

**Introduction:**

Crystals are the basic pillars of the modern technology. These are the solids in which the atoms are arranged in a closed manner. The physical structure of solid and its properties are closely related to the scheme of arrangement of atoms within the solid. The atomic arrangement in crystals is described by simple geometrical concepts of lattice and unit cell. The crystal structures are analyzed by X-ray diffraction technique invented by Laue and employed by Bragg. The study of crystal geometry helps to understand the diverse behavior of solids in their mechanical, metallurgical, electrical, magnetic and optical properties.

**Classification of solids:**

Based on the atomic arrangement the solids are classified into three categories.

- (1) Crystalline Solids: These have distinctive shape for each material and are bounded by smooth shiny faces and straight edges. Example: Metals
- (2) Amorphous Solids: These consist of atoms arranged distinctly and are non-crystalline. Glass, rubber and many polymers are amorphous solids.

Crystalline Solids	Amorphous Solids
Crystalline solids have regular and periodic arrangement of atoms	Amorphous Solids have irregular arrangement of atoms
Crystalline solids are anisotropic nature i.e these solids have different properties in different directions	Amorphous solids are isotropic in nature i.e these solids have same properties in all directions.
These have sharp melting points.	These don't have sharp melting points.
Crystalline solids have long range order of atomic interaction.	Amorphous solids have short range order of atomic interaction.
The cooling curve of crystalline solids has breaks.	The cooling curve of amorphous solids is smooth.
Crystalline solids have low lattice energy. Ex: Rock salt, calcite	Amorphous solids have high lattice energy. Ex: Glass, pitch, rubber etc..

The arrangement of atoms in specific relation to each other is called order. The atomic arrangement is specified by some basic definitions.

**Space lattice:**

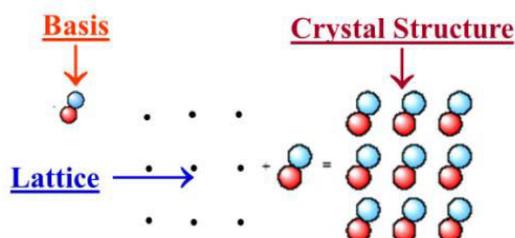
The most important feature of a crystal is regular and periodic arrangement of atoms. The actual arrangement of atoms is called structure. The atoms or group of atoms in a crystal are represented by points that correspond to their mean positions. Thus we obtain a regular distribution of points in space. These points are called lattice points or lattice sites.

*The three dimensional network of regularly arranged points is known as space lattice.*

**Basis set:**

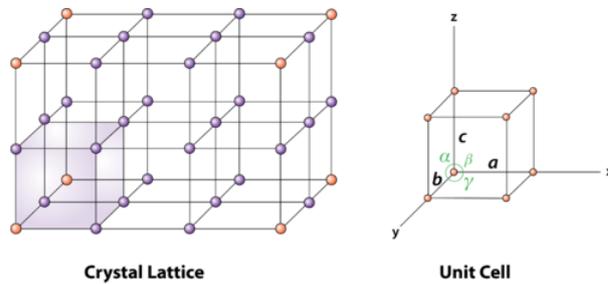
The crystal structure is formed when a group of atoms attached identically to each lattice point. *The group of atoms that is associated with every lattice point is called a Basis.*

A crystal structure is a unique arrangement of atoms in a crystal.



**Unit cell:**

Unit cell is the smallest geometrical unit which when repeated in space indefinitely generates a space lattice. It is described by lattice parameters. The unit cells are repeated over and over again in three dimensions as a result into the whole space lattice of the crystal.



The lines drawn parallel to the lines of intersection of any three faces of the unit cell that don't lie in the same plane are called crystallographic axes. Three translational vectors  $a$ ,  $b$  and  $c$  lie along the crystallographic axes. These three vectors are the intercepts that define the dimensions of unit cell are known as primitives.

**Basic lattice parameters:**

The axial lengths  $a$ ,  $b$ ,  $c$  and the three inter-axial angles  $\alpha$ ,  $\beta$ ,  $\gamma$  of a unit cell are known as basic lattice parameters.

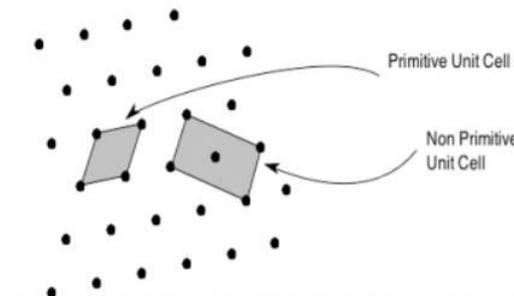
There are two types of unit cells: primitive and non-primitive.

**Primitive cell:**

A unit cell which has one atom or one lattice point is known as primitive cell. Thus a primitive cell is unit cell formed by primitives  $a$ ,  $b$ ,  $c$  having only one lattice point at each of the corners.

**Non-Primitive unit cell:**

A non- primitive unit cell has additional lattice points either on the face of the unit cell or within the unit cell.



**Bravais lattices:**

The concept of Bravais lattice was introduced by Bravais to study the crystal structures. A three dimensional space lattice is generated by repeated translations three co-planar vectors  $a$ ,  $b$ ,  $c$  and three inter-axial angles  $\alpha$ ,  $\beta$ ,  $\gamma$ . There are fourteen different ways of arranging identical points in three-dimensional space satisfying the condition of periodicity with a change in length of co-planar vectors and inter-axial angles. These are known as Bravais lattices. Of them there are seven primitive cells and seven non-primitive cells. Within the 14 types of lattices and on the basis of primitive cell, the crystals are grouped into 7 systems.

**Classification of Crystal Systems:**

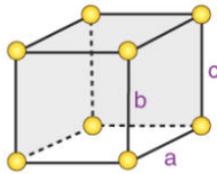
There are seven crystal systems depends on the edge lengths  $a$ ,  $b$ ,  $c$  and three inter-axial angles  $\alpha$ ,  $\beta$ ,  $\gamma$ . These seven crystal systems have 14 Bravais lattices.

**Cubic System:**

In cubic system the crystal axes are perpendicular to one another. That is  $\alpha = \beta = \gamma = 90^\circ$

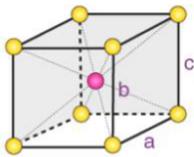
And the length of primitives is same along the three axes  $a = b = c$ . Cubic lattice has three bravais lattice possible arrangements.

(i) **Simple Cubic:** It has lattice points at all 8 corners of unit cell.



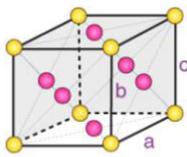
Simple cubic

(ii) **Body Centered Cubic:** It has lattice points at all 8 corners of unit cell and one lattice point at the center of the body.



Body-centred  
Cubic Unit Cell  
(BCC)

(iii) **Face-Centered Cubic:** It has lattice points at all 8 corners of unit cell and one lattice point at the face of the body.



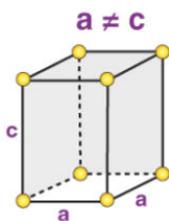
Face-centred  
Cubic Unit Cell  
(FCC)

**Tetragonal system:**

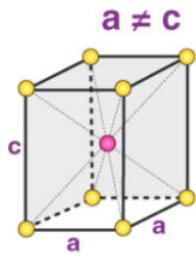
In this crystal the two lengths of cell are equal while the third is either shorter or longer. The crystal axes are perpendicular to one another.  $a = b \neq c$   $\alpha = \beta = \gamma = 90^\circ$

Tetragonal has two possible types of arrangements.

(i) **Simple Tetragonal:** It has lattice points at all 8 corners of unit cell



(ii) **Body centered tetragonal:** It has lattice points at all 8 corners of unit cell and one lattice point at the center of the body.

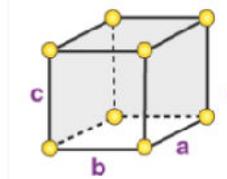


**Orthorhombic system:**

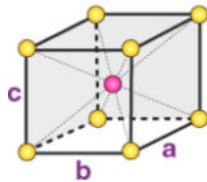
In this crystal system the lengths of unit cell are different but the axes are perpendicular.  $a \neq b \neq c$   $\alpha = \beta = \gamma = 90^\circ$

This lattice has four possible types of arrangements

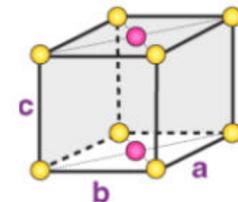
**(i) Simple Orthorhombic Lattice:** It has lattice points at all 8 corners of unit cell



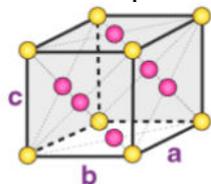
**(ii) Body centered orthorhombic lattice:** It has lattice points at all 8 corners of unit cell and one lattice point at the center of the body



**(iii) Base centered orthorhombic lattice:** It has lattice points at all 8 corners of unit cell and one lattice point at base and top of the body.

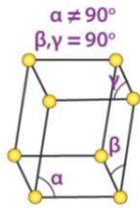


**(iv) Face centered orthorhombic lattice:** It has lattice points at all 8 corners of unit cell and six lattice points, one each at the center of six faces of the unit cell.

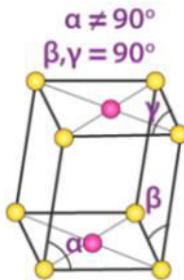


**Monoclinic system:** In this crystal the lengths of unit cell are different. Two axes are at right angles and the third is obliquely inclined  $a \neq b \neq c$   $\alpha = \beta = 90^\circ \neq \gamma$ . Monoclinic lattice has two possible types of arrangements.

**(i) Simple monoclinic:** It has lattice points at all 8 corners of unit cell



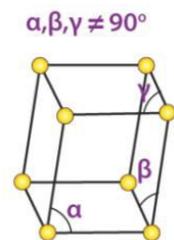
(ii) **Base centered monoclinic:** It has lattice points at all 8 corners of unit cell and one lattice point at base and top of the body.



Example:  $\text{Na}_2\text{SO}_3$ ,  $\text{FeSO}_4$

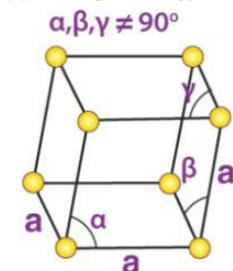
**Triclinic Crystal:** In this crystal the lengths of unit cell are different and the axes are oblique to each other.  $a \neq b \neq c$   $\alpha \neq \beta \neq \gamma$ . It has only one type of lattice.

(i) **Simple triclinic lattice:** It has lattice points at all 8 corners of unit cell



**Trigonal or Rhombohedral structure:** In this crystal all the three lengths of unit cell are equal and equally inclined to one another other than  $a = b = c$   $\alpha = \beta = \gamma \neq 90^\circ < 120^\circ$  It has only one type of lattice.

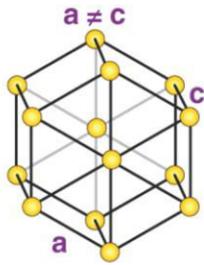
(i) **Simple trigonal lattice:** It has lattice points at all 8 corners of unit cell



**Hexagonal System:** In this crystal all the three lengths of unit cell are equal and two axes are equal inclined at  $90^\circ$  and third axis inclined at  $120^\circ$   $a = b \neq c$   $\alpha = \beta = 90^\circ \neq \gamma = 120^\circ$

It has only one possible type of arrangement

(i) **Simple hexagonal lattice:** It has lattice points at all 8 corners of unit cell



Thus, there are seven crystal systems with 14 Bravais lattices.

S.No	Name of the Crystal System	Relative length of axes of unit cell	Relation of angle between axes	Bravia's Lattice
1 C	Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$	P, I, F
2 T	Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	P, I
3 O	Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	P, I, C, F
4 Mr	Monoclinic	$a \neq b \neq c$	$\alpha = \beta = 90^\circ \neq \gamma$	P, C
5 Tri	Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$	P
6 Rho	Rhombohedral /Trigonal	$a = b = c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$	P
7 H	Hexagonal	$a = b \neq c$	$\alpha = \beta = 90^\circ \neq \gamma = 120^\circ$	P

**Calculation of parameters of a cubic lattice:**

A unit cell is characterized by a set of characteristics namely volume, effective number of atoms, coordination number and atomic packing fraction. Calculation of these parameters for cubic system is quite easy. There are three varieties of cubic lattice: (i) simple cubic (ii) body centered cubic (iii) face centered cubic

**Coordination Number:**

Coordination number is the number of equidistant neighbors that an atom has in the given structure. Larger the coordination number, the structure is more closely packed.

In simple cubic lattice any corner atom has four nearest neighbors in the same plane and two nearest neighbors one above and one below in a vertical plane. So, the coordination number is  $4+2=6$

In body centered cubic lattice, for any corner atom of the unit cell, the nearest atoms are the atoms which are the centers of unit cell. As such the corner atom is surrounded by eight unit cells. So, the coordination number is 8.

For any corner atom in a unit cell there will be 4 face centered atoms of the surrounding unit cells in its own plane 4 face centered atoms below this plane and 4 face centered atoms above this plane. So, the coordination number is  $4+4+4=12$ .

**Atomic Radius:**

The atomic radius  $r$  is defined as half of the distance between nearest neighbors in a crystal of pure element. The atomic radius is expressed in terms of cube edge ( $a$ ) or Lattice Constant ( $a$ ).

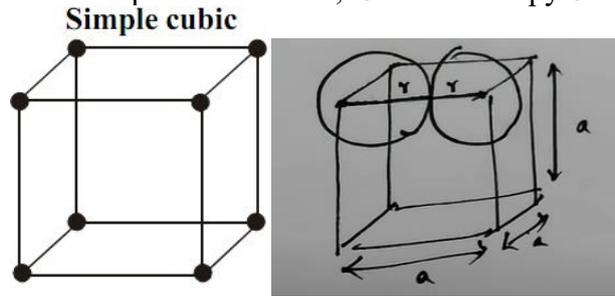
**Atomic Packing Fraction:**

*Atomic packing fraction is defined as the ratio of volume of atoms in unit cell to the total volume of the unit cell.*

$$PF = \frac{(Z_{\text{eff}})(\text{Volume occupied by atoms})}{\text{Total Number of atoms in unit cell}} \times 100$$

**APF for Simple Cubic:**

For a simple cubic lattice, 8 atoms occupy 8 corners of unit cell.



If  $a$  is the side of unit cell then from figure,

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

Number of atoms per unit cell =  $Z_{eff} = 8 \times \frac{1}{8} = 1$

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

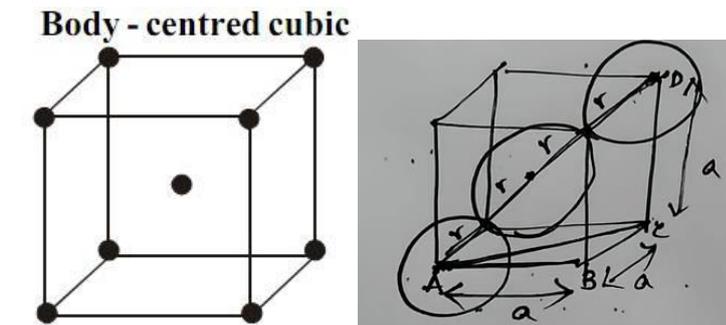
Side of unit cell  $a = 2r$

Volume of unit cell  $a^3$

$$\text{Packing density} = \frac{(4/3)\pi r^3}{a^3} = \frac{(4/3)\pi \left(\frac{a}{2}\right)^3}{(2r)^3} = \frac{\pi}{6} = 0.52 = 52\%$$

**APF for Body Centered Cubic:**

For body centered cubic lattice the calculation of  $r$  in terms of  $a$  is,



In Body Centered Cubic Lattice 8 atoms occupy 8 corners of unit cell and 1 atom at the center. Consider the corner atoms and center atom.

From Pythagoras theorem for  $\triangle ADC$

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

$(AC)^2$  is obtained using pythagoras theorem from  $\triangle ABC$ .

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

$$(AD)^2 = (AC)^2 + (BC)^2 \Rightarrow (4r)^2 = 2a^2 + a^2$$

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

Number of atoms per unit cell =  $Z_{eff} = 8 \times \frac{1}{8} + 1 = 1 + 1 = 2$

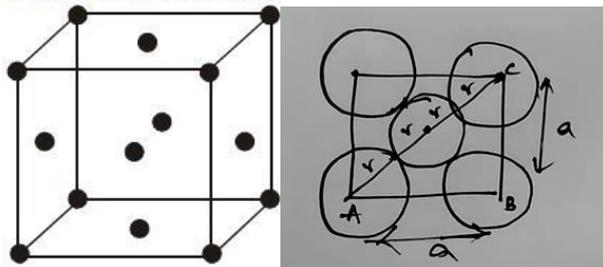
Side of unit cell  $a = \frac{4r}{\sqrt{3}}$

Volume of unit cell  $a^3$

Packing density  $\frac{2 \times (4/3)\pi r^3}{a^3} = \frac{2 \times (4/3)\pi r^3}{(4r/\sqrt{3})^3} = \frac{\sqrt{3}\pi}{8} = 0.68 = 68\%$

For face centered cubic lattice the calculation of  $r$  in terms of  $a$  is,

**Face - centred cubic**



In Face Centered Cubic Lattice 8 atoms occupy 8 corners of unit cell and 6 atoms occupy 6 faces. Consider a face of FCC lattice.

From Pythagoras theorem for  $\triangle ABC$

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

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

$$(4r)^2 = 2a^2 \Rightarrow 16r^2 = 2a^2 \Rightarrow r = \sqrt{\frac{2a^2}{16}} = \frac{a}{2\sqrt{2}}$$

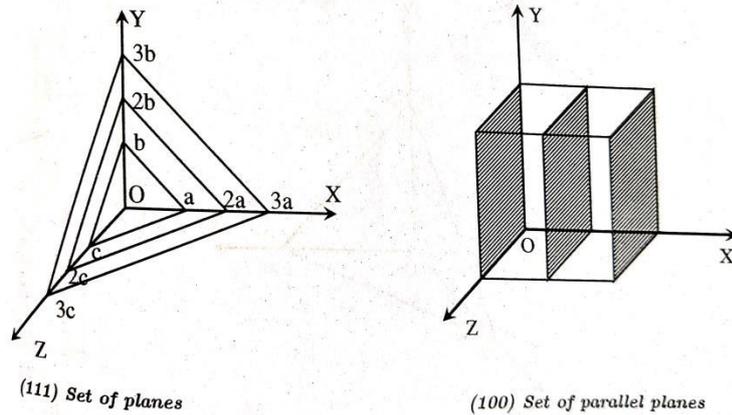
Number of atoms per unit cell =  $Z_{eff} = \left(8 \times \frac{1}{8}\right) + \left(6 \times \frac{1}{2}\right) = 1 + 3 = 4$

Volume of unit cell  $a^3$

Packing density  $\frac{4 \times (4/3)\pi r^3}{a^3} = \frac{4 \times (4/3)\pi r^3}{(a)^3} = \frac{4 \times (4/3)\pi \left(\frac{a}{2\sqrt{2}}\right)^3}{(a)^3} = 0.74 = 74\%$

**Miller Indices:**

A crystal is made up of a large number of parallel equidistant planes passing through lattice points are called lattice planes. The perpendicular distance between two adjacent crystal planes is called interplanar spacing  $d$



**Set of Planes**

A given space lattice may have infinite set of lattice planes each having its characteristic interplanar spacing. The crystal plane can have different orientations. Miller derived a method of representing the orientation of a crystal plane. *The directions of crystal planes are specified by a set of whole numbers called miller indices and are represented by (h k l) known as Miller indices. These are three smallest integers which have the same ratio as the reciprocals of the intercepts of the crystal plane with the coordinate axes.*

**Procedure for finding miller indices:**

- Let the intercepts of the desired plane on the three coordinate axes be  $(pa, qb, rc)$
- Divide the primitives  $(a, b, c)$  the intercepts are  $p, q, r$
- Take the reciprocals of intercepts *i.e.*,  
 $\frac{1}{p}, \frac{1}{q}, \frac{1}{r}$
- Find the LCM of denominators
- Reduce the reciprocals into integers by multiplying each of them with LCM
- These integers enclosed in brackets represent the Miller indices  $(h k l)$

**Example:**

Find the miller indices in a crystal plane which make intercepts  $2a, 3b,$  and  $2c$  along X,Y, and Z axes respectively, where  $a, b$  and  $c$  are lattice parameters.

Sol: The intercepts are multiples of  $a, b, c$

$2, 3, 2$

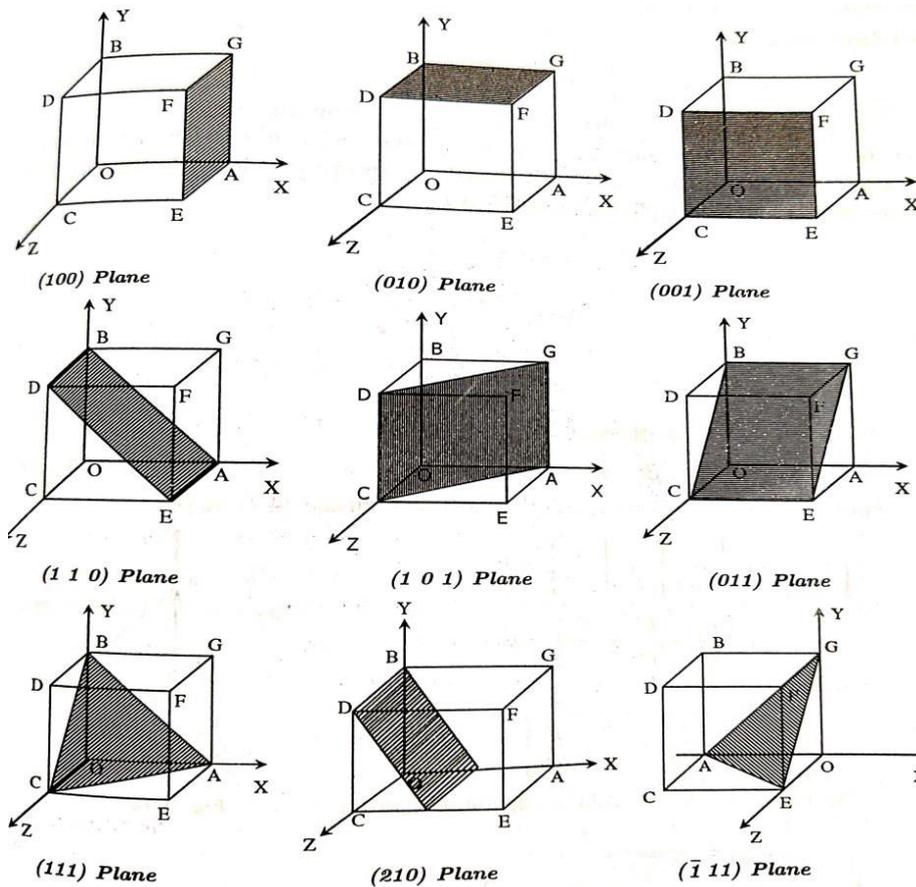
The reciprocals of intercepts

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

The LCM of denominators is 6.

Multiply with reciprocals to obtain integers.

Thus, Miller indices are  $(3 2 3)$



Representation of various planes

**Separation between successive *hkl* planes: or Inter planner distance (*d*)**

Consider a plane ABC making intercepts on the coordinate axes *OX, OY, OZ* at distances *OA, OB, OC* respectively as shown in figure. Let us consider any set of parallel planes with Miller indices (*h k l*) and any other plane which is parallel to the plane ABC, passing through the origin *O* as the reference plane. The plane ABC makes intercepts  $\frac{a}{h}, \frac{b}{k}, \frac{c}{l}$  on *X, Y* and *Z* axes

respectively. that is,  $OA = \frac{a}{h}, OB = \frac{b}{k}, OC = \frac{c}{l}$

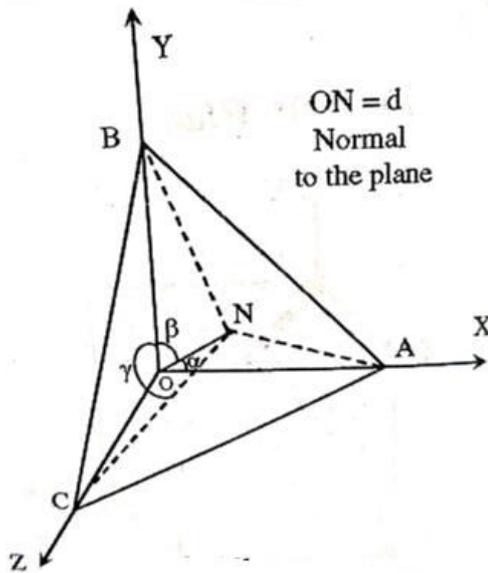
A normal *ON* is drawn to the plane ABC from origin. The distance of the plane ABC from the origin is the interplanar spacing *d* (*ON*). Let the angles made by the normal with the *X, Y* and *Z* axes be  $\alpha, \beta$  and  $\gamma$  respectively. Then the interplanar spacing *d* between the origin and

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

the plane is derived as follows

$$\cos \beta = \frac{ON}{OB} = \frac{d}{b/k}$$

$$\cos \gamma = \frac{ON}{OC} = \frac{d}{c/l}$$



According to law of directional cosines

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

Substituting the values of  $\cos \alpha$ ,  $\cos \beta$ ,  $\cos \gamma$  in the above equation,

$$\left[ \frac{d}{a/h} \right]^2 + \left[ \frac{d}{b/k} \right]^2 + \left[ \frac{d}{c/l} \right]^2 = 1$$

$$d^2 \left[ \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} \right] = 1$$

$$d^2 = \frac{1}{\left[ \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} \right]}$$

The expression for interplanar spacing is,

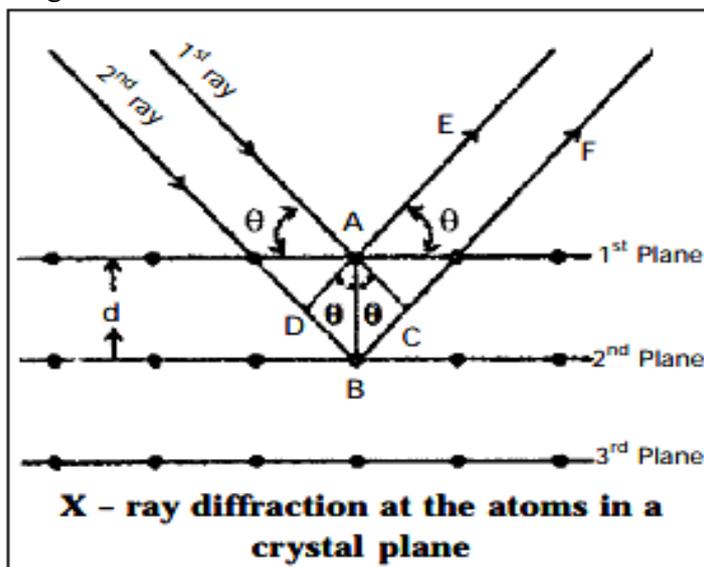
$$d_{hkl} = \frac{1}{\sqrt{\left[ \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} \right]}}$$

This is general expression for interplanar spacing. If  $a = b = c$  the expression becomes

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

**Bragg's law:**

When a beam of monochromatic X-rays falls on a crystal, each atom becomes a source of scattering radiation. In crystals there are certain planes which are rich in atoms. At certain glancing angles reflections from the set of these planes are in phase with each other to produce maximum intensity. For other angles that are out of phase produces less intensity. Consider a set of parallel lattice planes of a crystal separated by distance  $d$ . Suppose a narrow beam of X-rays of wavelength  $\lambda$  be incident upon these planes at angle  $\theta$  as shown in figure. The beam will be reflected in all directions by the atoms of various atomic planes. No particular bending of the rays occurs due to refractive index of crystal is nearly equal to 1. Consider a ray PA reflected at atom A in the direction of AR from the plane 1. Another ray QB reflected at another atom B in the direction BS. Now, from atom A drop perpendiculars on the incident ray QB and reflected ray BS. The path difference between these two rays is  $(CB+BD)$ . The two rays will be in phase out of phase depends upon the path difference. High intense spot will be produced when the path difference is equal to integral multiple of wavelength  $\lambda$ .



$$CB + BD = n\lambda$$

From figure,  $\Delta ACB$ ,

$$\sin \theta = \frac{AB}{CB} \Rightarrow CB = AB \sin \theta = d \sin \theta$$

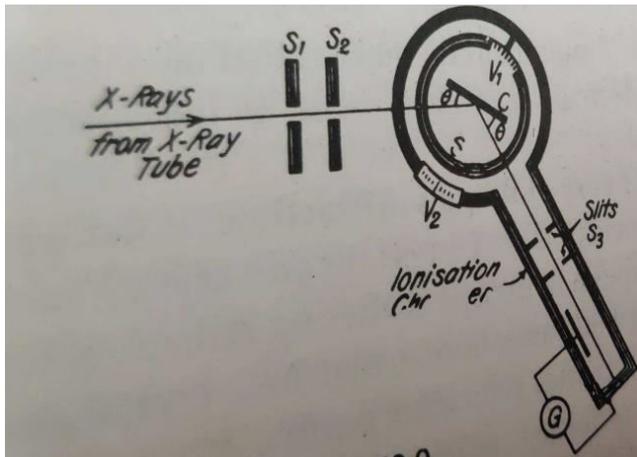
$$CB + BD = n\lambda \Rightarrow d \sin \theta + d \sin \theta = 2d \sin \theta$$

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

This is Bragg's law.

**Bragg's X-ray Spectrometer:**

Bragg X-ray spectrometer is used to study the structural properties of crystals by diffracting X-rays from the crystals. The experimental arrangement of Bragg spectrometer is shown in figure. X-rays from X-ray tube are narrowed to obtain a fine pencil of beam by passing through slits  $S_1$  and  $S_2$  provided in lead screens. The beam is now allowed to fall on crystal C (usually of NaCl with 100 face) mounted on a circular turn table of spectrometer.



This turn table is capable of rotation about vertical axis passing through its center. The rotation can be read on a circular graduated scale S with the help of vernier V<sub>1</sub>. The reflected beam then passes through S<sub>3</sub> and enters the ionization chamber. The ionization chamber is mounted on a special movable arm about the same axis of the crystal. The position of ionization chamber can be read by second vernier V<sub>2</sub>. The turn table and ionization chamber are linked together in such a way that when the turn table rotates through an angle  $\theta$ , the ionization chamber turns through angle  $2\theta$ .

The X-rays entering the ionization chamber ionize the gas which causes a current flow between two electrodes that can be measured by galvanometer G. The ionization current is measured for different values of  $\theta$ . A plot is drawn between  $\theta$  and ionization current. For certain values of glancing angle  $\theta$ , the intensity of ionization current increases abruptly.

From Bragg's equation,

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

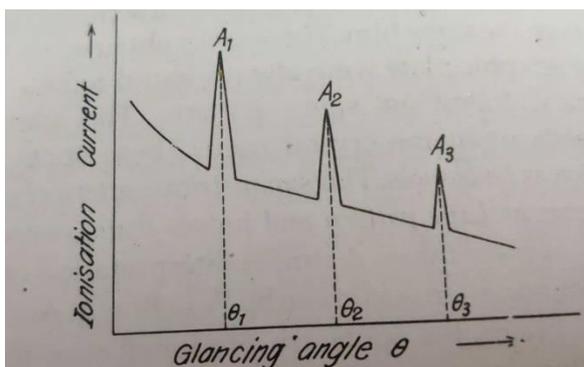
For first order spectrum,  $n = 1$  and  $2d \sin \theta_1 = \lambda$

For second order spectrum,

$$n = 2 \text{ and } 2d \sin \theta_2 = 2\lambda$$

For third order spectrum,

$$n = 3 \text{ and } 2d \sin \theta_3 = 3\lambda$$

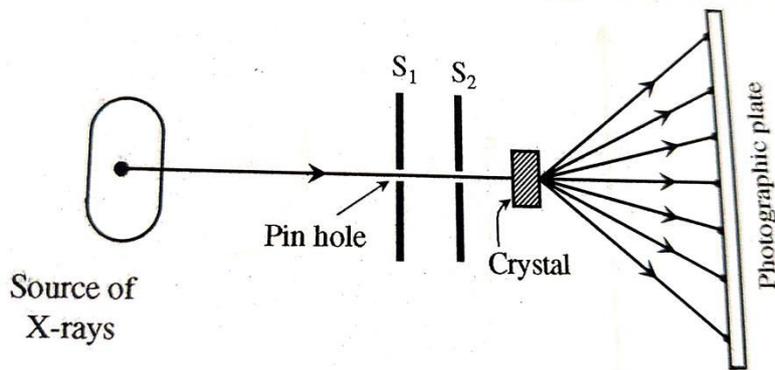


Thus,  $\sin \theta_1 : \sin \theta_2 : \sin \theta_3 = 1 : 2 : 3$

From the glancing angle  $\theta$  and ionization current, the glancing angles  $\theta_1, \theta_2$  and  $\theta_3$  or the first order, second order and third order reflections are measured. This shows X-rays get reflected like ordinary light is justified.

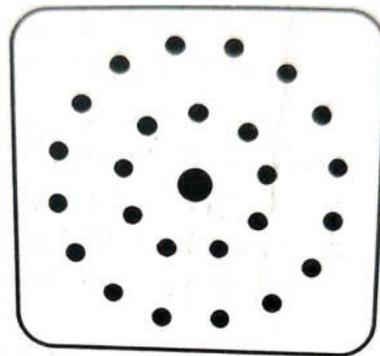
**Crystal structure determination by Laue's method:**

The Laue method is used for determination of the structure of a crystal. The experimental arrangement consists of source of X-rays, pin hole collimator, crystal holder and photographic film or florescent screen as shown in the figure.



**Fig. Experimental Arrangement of Laue Method**

The source produces X-rays of short wavelength ( $0.2 \text{ \AA}^0$  to  $2 \text{ \AA}^0$ ) which are allowed to pass through a slit system ( $S_1$  and  $S_2$ ) to become a fine and sharp beam. This beam is allowed to incident on a crystal, placed in crystal holder. After passing through the crystal, the X-rays are diffracted and recorded on photographic plate. As these X-rays penetrate into the crystal then scatter from different atomic direction centers. This is possible from a whole range of wavelengths in the continuous spectrum satisfying Bragg's law  $2d \sin \theta = n\lambda$



**Fig. Laue Pattern**

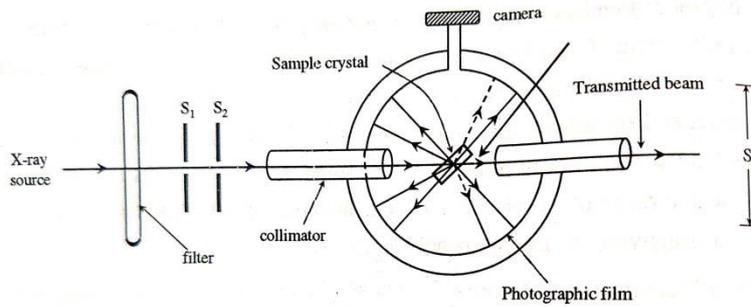
The diffraction consists of a central spot surrounded by concentric circular spots. The symmetrical pattern of spots is known as Laue pattern. Each spot in the Laue pattern corresponds to an interference maximum for a set of crystal planes satisfying Bragg's condition, for a particular wavelength scattered from the incident beam. The atomic arrangement can be understood from a study of the position and intensities of the Laue spots. From this method lattice constant and interplanar spacing can be found. This method is used to find structure single crystals. This method is also useful for the determination of crystal orientation, symmetry and also to study crystal imperfections.

#### **Powdered Method for Determination of Crystal Planes:**

Powdered crystal method is the standard technique to study the structure of micro crystals developed by Debye & Scherer in Germany. This method gives information about size of crystals, their orientation and presence of impurities and distortion.

#### **Experimental Arrangement:**

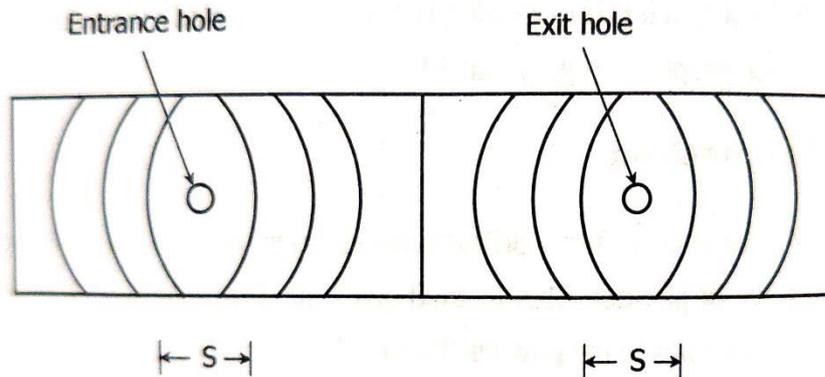
It consists of a cylindrical camera whose length is small as compared to the diameter. The fine powdered sample is filled in the capillary tube and mounted at the center of the camera. The x-rays are allowed to pass through a filter F to become monochromatic beam. The fine and sharp beam of X-rays enter the camera and made to fall on the crystal powder filled in the capillary tube.



**Fig. Experimental Arrangement of Powdered Method**

**Principle and Working:**

The principle of this method is millions of micro crystals have all possible random orientation among the large number of crystals satisfy Bragg’s relation. For a particular value of angle of incidence  $\theta$  numerous orientations of particular set of planes are possible. The diffracted rays corresponding to fixed values of  $\theta$  lie on the surface of a cone with its apex at the sample and the semi vertical angle is  $2\theta$ . Different cones are observed for different values of  $\theta$  with particular combinations. Each cone of the reflected beam levels two impressions on the photographic film, which are in the form of arcs on either side of exit hole.



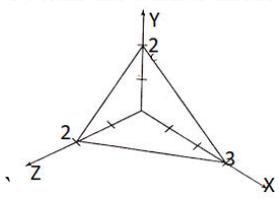
the film is exposed for a few hours in order to obtain arcs of sufficiently high intensity. It is removed from the camera and developed. The circular arcs are observed on the film as shown in figure. From the figure, the angle  $\theta$  corresponding to a particular pair of arcs is related to the distance S between the arcs.

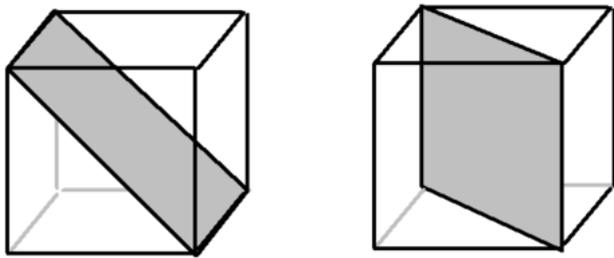
$$4\theta(\text{radians}) = \frac{S}{R}$$

$$4\theta(\text{degrees}) = \frac{S}{R} \left( \frac{180}{\pi} \right)$$

Using the value of  $\theta$  in Bragg’s relation  $2d \sin \theta = n\lambda$  the corresponding interplanar spacing can be calculated.

Q. No		Assignment Questions on Unit-2	M
1	A	Obtain the scattering angle of the crystal structure by X-ray diffraction powdered method	7
	B	A beam of X-rays of wavelength 0.071 nm is diffracted by (110) plane of rock salt with lattice constant of 0.28 nm. Find the glancing angle for the second order diffraction.	3
2	A	Sketch the seven crystal systems with lattice parameters and interfacial angles corresponding to the seven popular crystals.	10
3	A	Explain the FCC sub lattice with neat diagram and calculate its atomic packing factor.	7
	B	A beam of X-ray is incident on a CaCl crystal with lattice spacing 0.28 nm. Calculate the wavelength of X-ray if first order Bragg reflection takes place at a glancing angle of $9^{\circ}45'$ .	3
4	A	Illustrate the BCC sub lattice with neat diagram and calculate its atomic packing factor.	7
	B	Monochromatic X-rays of wavelength $1.5\text{\AA}$ are incident on a crystal face having an interplanar	3

		spacing of 1.6Å. Find the highest order for which Bragg's reflection maximum can be seen.	
5	A	What are Miller Indices? What are their important features?	6
	B	Draw the following crystals planes by using Miller indices. i. (100)                    ii. (111)	4
6	A	Obtain expressions for Coordination Number, Number of atoms in a unit cell, Nearest Neighbor Distance, Atomic Radius and Packing Fraction for Simple Cubic crystal structure.	7
	B	A beam of X-ray is incident on NaCl crystal with lattice spacing 0.282nm. Calculate the wavelength of X-ray if the first order Bragg's reflection takes place at a glancing angle of $8^{\circ}35'$ .	3
7	A	Describe the Bragg's law & deduce the expression for the same.	6
	B	Obtain the Miller Indices from the following figure 	4
8	A	Describe Laue's method for determination of crystal structure.	6
	B	Explain the important of lattice parameters in cubic crystals.	4
9	A	How the Bragg's spectrometer works? Explain with neat diagram.	6
	B	Calculate the interplanar spacing for (221) plane in an SC lattice, where lattice constant is $4.2 \times 10^{-10}$ m.	4
10	A	Deduce the expression for the interplanar distance in terms of successive hkl planes of a cubic system.	7
	B	X-ray beam is incident on a NaCl crystal with lattice spacing $0.26 \times 10^{-9}$ m. Calculate the wavelength of X-ray if first order Bragg reflection takes place at a glancing angle of $8^{\circ}30'$ .	3

Q. No	VIVA QUESTIONS	Marks	CO	RBT
1	Differentiate Primitive and Non-Primitive Unit cells	2	CO2	Apply
2	Identify the important of Miller Indices in a cubic crystals	2	CO2	Understand
3	Calculate the atomic radii in case of Simple cubic & BCC.	2	CO2	Apply
4	Describe Packing Factor of unit cell of lattice crystal.	2	CO2	Understand
5	Explain the Coordination number of FCC.	2	CO2	Understand
6	Mention the names of three main Cubic Crystals?	2	CO2	Understand
7	What are Miller indices?	2	CO2	Understand
8	Draw the planes of Miller Indices (111) in the unit cell of an cubic crystal	2	CO2	Apply
9	Mention any two applications of X – rays diffraction studies in crystal.	2	CO2	Apply
10	Find out the Miller Indices of the following figures 	2	CO2	Apply
11	Sketch the Miller Indices (011) in the unit cell of a cubic crystal.	2	CO2	Apply
12	Draw the Hexagonal cubic lattice crystal with examples	2	CO2	Apply
13	Attain the lattices parameters of Orthorhombic Crystal systems	2	CO2	Understand
14	Explain the Unit Cell with neat diagram.	2	CO2	Understand
15	Obtain the expression for interplanar spacing for a cubic crystal.	2	CO2	Understand