Introduction

It is a well known fact that matter consists of atoms and molecules. The properties of matter depend on the arrangement of atoms inside matter which depends on the chemical bonding between the atoms. To understand the bonding in solids, it is necessary to know the electronic structure of atoms.

Matter in the universe is mainly classified into three kinds; they are solids, liquids and gases. In solids, all the atoms and molecules are arranged in a fixed manner. Solids have a definite shape and size, whereas in liquids and gases, atoms or molecules are not fixed and cannot form any shape and size. These materials gain the shape and size of the vessel in which they are taken.

On the basis of arrangement of atoms or molecules, solids are broadly classified into two categories; they are crystalline solids and non-crystalline (or amorphous solids)

<table>
<thead>
<tr>
<th>Crystalline solids</th>
<th>Amorphous solids (non-crystalline solids)</th>
</tr>
</thead>
<tbody>
<tr>
<td>In crystalline solids, the atoms or molecules are arranged in a regular and periodic manner.</td>
<td>In amorphous solids the atoms or molecules are arranged in an irregular manner.</td>
</tr>
<tr>
<td>If a crystal breaks, the broken pieces also have regular in shape.</td>
<td>If an amorphous solid breaks, the broken pieces have irregular in shape.</td>
</tr>
<tr>
<td>These solids have directional properties and are therefore called anisotropic substances.</td>
<td>These solids have no directional properties and are therefore called isotropic substances.</td>
</tr>
<tr>
<td>The crystalline solids have sharp melting point.</td>
<td>The amorphous solids have wide range melting point.</td>
</tr>
</tbody>
</table>

Examples
Metallic solids - Cu, Ag, Au, Al
Non-Metallic solids – NaCl, MgO, CaO, Diamond, Si, Ge.

Examples
Glass, plastic, wood

1. Space lattice

A crystal is three dimensional body. Crystals are made up of regular and periodic three dimensional patterns of atoms are molecules in space. The crystal structure may be described in terms of idealized geometrical concept called a space lattice.

Let us consider the case of two dimensional arrays of points as shown in the figure. It is obvious from the figure that environment about any two points is the same and hence it represents a space lattice.

\[ \text{The space lattice may be defined as} \]

‘An array of points in space such that the environment about each point is the same’
If we choose a lattice point at a distance from the origin the translation vector can be written as
\[ \vec{r} = l \vec{a} + m \vec{b} \]
Where \( l, m \) are integers. In figure \( l = m = 1 \)
The three dimensional translation vector can be written as
\[ \vec{r} = l \vec{a} + m \vec{b} + n \vec{c} \]

Two dimensional space lattice:

Two dimensional space lattice can be defined as ‘An array of points in two dimensional space in which every point has the same environment with respect to all other points.

Three dimensional space lattice:

Three dimensional space lattice can be defined as ‘An array of points in three dimensional space in which every point has the same environment with respect to all other points.

2. Basis:

A group of atoms or molecules is attached identically to each lattice point then it gives the crystal structure, this group of atoms or molecules is called basis. The basis is identical in composition, and arrangement, which is repeated periodically in space to form the crystal structure.

\[
\begin{array}{c}
\text{Lattice} + \text{basis} = \text{crystal structure} \\
\bullet \bullet \bullet \bullet \bullet \bullet \quad \begin{pmatrix}
0^0 & 0^0 & 0^0 & 0^0 & 0^0 & 0^0 \\
0^0 & 0^0 & 0^0 & 0^0 & 0^0 & 0^0 \\
0^0 & 0^0 & 0^0 & 0^0 & 0^0 & 0^0 \\
0^0 & 0^0 & 0^0 & 0^0 & 0^0 & 0^0 \\
0^0 & 0^0 & 0^0 & 0^0 & 0^0 & 0^0 \\
0^0 & 0^0 & 0^0 & 0^0 & 0^0 & 0^0 \\
\end{pmatrix}
\end{array}
\]

Lattice \quad Basis \quad Crystal lattice

3. Unit cell:

In order to consider the idea of unit cell, let us consider a two dimensional crystal in which the atoms are arranged as shown in the figure. If we consider a parallelogram such as \( ABCD \) with side \( AB = a \) and \( AD = b \) then by rotating this parallelogram in all dimensions, the whole crystal lattice may be obtained. In this way this fundamental unit \( ABCD \) is called a unit cell. Thus a unit cell is defined as

“A smallest geometrical volume the repetition which gives the actual crystal structure”
4. Lattice parameters

The lines drawn parallel to the lines of interaction of any three faces of the unit cell which do not lie in the same plane are called crystallographic axes. The angles between the crystallographic axes represented by $\alpha, \beta$ and $\gamma$ are called interfacial angles. The intercepts, $a, b$ and $c$ on the respective crystallographic axes, are called primitives of the unit cell.

The combination of primitives $a, b$ and $c$ and three interfacial angles $\alpha, \beta$ and $\gamma$ are known as lattice parameters of the unit cell. Which determine the actual size and shape of the unit cell.

5. Crystal systems

On the basis of lattice parameters (or length and directions), the crystal systems may be classified into the following seven systems.

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

   **Lattice parameters**
   - All three sides are equal: \( a = b = c \)
   - All angles are right angles: \( \alpha = \beta = \gamma = 90^\circ \)

   **Bravais lattices**: \( P, I \& F \)
   **Examples**: \( \text{NaCl, po, Na, W, Ag, Au, Pb, } \alpha - \text{Fe} \)

2. **Tetragonal**

   **Lattice parameters**
   - Two sides are equal: \( a = b \neq c \)
   - All angles are right angles: \( \alpha = \beta = \gamma = 90^\circ \)

   **Bravais lattices**: \( P \& I \)
   **Examples**: \( \text{NiSO}_4, \text{SnO}_2, \text{TiO}_2, \text{KH}_2\text{PO}_4 \) etc

3. **Orthorhombic**

   **Lattice parameters**
   - All three sides are different: \( a \neq b \neq c \)
   - All angles are right angles: \( \alpha = \beta = \gamma = 90^\circ \)

   **Bravais lattices**: \( P, I, F \& B \)
   **Examples**: \( \text{KNO}_3, \text{BaSO}_4, \text{PbCO}_3, \text{K}_2\text{SO}_4, \alpha - S \) etc

4. **Monoclinic**

   **Lattice parameters**
   - All three sides are different: \( a \neq b \neq c \)
   - Two angles are right angles: \( \alpha = \beta = 90^\circ \neq \gamma \)

   **Bravais lattices**: \( P \& B \)
   **Examples**: \( \text{CaSO}_4 \cdot 2\text{H}_2\text{O}, \text{Na}_2\text{SO}_4, \text{FeSO}_4, \text{gypsum} \) etc

5. **Triclinic**

   **Lattice parameters**
   - All three sides are different: \( a \neq b \neq c \)
   - All angles are different: \( \alpha \neq \beta \neq \gamma \neq 90^\circ \)

   **Bravais lattices**: \( P \)
   **Examples**: \( \text{CuSO}_4 \cdot 5\text{H}_2\text{O}, \text{K}_2\text{Cr}_2\text{O}_7 \) etc

6. **Trigonal (or Rhombohedral)**

   **Lattice parameters**
   - All three sides are equal: \( a = b = c \)
   - All angles are equal but not right angles: \( \alpha = \beta = \gamma \neq 90^\circ \)

   **Bravais lattices**: \( P \)
   **Examples**: \( \text{CaSO}_4, \text{calcite}, \text{As, Sb}, \text{Bi} \) etc

7. **Hexagonal**

   **Lattice parameters**
   - Two sides are equal: \( a = b \neq c \)
   - Two angles are right angles: \( \alpha = \beta = 90^\circ \) and third is \( \gamma = 120^\circ \)

   **Bravais lattices**: \( P \)
   **Examples**: \( \text{quartz, Zn, Cd, SiO}_2, \text{AgI} \) etc
<table>
<thead>
<tr>
<th>S.No.</th>
<th>Name of the crystal system</th>
<th>Lattice parameters</th>
<th>Examples</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Cubic</td>
<td>$a = b = c$: $\alpha = \beta = \gamma = 90^\circ$</td>
<td>$\text{po, Na, W, Ag, CaF}_2$,</td>
</tr>
<tr>
<td>2</td>
<td>Tetragonal</td>
<td>$a = b \neq c$: $\alpha = \beta = \gamma = 90^\circ$</td>
<td>$\text{NiSO}_4, \text{SnO}_2, \text{TiO}_2$</td>
</tr>
<tr>
<td>3</td>
<td>Orthorhombic</td>
<td>$a \neq b \neq c$: $\alpha = \beta = \gamma = 90^\circ$</td>
<td>$\text{KNO}_3, \text{BaSO}_4, \text{PbCO}_3$,</td>
</tr>
<tr>
<td>4</td>
<td>Monoclinic</td>
<td>$a \neq b \neq c$: $\alpha = \beta = 90^\circ \neq \gamma$</td>
<td>$\text{CaSO}_4.2\text{H}_2\text{O}, \text{Na}_2\text{SO}_4$</td>
</tr>
</tbody>
</table>
| 5     | Triclinic                 | $a \neq b \neq c$: $\alpha \neq \beta \neq \gamma 
eq 90^\circ$ | $\text{CuSO}_4.5\text{H}_2\text{O}, \text{K}_2\text{Cr}_2\text{O}_7$ |
| 6     | Trigonal                  | $a = b = c$: $\alpha = \beta = \gamma 
eq 90^\circ$ | $\text{CaSO}_4, \text{As, Sb, Bi}$ |
| 7     | Hexagonal                 | $a = b \neq c$: $\alpha = \beta = 90^\circ; \gamma = 120^\circ$ | $\text{quartz, Zn, Cd, SiO}_2$ |

6. **Bravais lattices**

Bravais showed the 14 kinds of space lattices, on the basis of symmetry. These 14 kinds of space lattices are always belonging to the seven crystal systems. These are called as Bravais lattices.

**Cubic**

Lattice parameters
- All three sides are equal $\therefore a = b = c$
- All angles are right angles $\therefore \alpha = \beta = \gamma = 90^\circ$

Bravais lattices
$\therefore P, I & F$

![Cubic Bravais lattices](image1.png)

**Tetragonal**

Lattice parameters
- Two sides are equal $\therefore a = b \neq c$
- All angles are right angles $\therefore \alpha = \beta = \gamma = 90^\circ$

Bravais lattices
$\therefore P & I$

![Tetragonal Bravais lattices](image2.png)

**Orthorhombic**

Lattice parameters
- All three sides are different $\therefore a \neq b \neq c$
- All angles are right angles $\therefore \alpha = \beta = \gamma = 90^\circ$

Bravais lattices
$\therefore P, I, F & B$

![Orthorhombic Bravais lattices](image3.png)
Monoclinic
Lattice parameters
- All three sides are different \( a \neq b \neq c \)
- Two angles are right angles \( \alpha = \beta = 90^\circ \neq \gamma \)

Bravais lattices
\( P \quad & \quad B \)

Triclinic
Lattice parameters
- All three sides are different \( a \neq b \neq c \)
- All angles are different \( \alpha \neq \beta \neq \gamma \neq 90^\circ \)

Bravais lattices
\( P \)

Trigonal
Lattice parameters
- All three sides are equal \( a = b = c \)
- All angles are equal but not right angles \( \alpha = \beta = \gamma \neq 90^\circ \)

Bravais lattices
\( P \)
Hexagonal

Lattice parameters

- two sides are equal: $a = b 
eq c$
- two angles are right angles: $\alpha = \beta = 90^\circ$ and third is $\gamma = 120^\circ$

Bravais lattices

Here $P =$ primitive lattice
$I =$ Body centered lattice
$F =$ Face centered lattice
$B =$ Base centered lattice

7. Basic definitions

**Nearest neighboring distance** ($2r$)

The distance between the centers of two nearest neighboring atoms is called nearest neighboring distance. If $r$ is the radius of the atom, nearest neighboring distance is $2r$.

**Atomic radius** ($r$)

Atomic radius is defined as half the distance between the nearest neighboring atoms in the crystal.

**Coordination number** ($N$)

Coordination number is defined as the number of equidistance nearest neighbors that an atom has in a given structure.

**Atomic packing factor or packing factor or packing density:**

Atomic packing factor is the ratio of volume occupied by the atoms in a unit cell to the total volume of the unit cell.

$$\text{packing factor} = \frac{\text{volume of atoms in a unit cell}}{\text{volume of the unit cell}}$$

**Lattice points**

Lattice points denote the positions of atoms or molecules of the crystal.

**Effective number of atoms**

The total number of atoms appeared in a unit cell i.e., corner, centered and face centered is called Effective number of atoms.

**Void space or interstitial space**

The empty space available in a crystal lattice with atoms occupying their respective positions is called void space.
8. **Simple cubic (SC) structure or Primitive**

In simple cubic structure, the atoms are present at the corners of the cube. Each corner atom is shared by eight surrounding cubes. Hence in each atom, only 1/8 portion belonging to the cube. In SC structure, each atom is surrounded by six atoms; hence its coordination number is six.

The number of atoms present in a simple cube = \( 8 \times \frac{1}{8} = 1 \)

Volume occupied by the atom = \( 1 \times \frac{4}{3} \pi r^3 \)

Volume of unit cell = \( a^3 \)

If ‘\( r \)’ is the radius of the atom and ‘\( a \)’ is the side of the cube then

In simple structure \( a = 2r \) (from fig \( AB = a = 2r \) )

packing factor = \( \frac{\text{volume of atoms in a unit cell}}{\text{volume of the unit cell}} \)

\[
\text{packing factor} = \frac{\frac{4}{3} \pi r^3}{a^3} =
\]

\[
= \frac{4}{3} \pi r^3 \div \frac{2r}{3} = \frac{4}{3} \pi r^3 \div \frac{8r^3}{3} = \frac{4}{8r^3} \pi r^3 = \frac{\pi}{6} = 0.52 \quad \text{or} \quad 52\%
\]

Thus, the packing fraction for simple cubic structure is 52% i.e., the atoms occupy only 52% of the space and the rest 48% is void space.
9. **Body centered cubic (BCC) structure**

In body centered cubic structure the atoms are present at the corners of the cube and one atom is present at the center of the cube. Each corner atom is shared by eight surrounding cubes. Hence in each atom, only 1/8 portion belonging to the cube and the centered atom is completely belonging to the cube. In BCC structure each atom is surrounded by eight atoms; hence its coordination number is eight.

The total number of atoms present in BCC = \(8 \times \frac{1}{8} + 1 = 2\)

Volume occupied by the atoms = \(2 \times \frac{4}{3} \pi r^3\)

Volume of unit cell = \(a^3\)

If \(r\) is the radius of the atom and \(a\) is the side of the cube then

In a body centered cubic structure \(\sqrt{3} a = 4 r\)

From fig \(AC^2 = AB^2 + BC^2 = a^2 + 2a^2 = 3a^2 = (4r)^2\)

packing factor = \(\frac{\text{volume of atoms in a unit cell}}{\text{volume of the unit cell}}\)

\[
\text{packing factor} = \frac{2 \times \frac{4}{3} \pi r^3}{a^3} = \frac{8}{3} \pi r^3 = \frac{8}{3} \pi \left(\frac{4r}{\sqrt{3}}\right)^3 = \frac{64}{3} \pi \frac{r^3}{\sqrt{3}} = \frac{64r^3}{3\sqrt{3}}
\]

\[
\therefore a = \frac{4r}{\sqrt{3}}
\]

\[
= \frac{\sqrt{3} \pi}{8} = 0.68 \quad \text{or} \quad 68\%
\]

Thus, the packing fraction for BCC structure is 68% i.e., the atoms occupy only 68% of the space and the rest 32% is void space.
10. **Face centered cubic (FCC) structure**

In FCC structure, the atoms are present at the corners of the cube and as also the atoms are present at the center of its six faces. Each corner atom is shared by eight surrounding cubes. Hence in each atom only $\frac{1}{8}$ portion belonging to the cube. Each face centered atom is shared by two surrounding cubes; hence in each face centered atom, only $\frac{1}{2}$ portion is belonging to the cube. In FCC structure each atom is surrounded by 12 atoms; hence its coordination number is 12.

Total number of atoms present in a FCC = $8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 4$

Volume occupied by the atom = $4 \times \frac{4}{3} \pi r^3$

Volume of unit cell = $a^3$

If $r$ is the radius of the atom and $a$ is the side of the cube then

In simple structure \[ \sqrt{2} a = 4r \]

(From fig $AC^2 = AB^2 + BC^2$; $(4r)^2 = 2a^2$)

packing factor = \[ \frac{\text{volume of atoms in a unit cell}}{\text{volume of the unit cell}} \]

\[ \text{packing factor} = \frac{4 \times \frac{4}{3} \pi r^3}{a^3} = \frac{16 \pi r^3}{3} = \frac{16 \pi r^3}{16 \sqrt{2} r^3} = \frac{\pi}{3\sqrt{2}} = 0.74 \] or 74%

Thus, the packing fraction value for FCC structure is 0.74 i.e., the atoms occupy only 74% of the space and the rest 26% is void space.

The packing factor is more for FCC structure. Hence it is proved that, FCC structure is closely packed than the simple structure and body centered cubic structure.
11. **Miller indices – crystal planes**

A crystal consists of a large number of lattice points. *The plane which is passing through the lattice points is called crystal plane or lattice plane.* The parallel equidistance lattice planes can be chosen in various number of ways as represented in the figure. The problem is that how to designate a plane in the crystal. Miller evolved a method to designate a plane in crystal by three smallest integers \((h \ k \ l)\) known as miller indices.

**Definition**

_Miller indices are three smallest integers which have same ratio as the reciprocals of intercepts of the crystal plane with the coordinate axis.

The procedure for finding Miller indices

I. First of all determine the intercepts of the plane on the three coordinate axes.

II. Secondly take the reciprocals of the intercepts.

III. Lastly reduce the reciprocals into whole numbers. This can be done by multiplying each reciprocal by a number obtained after taking the L.C.M of denominator.

**Example**

Let us consider a plane ABC, its intercepts along three axes are 2, 3, and 4. Miller indices of the plane ABC can be obtained as follows

(i) intercepts are 2, 3, 4
(ii) reciprocals of these are \(
\frac{1}{2}, \frac{1}{3}, \frac{1}{4}
\)
(iii) L.C.M of denominators, i.e., 2, 3 and 4 is 12. hence multiplying by 12, we have 6, 4, 3

Thus the miller indices of the plane is \((6 \ 4 \ 3)\)

**Important features of miller indices – crystal planes**

1. When a plane is parallel to any axis, the intercepts of the plane on that axis is infinity. Hence its miller index for that axis is zero.
2. When the intercept of a plane on any crystallographic axis is negative then a bar should be kept on the corresponding miller index.
3. All equally spaced parallel planes of a crystal have the same miller indices.
4. A plane passes through origin is defined in terms of parallel plane having non-zero intercepts.
5. If a normal drawn to a plane \((h \ k \ l)\), the direction of normal is \([h \ k \ l]\)
(v) Miller indices represent the orientation of crystal plane in a crystal lattice.
(vi) If \((h \ k \ l)\) is the miller indices of a crystal plane, then the intercepts made by the plane with the coordinate axis is \(a/h, b/k\) and \(c/l\) where \(a, b\) and \(c\) are primitives.

1.2. Miller indices – crystal directions

In a crystal system, the line joining the origin and lattice point presents the direction of lattice point. To find the miller indices of crystal direction of lattice point first note down the coordinates of lattice points and enclose them in bigger parenthesis as \([h \ k \ l]\).

For the unit cell, the directions of lattice points are

\[
\begin{align*}
AB &- [100] \\
AC &- [110] \\
AD &- [010] \\
AE &- [001] \\
AF &- [101] \\
AG &- [111] \\
AH &- [011]
\end{align*}
\]

The line joining the origin to the crystal plane represents the direction of crystal plane. The miller indices of the crystal plane enclosed within the bigger parenthesis i.e., \([h \ k \ l]\).

13. Separation between successive \((hkl)\) planes

Let us consider a plane ABC having miller indices \((h \ k \ l)\). Let ON be the normal to the plane passing through the origin O. Let ON makes angles \(\alpha', \beta'\) and \(\gamma'\) With X, Y and Z axes respectively. Let a, b and c is the intercepts of the unit cell. The intercepts of OA, OB and OC of the plane ABC along X, Y and Z axes are

\[
\begin{align*}
OA &= \frac{a}{h} \\
OB &= \frac{b}{k} \\
OC &= \frac{c}{l}
\end{align*}
\]
The direction cosines of the perpendicular ON are 

\[
\cos \alpha' = \frac{ON}{OA} = \frac{ON \cdot h}{a}
\]

\[
\cos \beta' = \frac{ON}{OB} = \frac{ON \cdot k}{b}
\]

\[
\cos \gamma' = \frac{ON}{OC} = \frac{ON \cdot l}{c}
\]

From cosine law

\[
\cos^2 \alpha' + \cos^2 \beta' + \cos^2 \gamma' = 1
\]

Hence

\[
\left(\frac{ON}{a}\right)^2 + \left(\frac{ON}{b}\right)^2 + \left(\frac{ON}{c}\right)^2 = 1
\]

\[
\frac{ON^2 \cdot h^2}{a^2} + \frac{ON^2 \cdot k^2}{b^2} + \frac{ON^2 \cdot l^2}{c^2} = 1
\]

\[
ON^2 \left(\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right) = 1
\]

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

Let the next plane \(A'B'C'\) is parallel to \(ABC\) plane and passing through the origin O. Then the distance between the \(A'B'C'\) and \(ABC\) planes is equal to \(ON\). Hence, the interplanar distance \((d)\) between the adjacent planes is equal \(ON\) i.e., \(ON = d\) so

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

For a cubic lattice \(a = b = c\)

Then

\[
d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}
\]

For tetragonal system \(a = b \neq c\)

Then

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

For orthorhombic system \(a \neq b \neq c\)

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

Note: This relation is only applicable for the crystal systems which systems have all angles are right angles i.e., cubic, tetragonal and orthorhombic.

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14. **X-Ray Diffraction:**
Diffraction of visible light rays can be produced from a diffraction grating. If the grating consists of 6000 lines/cm; the spacing between any two successive lines in the grating is in the order of the wavelength of visible light so it produces diffraction. The wavelength of X-rays is in the order of an angstrom, so X-rays are unable to produce diffraction with a diffraction grating. To produce diffraction with X-rays, the spacing between the consecutive lines of the grating should be of the order of few angstroms. Practically, it is not possible to construct such a grating. In the year 1912, Laue suggested that the crystal can be served as a three-dimensional grating due to the three-dimensional arrangement of atoms in crystal.

There are three main diffraction methods by which the crystal structures can be analyzed.

a. Laue method : applicable to single crystals
b. Powder method : applicable to finely divided crystalline or Polycrystalline specimen powder
c. Rotating crystal method : applicable to single crystals.

15. **Bragg's law**

**Statement**

Bragg's law states that the path difference between the two reflected X-rays by the crystal planes should be an integral multiple of the wavelength of incident X-rays for producing maximum or constructive interference.

Path difference = nλ

Let us consider a set of parallel lattice planes I and II of a crystal separated by a distance d apart. Suppose a narrow beam of X-rays of wavelength λ be incident upon these planes at an angle θ as shown in the figure. Consider a ray PA reflected at the atom A in the direction AR from plane I and another ray QB reflected at another atom B in the direction of BS from plane II. The path difference between the two rays is (CB+BD). When the path difference between the two rays is an integral multiple of X-rays wavelength, the constructive interference phenomenon will occur.

Thus the condition for constructive interference is

\[(CB + BD) = n\lambda\]

From \[\triangle ABC\]

\[
\sin \theta = \frac{CB}{AB} = \frac{CB}{d}
\]

\[CB = d \sin \theta\]
From \[ \Delta ABD \quad \sin \theta = \frac{BD}{AB} = \frac{BD}{d} \]

\[ BD = d \sin \theta \]

\[ (CB + BD) = 2d \sin \theta \]

\[ 2d \sin \theta = n \lambda \]

Where \( n = 1, 2, 3 \ldots \) etc we obtain first, second, third \ldots etc order diffraction spots. Since maximum possible value of \( \theta \) is 1. We get

\[ 2d = n \lambda \]

\[ \lambda \leq 2d \]

Thus, the wavelength \( \lambda \) should not be exceed twice the interplanar spacing for diffraction to occur.

16. **Powder method**

The powder method was developed by Debye and Sherrer in Germany and by Hill in America simultaneously. This method is used to study the structure of crystals which cannot be obtained in the form of perfect crystals of appreciable size. This method can be used for pure metals, compounds and alloys.

**Basic Principle**

The basic principle underlying this powder technique is that, the specimen contains a large number of micro crystals (~10^12 in 1 mm^3 of powder sample) with random orientations, almost all the possible \( \theta \) and \( d \) values are available. The diffraction takes place for these values of \( \theta \) and \( d \) which satisfy Bragg’s condition, i.e., \( 2d \sin \theta = n \lambda \).

**Experimental arrangement:**

The experimental arrangement is shown in figure. The finely powdered sample is filled in a thin capillary tube and mounted at the center of the drum shaped cassette with photographic film at the inner circumference. Collect the X-rays (non-monochromatic) from an X-ray tube. We obtain the monochromatic X-ray radiation by passing through the filter. This monochromatic X-ray radiation can be converted into fine pencil beam by passing through the lead diaphragms or collimators. The pencil beam of X-rays is allowed to fall on the thin walled capillary tube \( P \) containing the powdered crystal.
Theory

The basic principle underlying this powder technique is that, the specimen contains a large number of micro crystals (~$10^{12}$ in $1mm^3$ of powder sample) with random orientations, almost all the possible $\theta$ and $d$ values are available. The diffraction takes place for these values of $\theta$ and $d$ which satisfy Bragg’s condition, i.e., $2d \sin \theta = n\lambda$.

For the value of $\theta$, the beam appears at the corresponding $2\theta$ deviation.

The pattern recorded on the photographic film is shown in the figure when the film is laid flat. Due to the narrow width of the film, only parts of circular rings are register on it. The curvature of arcs reverses when the angle of diffraction exceeds $90^\circ$.

Knowing the distances between the pair of arcs, various diffraction angles $4\theta''$ can be calculated by using the formula.

$$4\theta = \frac{S}{R} \cdot 180^\circ = 57.296 \frac{S}{R}$$

Where $r$, is the radius of the camera.

By knowing the value of $\theta$ from the above equation, the interplanar spacing ($d$) can be calculated for first order diffraction from Bragg’s equation.

$$d = \frac{n\lambda}{2 \sin \theta}$$

Knowing all parameters, the crystal structure can be studied.

Merits:-
- Using filter, we get monochromatic x-rays
- All crystallites are exposed to x-rays and diffraction takes place with all available planes.
- This method is used for determination of crystal structure, impurities, dislocation density etc.,

17. Laue method

The Laue method is one of the X-ray diffraction technique used for crystal structure studies.

Basic principle
The basic principle underlying this Laue technique is that, each reflecting plane selects a wave length according with the Bragg’s relation, i.e., $2d \sin \theta = n\lambda$. The resulting diffraction is recorded on the photographic plate.

Experimental arrangement
The experimental arrangement of the Laue technique is shown in the figure.