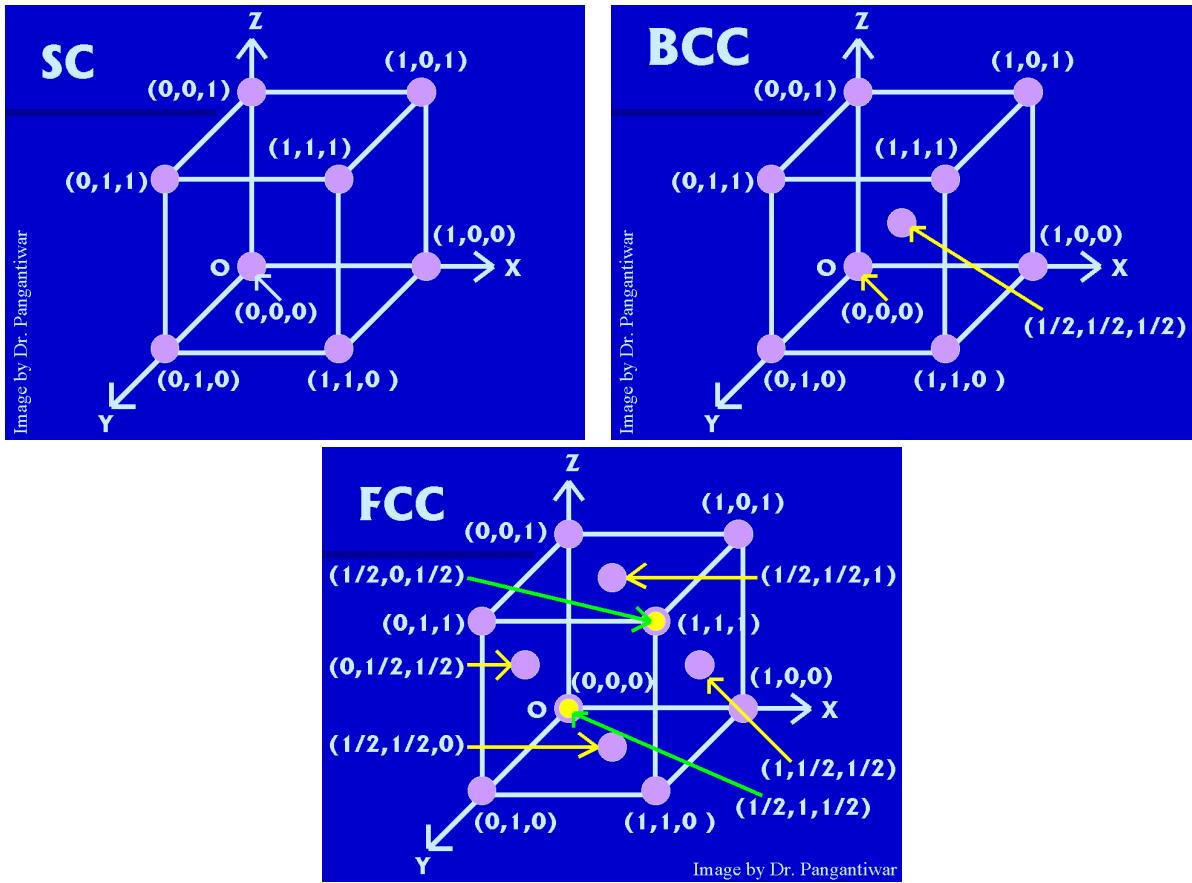
So, putting these values in equation (1), we get

$$(dh/a)^2 + (dk/a)^2 + (dl/a)^2 = 1$$

$$\text{i.e. } [d^2/a^2] (h^2 + k^2 + l^2) = 1$$

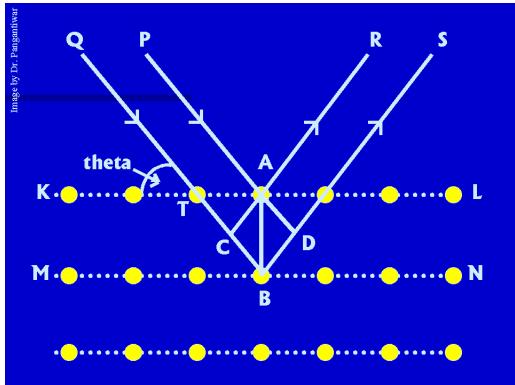
$$\text{i.e. } d^2 = a^2 / (h^2 + k^2 + l^2)$$

$$\text{i.e. } d_{hkl} = a / [\text{square root of } (h^2 + k^2 + l^2)]$$



i.e. we have to obtain the expression for Bragg's law,  $2d \sin (\theta) = n (\lambda)$ , where  $d$  is the interplaner distance,  $(\theta)$  is the angle between the Bragg plane and the direction of the incident beam and  $n = 1, 2, 3 \dots$  etc., for first order, second order, third order ..... etc., maxima respectively.

Let us consider a set of parallel lattice planes of a crystal separated by a distance  $d$  apart, i.e.  $AB = d$ . Suppose a narrow beam of X-rays of wavelength  $(\lambda)$  be incident upon these planes at an angle  $(\theta)$  as shown in figure. The beam will be reflected in all directions by the atoms of various atomic planes. Because the refractive index of the matter of the crystal is very nearly equal to unity, there is practically no bending of the rays entering or leaving the crystal.



Consider a ray PA reflected at atom A in the direction AR from plane KL and another ray QB reflected at another atom B from plane MN in the direction BS. Now from the atom A, draw two perpendiculars AC and AD on the incident ray QB and reflected ray BS respectively. The path difference between these two rays is (CB+BD). The two reflected rays will be in phase or out of phase, will depend upon this path difference. When the path difference (CB+BD) is an integral multiple of the wavelength ( $\lambda$ ), then the

two reflected rays will reinforce each other and produce an intense spot. Thus the condition of reinforcement is  $CB + BD = n(\lambda)$

From figure,

$$\text{angle } \text{PAT} = \text{angle } \text{QTK} = \theta$$

$$\text{But angle } \text{PAC} = 90^\circ$$

$$\text{So, angle } \text{TAC} = 90^\circ - \theta$$

$$\text{Now angle TAB} = 90^\circ$$

$$\text{So, as angle TAC} = 90^\circ - \theta, \text{ angle CAB} = \theta$$

Now in right angled triangle ACB,

$$\sin(\text{angle CAB}) = \sin(\theta) = CB / AB = CB / d$$

$$\text{So, } CB = d \sin(\theta).$$

Similarly, it can be shown that  $BD = d \sin(\theta)$

$$\text{So, } CB + BD = 2d \sin(\theta) = n(\lambda)$$

where  $n = 1, 2, 3, \dots$  etc., for first order, second order, third order ..... etc., maxima respectively. This relation is known as Bragg's law.

Bragg's law is a necessary but not sufficient condition for diffraction. It specifies the diffraction for primitive unit cells such as simple cubic cells. If the given natural crystal is nonprimitive cell, some of the diffractions predicted by Bragg's law do not occur.

Miller indices are the reciprocals of the intercepts, made by the plane on the crystallographic axes, when reduced to smallest integers.

Miller indices are used to designate the planes in a crystal lattice.

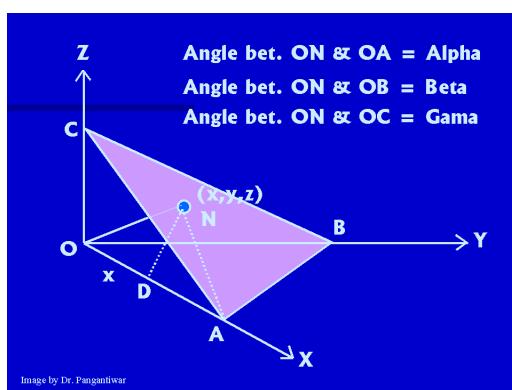
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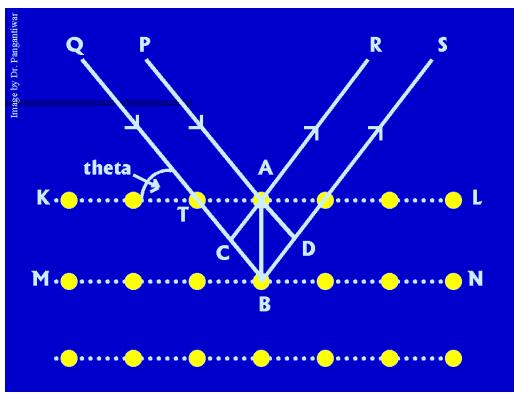
$$\text{i.e. } d^2 = a^2 / (h^2 + k^2 + l^2)$$

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## $2d \sin (\theta) = n (\lambda)$ ,

where  $d$  is the interplaner distance,  $(\theta)$  is the angle between the Bragg plane and the direction of the incident beam and  $n = 1, 2, 3 \dots$  etc., for first order, second order, third order ..... etc., maxima respectively, is known as Bragg's law.

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$$\text{But angle PAC} = 90^\circ$$

$$\text{So, angle TAC} = 90 - \theta$$

$$\text{Now angle TAB} = 90^\circ$$

$$\text{So, as angle TAC} = 90 - \theta, \text{ angle CAB} = \theta$$

Now in right angled triangle ACB,

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**GIVEN :-**

$$r = 1.746 \text{ Å}^0 = 1.746 \times 10^{-10} \text{ m.}$$

For FCC,  $a = 2$  (square root of 2)  $r$

$$\text{i.e. } a = 2 \times 1.414 \times 1.746 \times 10^{-10} \text{ m}$$

$$\text{i.e. } a = 4.94 \times 10^{-10} \text{ m}$$

$$\text{Spacing of (hkl) plane} = d_{hkl} = [a / \text{square root of (} h^2 + k^2 + l^2 \text{)}]$$

$$\text{So, spacing of (202) plane} = d_{202} = [4.94 \times 10^{-10} / \text{square root of (} 2^2 + 0^2 + 2^2 \text{)}]$$

$$\text{i.e. } d_{202} = 1.75 \times 10^{-10} \text{ m.}$$

$$\text{So, spacing of (220) plane} = d_{220} = [4.94 \times 10^{-10} / \text{square root of (} 2^2 + 2^2 + 0^2 \text{)}]$$

$$\text{i.e. } d_{220} = 1.75 \times 10^{-10} \text{ m.}$$

$$\text{So, spacing of (111) plane} = d_{111} = [4.94 \times 10^{-10} / \text{square root of (} 1^2 + 1^2 + 1^2 \text{)}]$$

$$\text{i.e. } d_{111} = 1.01 \times 10^{-10} \text{ m.}$$

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The number of equidistant neighbours that an atom has in the given structure, is the coordination number.

When the coordination number is large, the structure is more closely packed.

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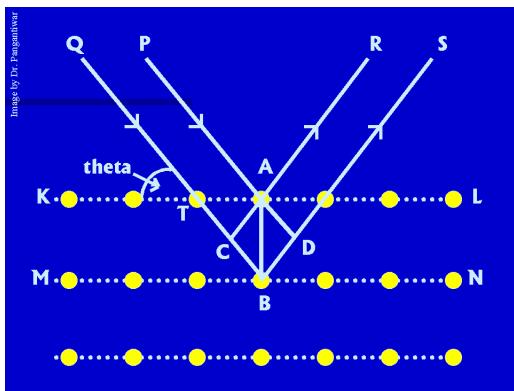
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**$2d \sin(\theta) = n \lambda$** ,

where  $d$  is the interplaner distance,  $(\theta)$  is the angle between the Bragg plane and the direction of the incident beam and  $n = 1, 2, 3 \dots$  etc., for first order, second order, third order ..... etc., maxima respectively, is known as Bragg's law.

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where  $n = 1, 2, 3, \dots$  etc., for first order, second order, third order ..... etc., maxima respectively. This relation is known as Bragg's law.

The packing density (PD) in SC :-

$$1 \times (4/3) \pi (R)^3 / (a)^3$$

$$\text{i.e. } 1/1 \times 4/3 \times \pi/1 \times [a/2]^3 \times 1/(a)^3$$

- i.e.  $\pi / 6$   
 i.e. 0.52  
 i.e. percentage of packing density = 52 %

The percentage of void space in SC :-

$$(1 - PD) \times 100$$

$$\text{i.e. } (1 - 0.52) \times 100 = 48\%$$

The packing density in BCC :-

$$2 \times (4/3) \pi (R)^3 / (a)^3$$

$$\text{i.e. } 2/1 \times 4/3 \times \pi/1 \times [(square root of 3) \times a /4]^3 \times 1/ (a)^3$$

$$\text{i.e. } (square root of 3) \times (\pi / 8)$$

$$\text{i.e. } 0.68.$$

$$\text{i.e. percentage of packing density} = 68 \%$$

The percentage of void space in BCC :-

$$(1 - PD) \times 100$$

$$\text{i.e. } (1 - 0.68) \times 100 = 32\%$$

The packing density in FCC :-

$$4 \times (4/3) \pi (R)^3 / (a)^3$$

$$\text{i.e. } 4/1 \times 4/3 \times \pi/1 \times [(square root of 2) \times a /4]^3 \times 1/ (a)^3$$

$$\text{i.e. } \pi / (3 \times square root of 2)$$

$$\text{i.e. } 0.74.$$

$$\text{i.e. percentage of packing density} = 74 \%$$

The percentage of void space in FCC :-

$$(1 - PD) \times 100$$

$$\text{i.e. } (1 - 0.74) \times 100 = 26\%$$

Hence the SC structure possesses minimum percentage of packing density and maximum percentage of void space among the three cubiccrystal structures.

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GIVEN :-

$$r = 1.746 \text{ \AA}^0 = 1.746 \times 10^{-10} \text{ m.}$$

$$\text{For FCC, } a = 2 \text{ (square root of 2)} r$$

$$\text{i.e. } a = 2 \times 1.414 \times 1.746 \times 10^{-10} \text{ m}$$

$$\text{i.e. } a = 4.94 \times 10^{-10} \text{ m}$$

Spacing of (hkl) plane =  $d_{hkl} = [a / \text{square root of } (h^2 + k^2 + l^2)]$

So, spacing of (111) plane =  $d_{111} = [4.94 \times 10^{-10} / \text{square root of } (1^2 + 1^2 + 1^2)]$   
i.e.  $d_{111} = 1.01 \times 10^{-10}\text{m}$ .

So, spacing of (220) plane =  $d_{220} = [4.94 \times 10^{-10} / \text{square root of } (2^2 + 2^2 + 0^2)]$   
i.e.  $d_{220} = 1.75 \times 10^{-10}\text{m}$ .

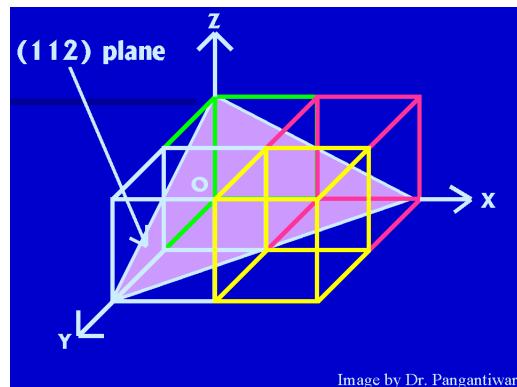
So, spacing of (200) plane =  $d_{200} = [4.94 \times 10^{-10} / \text{square root of } (2^2 + 0^2 + 0^2)]$   
i.e.  $d_{200} = 2.47 \times 10^{-10}\text{m}$ .

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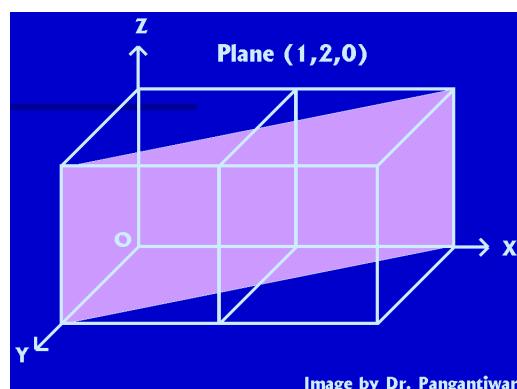
Now we have to draw (112) plane. Let intercepts by this plane on x, y and z axes are OA, OB



and OC.

The reciprocals of intercepts :-  $1/\text{OA}$ ,  $1/\text{OB}$ ,  $1/\text{OC}$   
Reciprocals are reduced to smallest set of integers by taking LCM :-  $a/\text{OA}$ ,  $a/\text{OB}$ ,  $a/\text{OC}$   
But, miller indices of this plane are:- 1, 1, 2  
So,  $1 = a/\text{OA}$ ,  $1 = a/\text{OB}$ ,  $2 = a/\text{OC}$   
So,  $\text{OA} = a$ ,  $\text{OB} = a$  and  $\text{OC} = a/2$ .  
or,  $\text{OA} = 2$ ,  $\text{OB} = 2$  and  $\text{OC} = 1$ .

Now we have to draw (120) plane. Let intercepts by this plane on x, y and z axes are OA, OB



and OC.

The reciprocals of intercepts :-  $1/\text{OA}$ ,  $1/\text{OB}$ ,  $1/\text{OC}$   
Reciprocals are reduced to smallest set of integers by taking LCM :-  $a/\text{OA}$ ,  $a/\text{OB}$ ,  $a/\text{OC}$   
But, miller indices of this plane are:- (1,2,0)  
So,  $1 = a/\text{OA}$ ,  $2 = a/\text{OB}$ ,  $0 = a/\text{OC}$   
So,  $\text{OA} = a$ ,  $\text{OB} = a/2$  and  $\text{OC} = \infty$  i.e plane is parallel to z axis.  
i.e.  $\text{OA} = 2a$ ,  $\text{OB} = 1a$  and plane is parallel to z axis.  
or,  $\text{OA} = 2$ ,  $\text{OB} = 1$  and plane is parallel to z axis.

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### GIVEN :-

$$r = 0.1278 \text{ nm} = 0.1278 \times 10^{-9} \text{ m.}$$

For FCC,  $a = 2$  (square root of 2)  $r$

$$\text{i.e. } a = 2 \times 1.414 \times 0.1278 \times 10^{-9} \text{ m}$$

$$\text{i.e. } a = 3.61 \times 10^{-10} \text{ m}$$

$$\text{Spacing of (hkl) plane} = d_{hkl} = [a / \text{square root of (} h^2 + k^2 + l^2 \text{)}]$$

$$\text{So, spacing of (111) plane} = d_{111} = [3.61 \times 10^{-10} / \text{square root of (} 1^2 + 1^2 + 1^2 \text{)}]$$

$$\text{i.e. } d_{111} = 2.08 \times 10^{-10} \text{ m.}$$

$$\text{So, spacing of (321) plane} = d_{321} = [3.61 \times 10^{-10} / \text{square root of (} 3^2 + 2^2 + 1^2 \text{)}]$$

$$\text{i.e. } d_{321} = 9.65 \times 10^{-11} \text{ m.}$$

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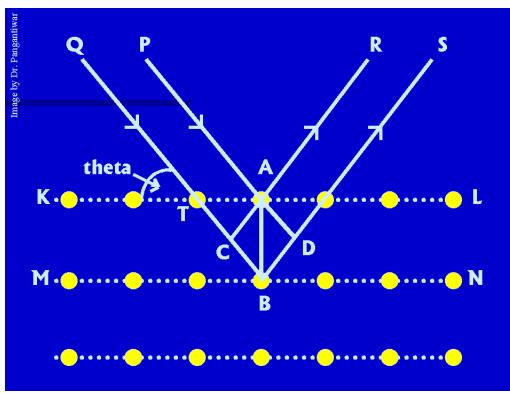
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Sr. No.	Properties	Unit Cell		
		SC	BCC	FCC
1	No. of atoms per unit cell, $n$	1	2	4
2	Atomic radius, $r$	$a/2$	$[a (\text{square root of 3})] / 4$	$a / [2 (\text{square root of 2})]$
3	Nearest neighbour distance, $2r$	$a$	$[a (\text{square root of 3})] / 2$	$a / (\text{square root of 2})$
4	Coordination number, CN	6	8	12
5	Atomic packing fraction, APF	$(\pi / 6) = 0.52$	$[\pi (\text{square root of 3})] / 8 = 0.68$	$\pi / [3 (\text{square root of 2})] = 0.74$
6	Void space	48 %	32 %	26 %
7	Density	$M / [n (a)^3]$	$2 M / [n (a)^3]$	$4 M / [n (a)^3]$

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Let us consider a set of parallel lattice planes of a crystal separated by a distance  $d$  apart, i.e.  $AB = d$ . Suppose a narrow beam of X-rays of wavelength ( $\lambda$ ) be incident upon these planes at an angle ( $\theta$ ) as shown in figure. The beam will be reflected in all directions by the atoms of various atomic planes. Because the refractive index of the matter of the crystal is very nearly equal to unity, there is practically no bending of the rays entering or leaving the crystal.



Consider a ray  $PA$  reflected at atom  $A$  in the direction  $AR$  from plane  $KL$  and another ray  $QB$  reflected at another atom  $B$  from plane  $MN$  in the direction  $BS$ . Now from the atom  $A$ , draw two perpendiculars  $AC$  and  $AD$  on the incident ray  $QB$  and reflected ray  $BS$  respectively. The path difference between these two rays is  $(CB+BD)$ . The two reflected rays will be in phase or out of phase, will depend upon this path difference. When the path difference  $(CB+BD)$  is an integral multiple of the wavelength ( $\lambda$ ), then the

two reflected rays will reinforce each other and produce an intense spot. Thus the condition of reinforcement is  $CB + BD = n(\lambda)$

From figure,

$$\text{angle } PAT = \text{angle } QTK = \theta$$

$$\text{But angle } PAC = 90^\circ$$

$$\text{So, angle } TAC = 90^\circ - \theta$$

$$\text{Now angle } TAB = 90^\circ$$

$$\text{So, as angle } TAC = 90^\circ - \theta, \text{ angle } CAB = \theta$$

Now in right angled triangle  $ACB$ ,

$$\sin(\text{angle } CAB) = \sin(\theta) = CB / AB = CB / d$$

$$\text{So, } CB = d \sin(\theta).$$

Similarly, it can be shown that  $BD = d \sin(\theta)$

$$\text{So, } CB + BD = 2d \sin(\theta) = n(\lambda)$$

where  $n = 1, 2, 3 \dots$  etc., for first order, second order, third order ..... etc., maxima respectively. This relation is known as Bragg's law.

X-ray diffraction technique can be used to analyze different types of crystal structures using Bragg's X-ray spectrometer.

---

GIVEN :-

Edge of unit cell,  $a = 4.3 \text{ \AA}^0 = 4.3 \times 10^{-10} \text{ m}$

Density of sodium, Density =  $963 \text{ kg / m}^3$

Atomic weight,  $M = 23 \text{ kg / k. mol}$

Avogadro's number,  $N = 6.02 \times 10^{26} \text{ atoms / k. mol.}$

$$\text{Density} = nM / N (a)^3$$

$$\text{So, } n = [\text{Density } N (a^3)] / M$$

$$\text{i.e. } n = [(963 \text{ kg / m}^3) (6.02 \times 10^{26} \text{ atoms / k.mol}) (4.3 \times 10^{-10} \text{ m})^3] / (23 \text{ kg / k.mol})$$

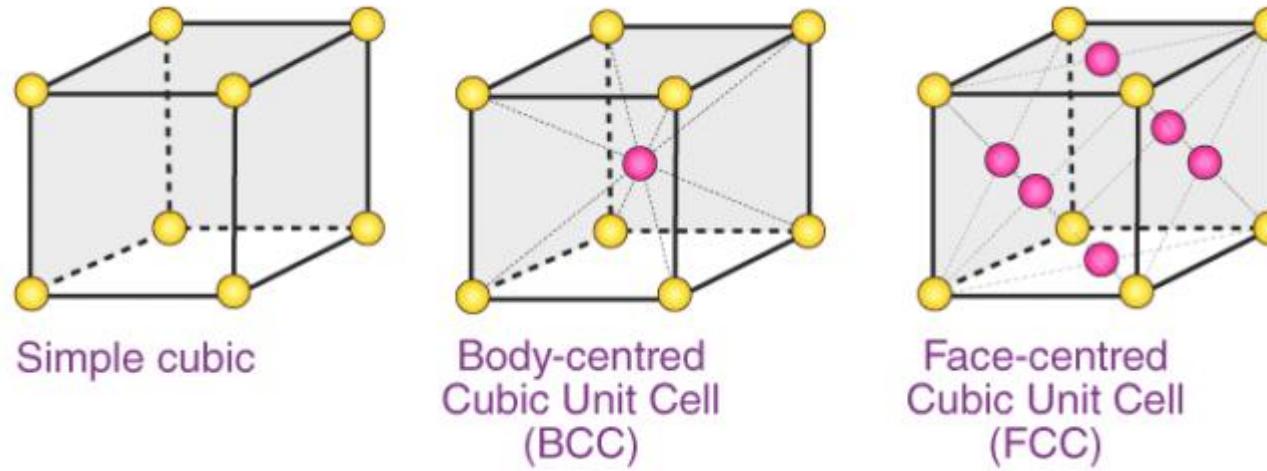
$$\text{i.e. } n = 46.09 / 23 \text{ atoms} = 2 \text{ atoms}$$

As, number of atoms per unit cell in BCC is 2, sodium crystallizes in a BCC cell.

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# Introduction to Solid State Physics

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The science of **crystallography** is concerned with the enumeration and classification of all possible types of crystal structures and determination of the actual structure of the crystalline solids.

Based on their crystal structures, solids can be classified into the following categories:

- 1. Crystalline solids**
- 2. Amorphous solids**

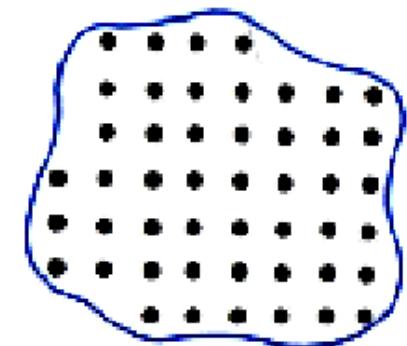
**Crystalline:** Elements and their chemical compounds are found to occur in three states, i.e., solids, liquids and gases. If the atoms or molecules in a solid are arranged in some regular fashion, it is known as crystalline materials.

Or,

The solids featuring highly ordered arrangements of their particles (atoms, ions, and molecules) in microscopic structures are called crystalline solids.

Examples of crystalline solids include **salt (sodium chloride)**, **diamond**, and **sodium nitrate**.

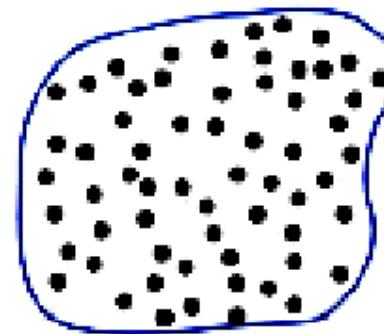
Dr. M M Hossain



**Crystalline**

**Non-crystalline or amorphous:** When the atoms or molecules in a solid are arranged in an irregular fashion, it is known as non-crystalline or amorphous.

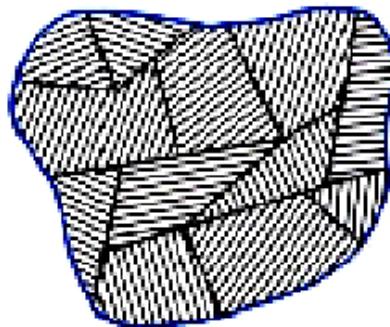
Or, The solids in which the particles are not arranged in any specific order or the solids that lack the overall order of a crystal lattice are called amorphous solids.



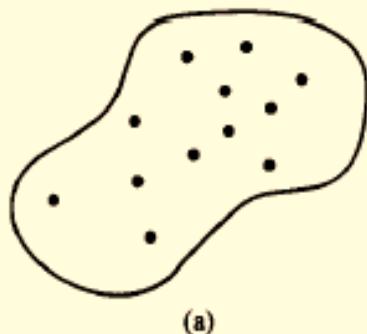
**Amorphous**

In **single crystals** the same periodicity extends throughout the material.

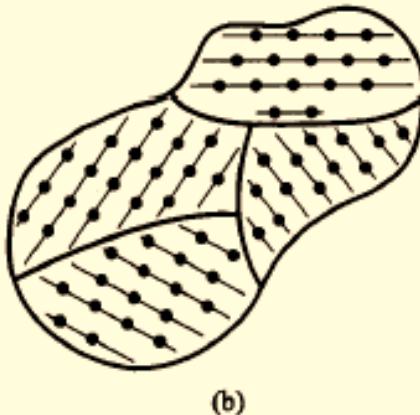
Whereas in **polycrystalline crystals** the same periodicity does not extend throughout the crystal but is interrupted at grain boundaries.



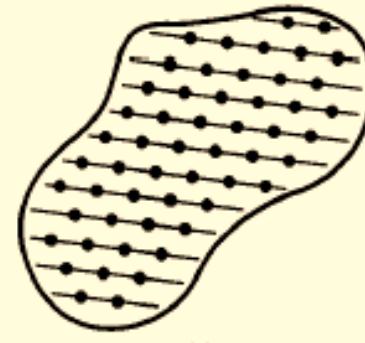
**Polycrystalline**



(a)



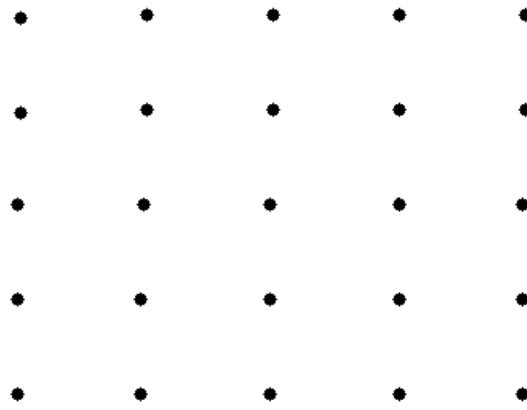
(b)



(c)

**Figure 1–1** Schematics of three general types of crystals: (a) amorphous, (b) polycrystalline, (c) single crystal.

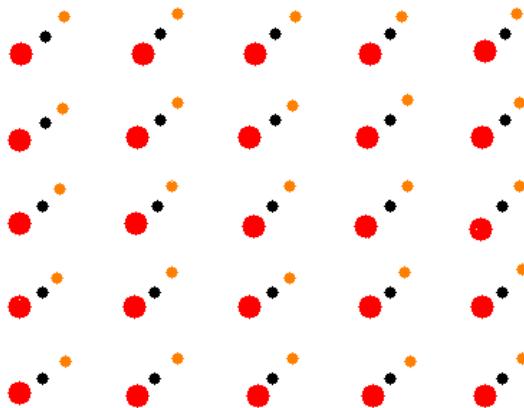
**Lattice:** A lattice is a hypothetical regular and periodic arrangement of points in space. It is used to describe the structure of a crystal.



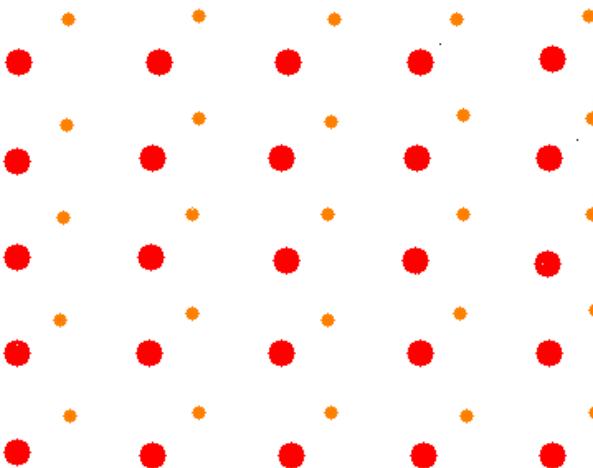
**Basis:** A basis is a collection of atoms in particular fixed arrangement in space. We could have a basis of a single atom as well as a basis of a complicated but fixed arrangement of hundreds of atoms. Below we see a basis of two atoms inclined at a fixed angle in a plane.



Let us now attach the above basis to each lattice point (in black) as follows.



Next remove the lattice points in black (remember that the lattice is an abstract entity). Lets see what we have got?



We have got the actual two-dimensional crystal in real space. So we may write:

$$\text{lattice} + \text{basis} = \text{crystal}$$

### Unit cell:

We have seen that the atomic order in crystalline solids indicates that **the smallest groups of atoms form a repetitive pattern**. Thus in describing crystal structures, it is often convenient to subdivide the structure into repetitive small repeat entities called *unit cell*, i.e. in every crystal some fundamental grouping of particles is repeated.

## In Summary.....

**CRYSTAL:** Translationally periodic arrangement of ATOMS in space.

**LATTICE:** Translationally periodic arrangement of POINTS in space.

**BASIS (or MOTIF):** An atom or a group of atoms associated with each lattice point in crystal

.

**CRYSTAL=LATTICE+BASIS**

**LATTICE** of a crystal tells how to repeat (the periodicity of the crystal).

**BASIS** tells what to repeat according to the lattice to get the crystal.

**LATTICE TRANSLATION:** A vector from one lattice point to another.

**UNIT CELL:** A finite region of space which when translated by all lattice translations, or a subset of lattice translations, can fill the entire space without gaps or overlaps (i.e., it tiles the space).

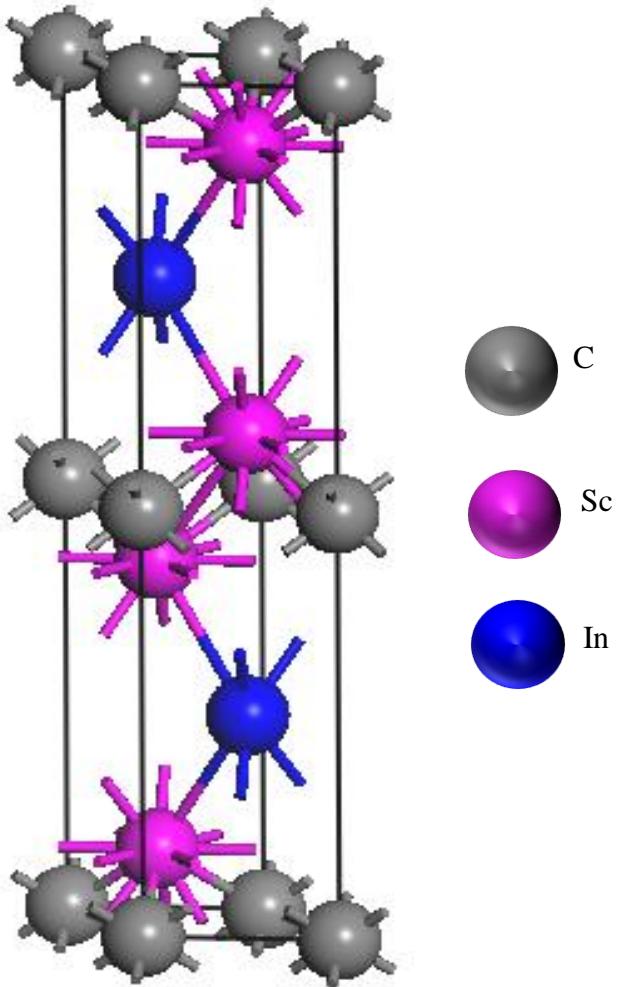


Fig.: Optimized unit cell of the  $\text{Sc}_2\text{InC}$  compound.

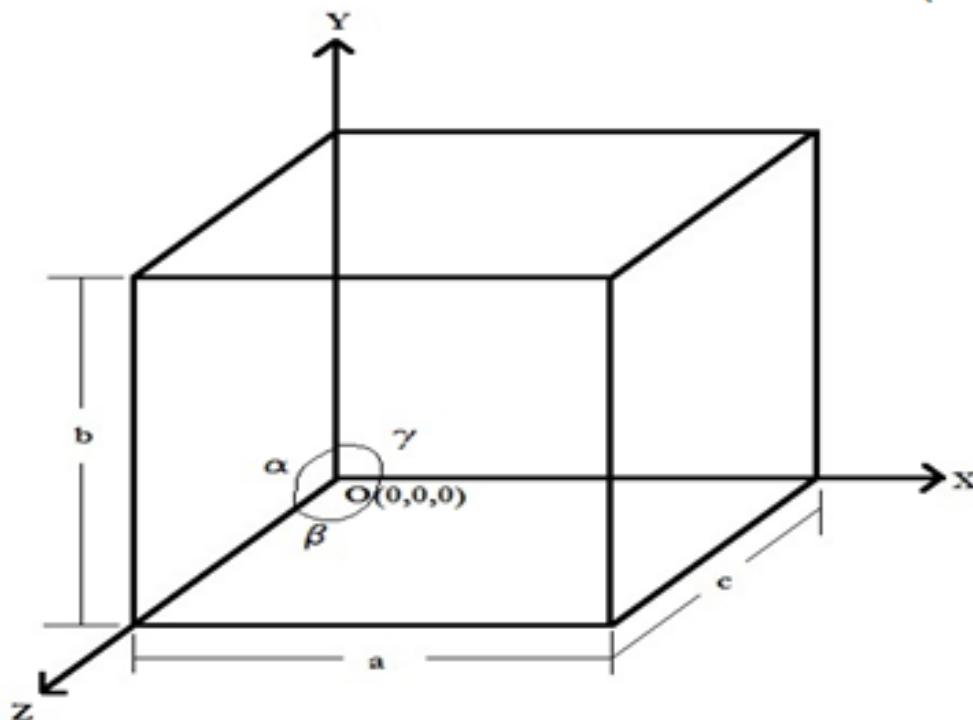
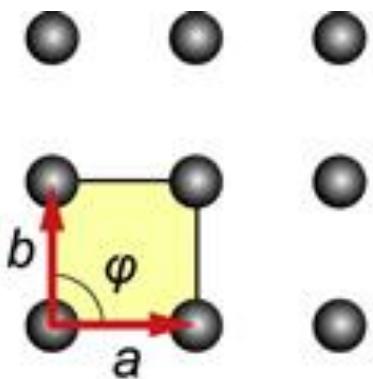


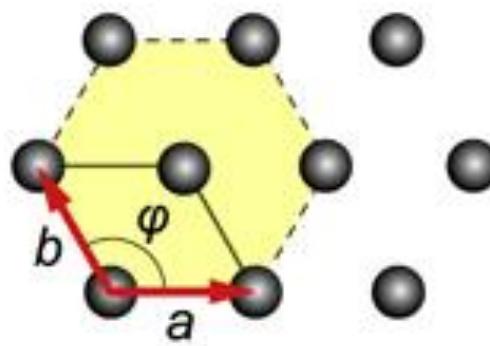
Fig. 1.1: Lattice Parameters

## Lattice types in 2 dimensional system



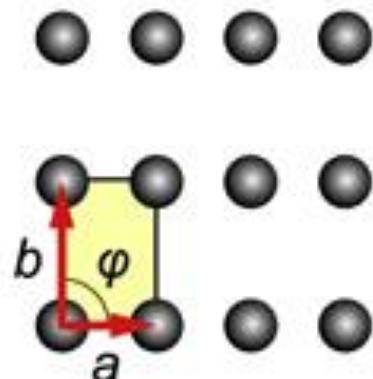
$$|a| = |b|, \varphi = 90^\circ$$

Square



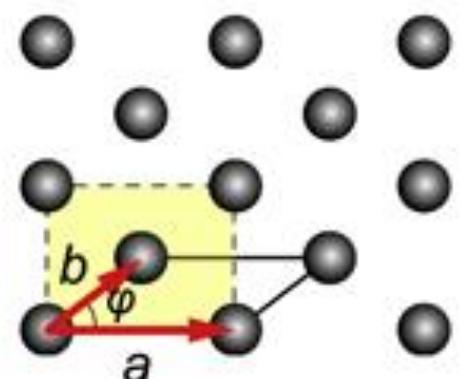
$$|a| = |b|, \varphi = 120^\circ$$

Hexagonal



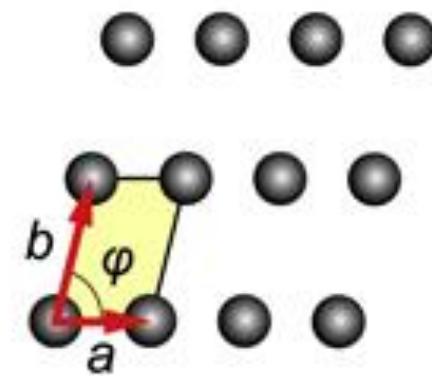
$$|a| \neq |b|, \varphi = 90^\circ$$

Rectangular



$$|a| \neq |b|, \varphi = 90^\circ$$

Centered Rectangular



$$|a| \neq |b|, \varphi \neq 90^\circ$$

Oblique

# Bravais space lattice in three dimensions

<i>Crystal system</i>	<i>Lattice Type</i>	<i>Relation between primitives</i>	<i>Relation between interfacial angles</i>	<i>Example</i>
Cubic	P, F, C	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$	Au, NaCl, CaF <sub>2</sub>
Monoclinic	P, B	$a \neq b \neq c$	$\alpha = \beta = 90^\circ \neq \gamma$	CaSO <sub>4</sub> , FeSO <sub>4</sub> , Na <sub>2</sub> SO <sub>4</sub>

P = primitives

C = body-centered

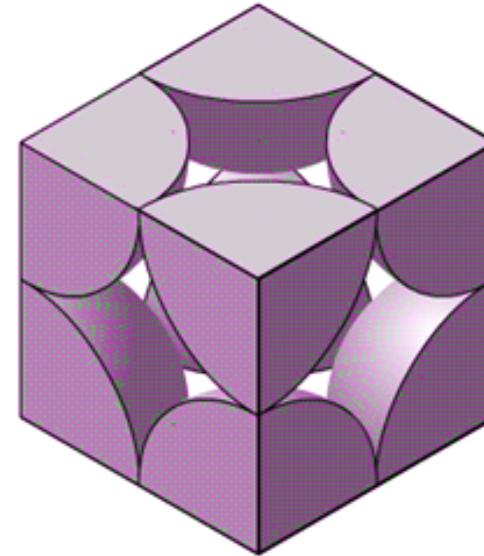
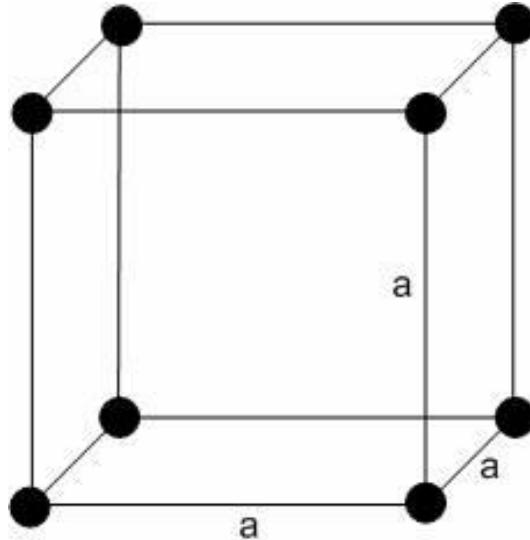
B = base-centered

F = face-centered

<i>Crystal system</i>	<i>Lattice Type</i>	<i>Relation between primitives</i>	<i>Relation between interfacial angles</i>	<i>Example</i>
Triclinic	P	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$	$\text{CuSO}_4$
Tetragonal	P, C	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	$\text{TiO}_3, \text{NiSO}_4, \text{SnO}_4$
Orthorhombic (orthogonal)	P, C, B, F	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	$\text{KNO}_3, \text{BaSO}_4$
Rhombohedral (trigonal)	P or R	$a = b = c$	$\alpha = \beta = \gamma \neq 90^\circ$	$\text{CaSO}_4, \text{CaCO}_3$
Hexagonal	P	$a = b \neq c$	$\alpha = \beta = 90^\circ, \gamma = 120^\circ$	$\text{SiO}_2, \text{Zn}$

## Simple cubic (sc) cell

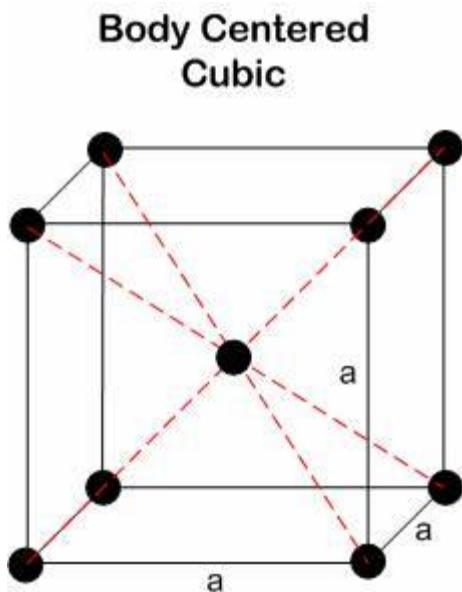
As stated in the previous slide, each corner atom in a cubic cell is shared by a total number of eight unit cells so that each corner atom contributes only  $1/8$  of its effective part to a unit cell. Since there are in all 8 corner atoms there total contribution is equal to  $\frac{1}{8} \times 8 = 1$ . Thus the number of atoms per unit simple cubic cell is one.



## Body centered cubic (bcc) cell

The contribution of body centered is full, i.e., one. This is in addition to eight corner atoms. So number of atoms per unit body centered cubic cell.

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

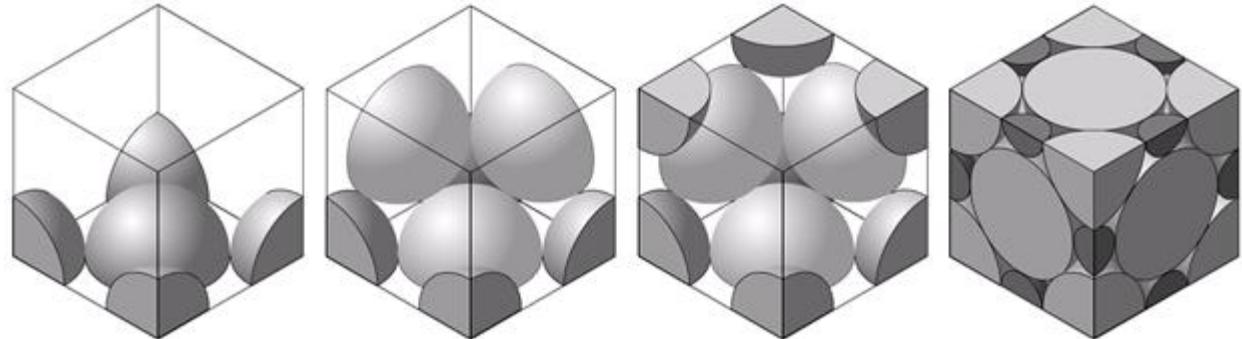
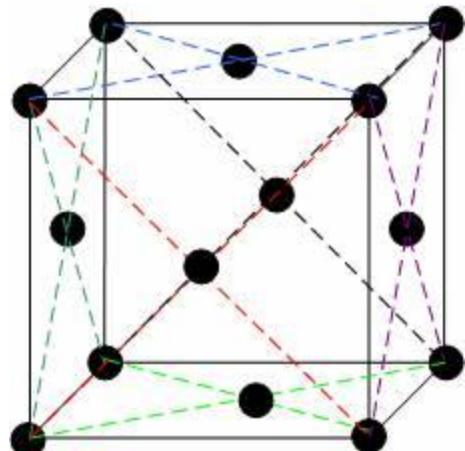


## Face centered cubic (fcc) cell

Each face centered atom is shared by two unit cells. There are six faces of a cube and there are eight corner atoms. So Number of atoms per unit face centered cubic cell

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

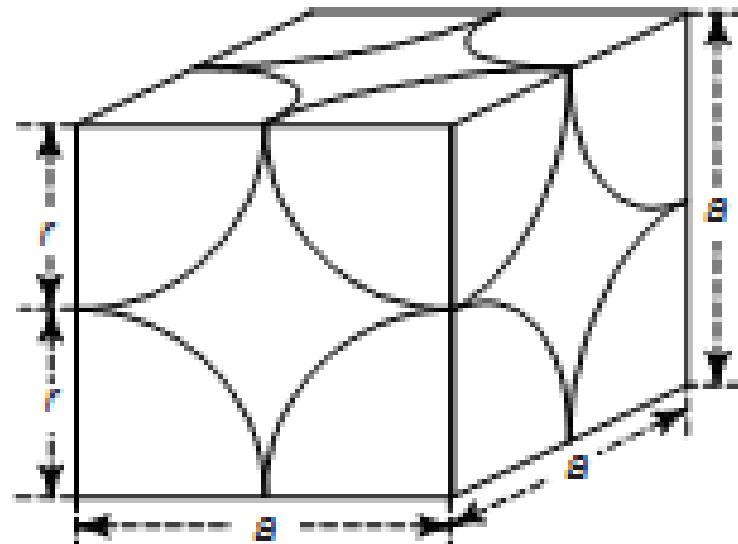
Face Centered Cubic



# Atomic Radius

Atomic radius is denoted by  $r$  and expressed in terms of cube edge element  $a$ . Atomic radius can be calculated by assuming that atoms are spheres in contact in crystal.

In the case of a *simple cube*, if  $r$  be the atomic radius and lattice parameter is ‘ $a$ ’ then  $a = 2r$  or  $r = a/2$ . And area



$$a^2 = 4r^2$$

In case of a *body centered cube*, the atoms touch each other along the diagonal of the cube as shown below.

Obviously, the diagonal in this case is  $4r$ . Also,

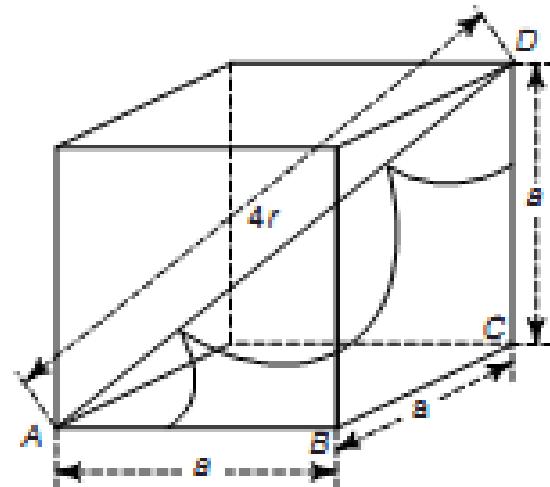
$$AC^2 = AB^2 + BC^2 = a^2 + a^2 = 2a^2$$

$$AD^2 = AC^2 + CD^2 = 2a^2 + a^2 = 3a^2$$

$$a = \frac{4r}{\sqrt{3}} \quad \text{and} \quad 2r = \frac{a\sqrt{3}}{2}$$

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

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



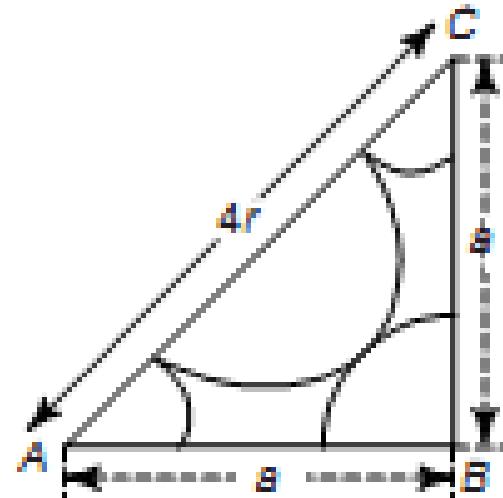
In case of a ***face centered cube*** the atoms are in contact along the diagonal of the faces as shown below. The diagonal has a length of  $4r$ .

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

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

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

$$a^2 = 8r^2$$



**Example1: A compound formed by elements A and B has a cubic structure in which A atoms are at the corners of the cube and B atoms are at face centres. Derive the formula of the compound.**

**Solution:**

As ‘A’ atom are present at the 8 corners of the cube therefore no of atoms of A in the unit cell =  $\frac{1}{8} \times 8 = 1$

As B atoms present at the face centres of the cube, therefore no of atoms of B in the unit cell =  $\frac{1}{2} \times 6 = 3$

Hence the formula of compound is  $\text{AB}_3$ .

## Atomic packing fraction

The packing fraction is the maximum proportion of the available volume that can be filled hard spheres.

Or,

The fraction of volume occupied by spherical atoms as compared to the total available volume of the structure.

In a ***simple cubic (sc)*** structure the number of atoms per unit cell is one. The atomic radius is given by half the primitive, i. e.,  $a/2$ .

So the volume occupied by the atom in the unit cell

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

Volume of the unit cell =  $a^3$  ; so the packing fraction

$f$  = volume of spheres/volume of cube

$$f = \frac{\frac{4}{3} \pi \left(\frac{a}{2}\right)^3}{a^3} = \frac{\pi}{6} = 52\%$$

Thus the atoms are loosely packed. Polonium at a certain temperature exhibits such structure.

# Body Centered Cube (bcc)

In a *body centered cubic* lattice there are two atoms per unit cell.

The atomic radius  $r = \frac{a\sqrt{3}}{4}, a = \frac{4r}{\sqrt{3}}$

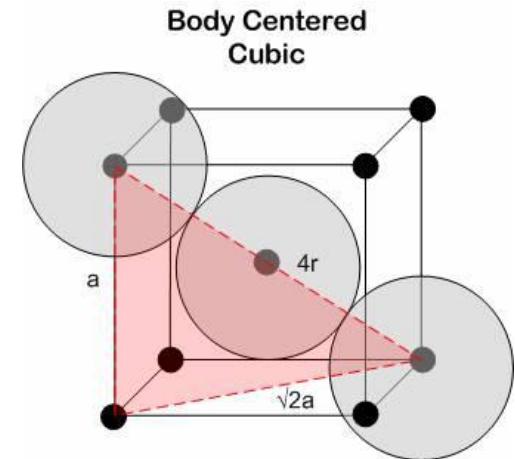
So volume occupied by the atoms in the unit cell

$$= 2 \times \frac{4}{3} \pi r^3 = 2 \times \frac{4}{3} \pi \frac{3^{\frac{3}{2}}}{4^3} a^3 = \frac{\sqrt{3}}{8} \pi a^3$$

Volume of the unit cell =  $a^3$

So, packing fraction  $f = \frac{\frac{\sqrt{3}}{8} \pi a^3}{a^3} = \frac{\sqrt{3}\pi}{8} = 68\%$

Common substances with bcc lattice are barium, chromium, sodium, iron and cesium chloride.



# Face Centered Cube (fcc)

In a face centered cubic lattice there are four atoms per unit cell.

The atomic radius  $r = \frac{a}{2\sqrt{2}}$

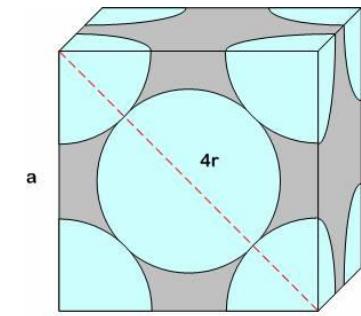
So the volume occupied by the atoms in the unit cell  $a^3$

Volume of the unit cell  $= 4 \times \frac{4}{3}\pi r^3 = \frac{16}{3}\pi \frac{a^3}{2^3 2\sqrt{2}} = \frac{\pi}{3\sqrt{2}} a^3$

So packing fraction

$$f = \frac{\frac{\pi}{3\sqrt{2}} a^3}{a^3} = \frac{\pi}{3\sqrt{2}} = 74\%$$

Common examples of this type of structure is Ni, Cu, Au, Al, Ag, Li, K, etc.



## Hexagonal Closed Packed (hcp)

In hexagonal closed packed (hcp) structure unit cell contains one atom at each corner of the hexagonal prism, one atom at each at the center of the hexagonal faces and three more atoms within the body of the cell. This type of structure is denser than the simple hexagonal structure. Total number of atoms inside is 6.

Each corner atoms is shared by 6 other unit lattices or each corner has  $\frac{1}{6}$  atom.  
Number of atoms in upper hexagonal plane

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

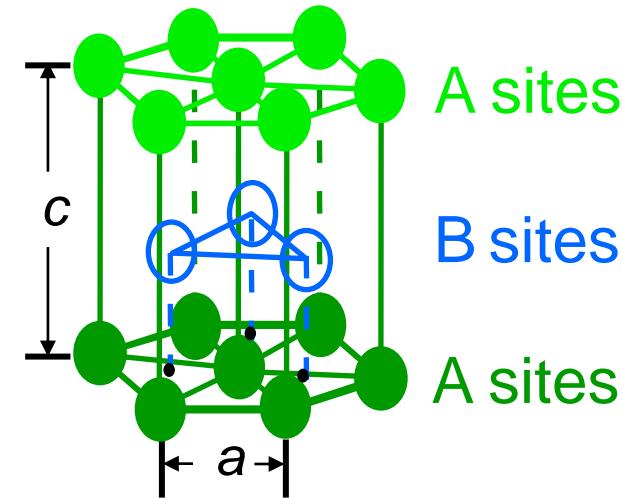
Number of atoms in lower hexagonal plane

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

We note that each central atom is shared by two unit cells which means upper and lower planes contain atom each.

So, total number of central atom in both, upper and lower planes and there are three interstitial atoms.

So, Total number of atoms in hcp crystal =  $1 + 1 + 1 + 3 = 6$



# Volume of HCP unit cell:

## 4. Hexagonal Close Packed (HCP) Structures

The volume of the unit cell for HCP can be found by finding out the area of the basal plane and then multiplying this by its height

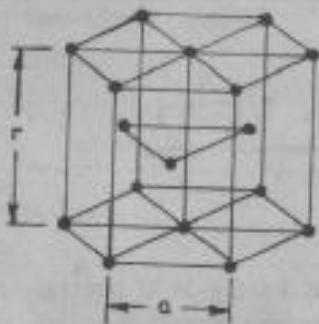
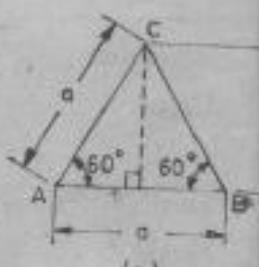
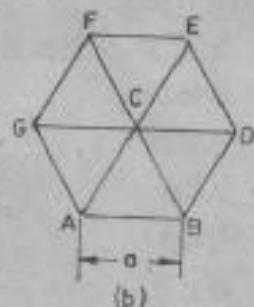
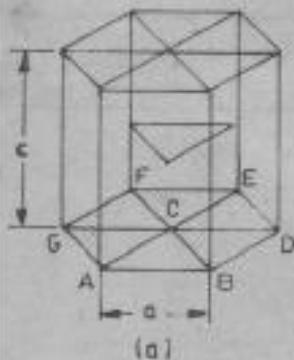


Fig. 1.15 : Hexagonal close packed structure,

The area of the base of the unit cell is the area ABDEFG  
Fig.1.16 (a).



This area is six times the area of equilateral triangle ABC

$$\text{Area of triangle ABC} = \frac{1}{2} a^2 \sin 60$$

$$\begin{aligned}\text{Total area ABDEFG} &= 6 \times \frac{1}{2} a^2 \sin 60 \\ &= 3 a^2 \sin 60\end{aligned}$$

$$\text{Now volume of unit cell} = 3 a^2 \sin 60 \times c$$

For HCP structures, the corner atoms are touching the centre atoms, i.e. atoms at ABDEFG are touching the C atom.  
Therefore  $a = 2r$  or  $r = a / 2$

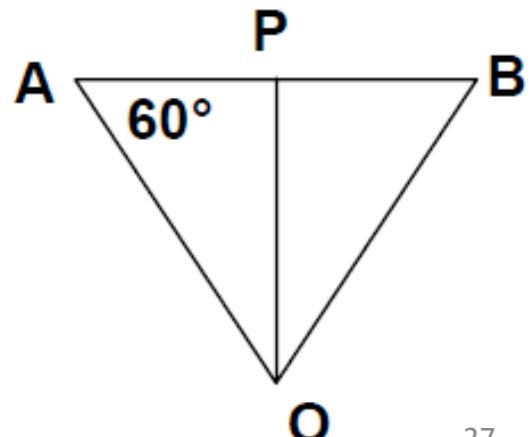
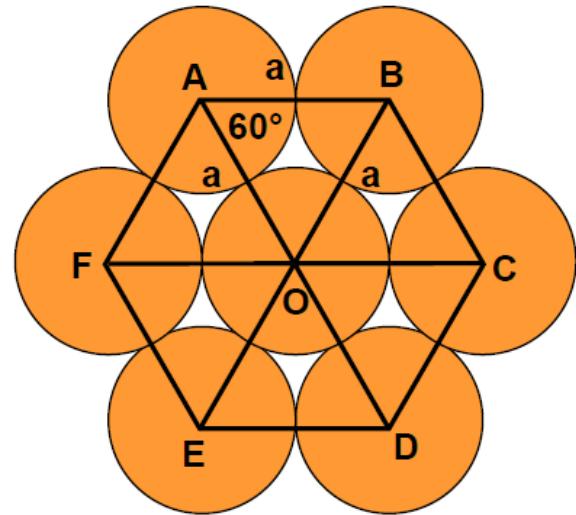
Atomic packing fraction

$$= \frac{6\left(\frac{4}{3}\pi r^3\right)}{3a(a \sin 60^\circ)c}$$

where  $r$  is the atomic radius, using  $c = 1.633a$

and  $a = 2r$ , we get,

$$= \frac{\pi\sqrt{2}}{6} = 0.74 = 74\%$$



## Calculation of lattice constant

Let us consider the case of a cubic lattice of lattice constant  $a$ . If  $\rho$  be the density of the crystal then,

Volume of the unit cell= $a^3$

$$\therefore \text{Mass of each unit cell} = \rho a^3 \quad \dots \dots \dots (1)$$

Let there be  $n$  molecules (lattice point) per unit cell,  $M$  be the molecular weight and  $N$  be the Avogadro's number. Then,

$$\text{Mass of each molecule} = \frac{M}{N}$$

$$\text{Mass of each unit cell} = n \times \frac{M}{N} \quad \dots \dots \dots (2)$$

From equation (1) and (2), we have

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

$$a^3 = \frac{nM}{\rho N}$$

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

The value of lattice constant  $a$  can be calculated using equation (3).

**Problem-1:** Iron has a BCC crystal structure. If the density of 7.86 g/cm<sup>3</sup>, what is the radius of the Iron atom?

**Answer:**

$$\rho = 7.86 \text{ g/cc}, n = 2, \text{Atomic weight } M = 55.85$$

We know,

$$a^3 = \frac{nM}{\rho N} \quad \text{and} \quad a = \frac{4r}{\sqrt{3}}$$

$$a = \left( \frac{2 \times 55.85}{6.023 \times 10^{23} \times 7.86} \right)^{1/3} = 2.87 \text{ \AA}$$

$$r = \frac{\sqrt{3}a}{4} = \frac{\sqrt{3} \times 2.87}{4} = 1.242 \text{ \AA}$$

The radius of Iron atom = 1.242 \AA

**Problem-2:** NaCl crystals have FCC structure. The density of sodium chloride is 2.18 g/cm<sup>3</sup>. Calculate the distance between two adjacent atoms. Atomic weight of sodium=23 and that of chloride=35.5.

**Answer:** We know,

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

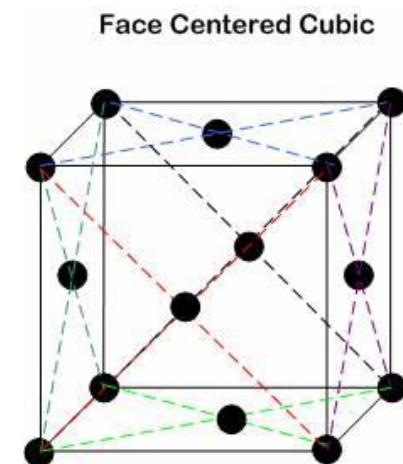
$$\text{here, } n = 4, M = 23 + 35.5 = 58.5$$

$$N = 6.02 \times 10^{23} \text{ g/mol}, \rho = 2.18 \text{ g/cm}^3$$

$$a = 5.63 \times 10^{-8} \text{ cm}$$

The distance between two adjacent atoms is half of this value, i. e.,

$$d = \frac{a}{2} = 2.8 \times 10^{-8} \text{ cm} = 2.811.24$$

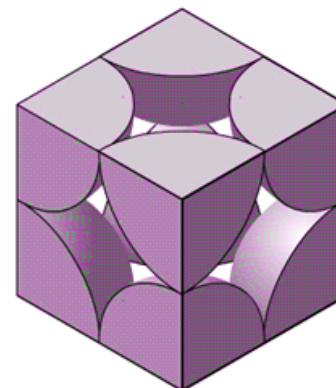


## Miller Indices

Miller index of a crystal face or plane is given by three smallest figures which are inversely proportional to the numerical parameters of the face.

In order to make the designation the following procedure has been adopted.

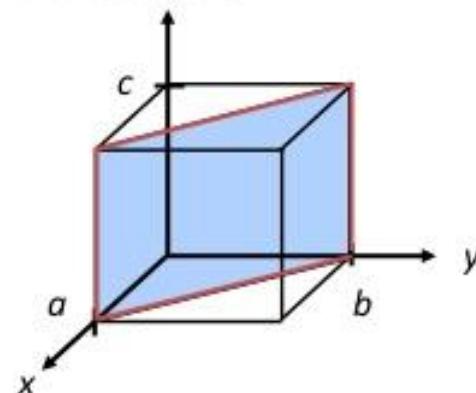
1. Determine the intercepts of the plane along a, b, c in terms of lattice constants.
2. Invert the intercepts, that is, write the numbers as their reciprocals.
3. If fraction results, multiply them by lowest common denominator.



# Crystallographic Planes

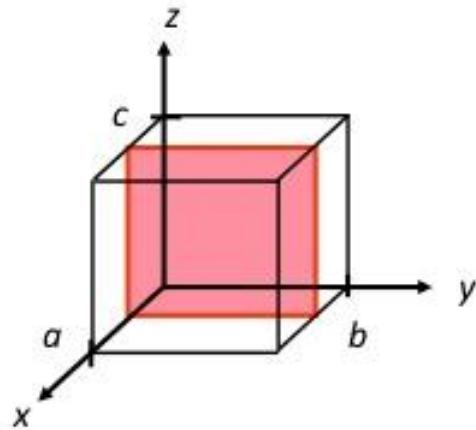
example

	$a$	$b$	$c$
1. Intercepts	1	1	$\infty$
2. Reciprocals	$1/1$	$1/1$	$1/\infty$
	1	1	0
3. Reduction	1	1	0
4. Miller Indices	(110)		



example

	$a$	$b$	$c$
1. Intercepts	$1/2$	$\infty$	$\infty$
2. Reciprocals	$1/\frac{1}{2}$	$1/\infty$	$1/\infty$
	2	0	0
3. Reduction	2	0	0
4. Miller Indices	(200)		



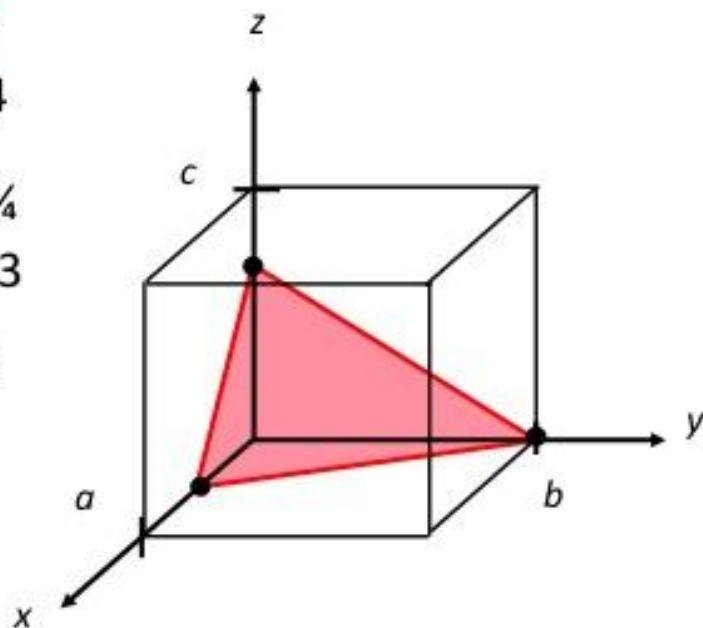
The resulting integers are called Miller indices of a plane and conventionally closed in parentheses  $(h k l)$ .

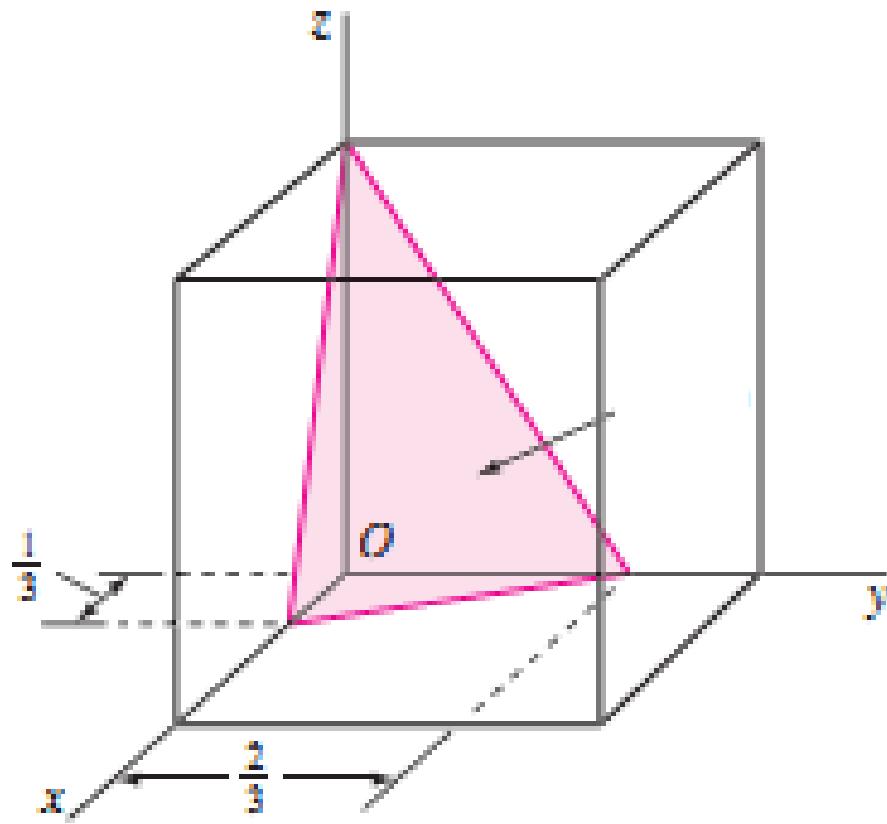
The meaning of these indices is that a set of parallel planes  $(h k l)$  cuts the a-axis into  $h$  parts, the b-axis into  $k$  parts and the c-axis into  $l$  parts.

# Crystallographic Planes

example

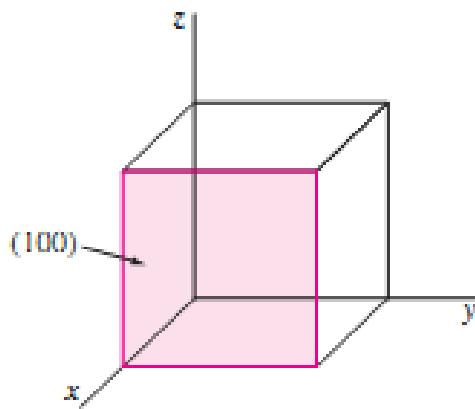
	<i>a</i>	<i>b</i>	<i>c</i>
1. Intercepts	1/2	1	3/4
2. Reciprocals	1/½	1/1	1/¾
	2	1	4/3
3. Reduction	6	3	4
4. Miller Indices	(634)		



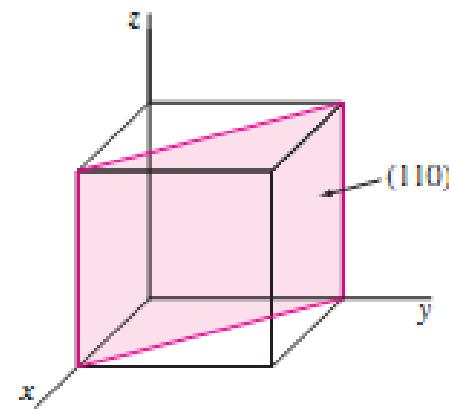


(632)

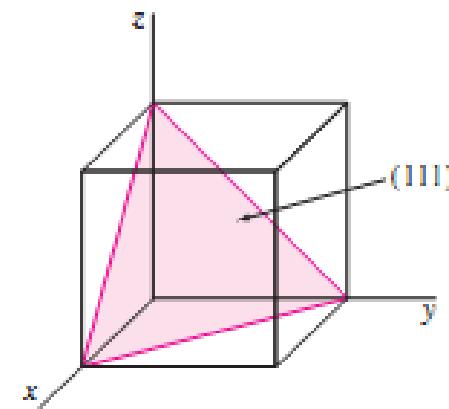
# Draw the planes



$(100)$  plane



$(110)$  plane



$(111)$  plane

