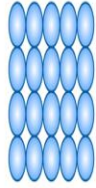
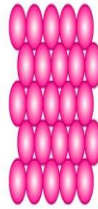


Intermolecular structure of solid

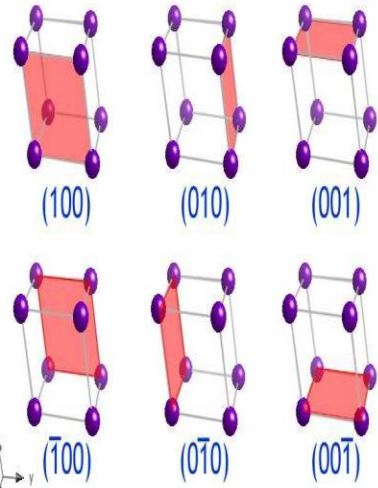
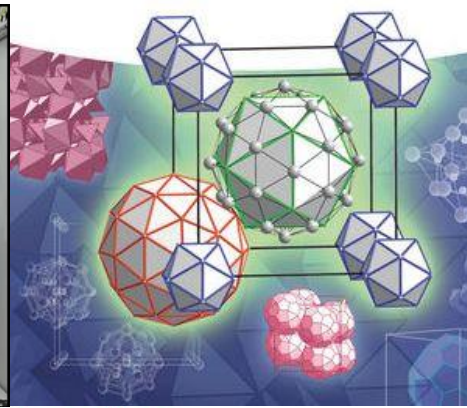
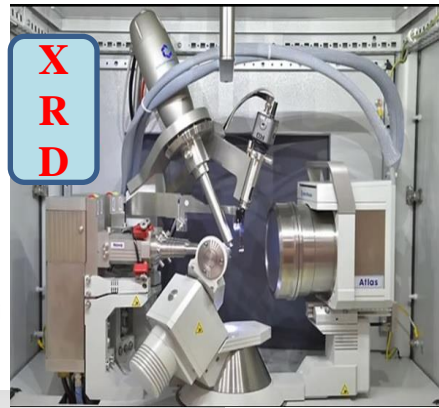


Square packing

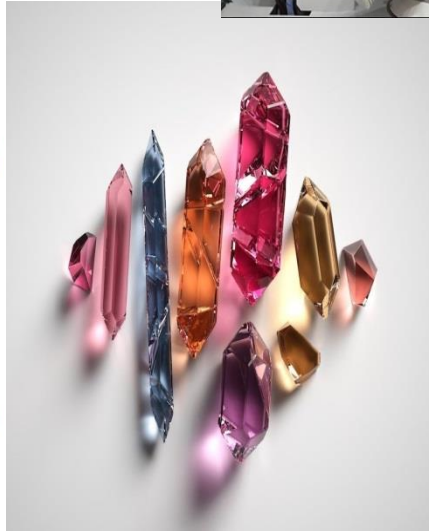


Hexagonal packing

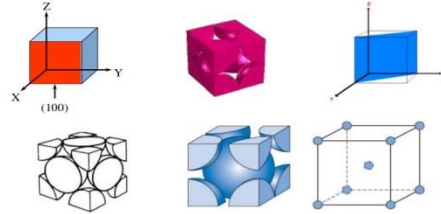
**X
R
D**



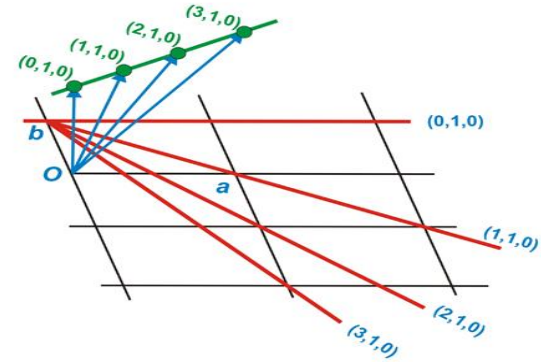
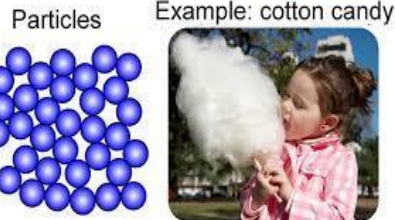
Crystalline Solid



Miller Indices



Amorphous Solid

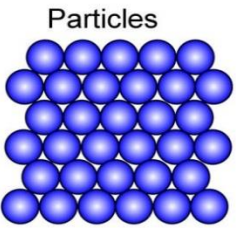


Solid State

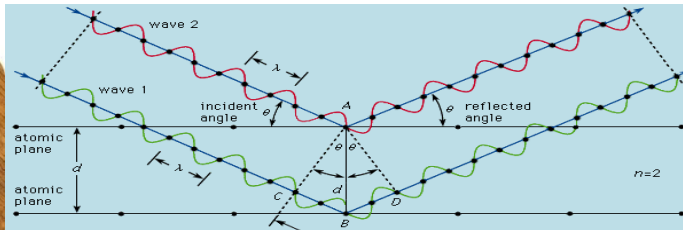
Prof.(Dr) Suryawanshi V.S.

Dept. of Chemistry,
Shri Chhatrapati Shivaji
College, Omerga

vssurya11@gmail.com



Example: Table Salt

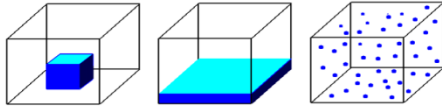


Introduction:

- Solid state is a state of matter besides liquid and gaseous state.
- In case of solids the intermolecular forces are very strong and empty spaces between the atoms/ions/molecules is very less.
- That is why they have a fixed shape and volume and high rigidity.

Characteristics of solids:

1. Definite shape and volume



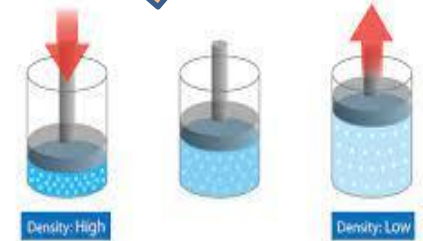
Solid
Holds Shape
Fixed Volume

Liquid
Shape of Container
Free Surface
Fixed Volume

Gas
Shape of Container
Volume of Container

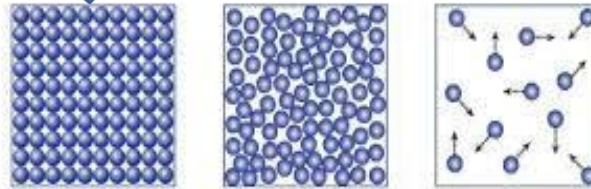
2. High density and low compressibility:

This is due to close packing of molecules which eliminates free space between molecule.



3. Very slow diffusion:

Negligible or very slow diffusion as particles have permanent position from which they do not move easily.



Solid Liquid Gas

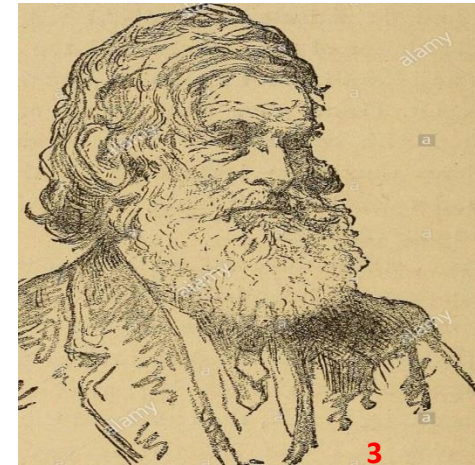
Slow diffusion in Solids

4. Vapor Pressure:

V.P. of solids is generally much less than V.P. of liquids at definite temperature.

Crystallography:

- It is science of crystals which is devoted to the study of crystal development and growth, their external form, internal structure and physical properties.
- For long time crystallography was regarded as mineralogy.
- Crystalline substances are very widespread; majority of bodies/objects surrounding us have crystalline structure.
- **Abbe R.J.Haüy (1784):** Studied regularity of the crystal growth and observed that crystal is made up of very large identical units called as space lattice, it describes three dimensional arrangement of atoms, molecules or ions in crystal lattice.



Classification of Solids: Solids are classified on the basis of following parameters.

1. Based on various properties 2. Based on bonding present in building blocks.

➤ On the basis of various properties solids can be classified as,

1. Crystalline solid 2. Amorphous solid

✓ **Crystalline solid:**

1. They have regular and well defined ordered arrangement of particles.
2. Crystalline solids have same geometry and regularity of crystal lattice.
3. Atoms are closely packed.
4. Examples are KCl, NaCl, ice etc.

✓ **Amorphous solid:**

1. They have no regular and well defined ordered arrangement of particles.
2. Amorphous solid does not have same geometry and regularity of crystal lattice.
3. Examples are Rubber, amorphous sulphur etc. glasses are sometime called amorphous solids and sometimes super cooled liquids of high viscosity.

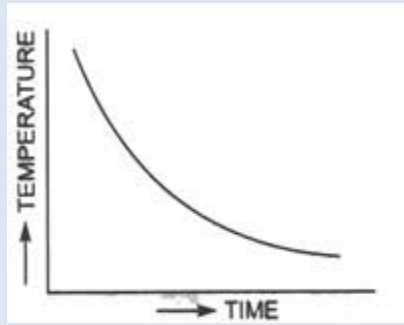
Difference between Crystalline and Amorphous solid

Sr.	Property	Crystalline solid	Amorphous solid
1	Shape	Have Long range order	Have short range order
2	Melting point	Have definite Melting point	Do not have definite Melting point
3	Heat of fusion	They have definite heat of fusion.	Do not have definite heat of fusion.
4	Compressibility	They are rigid and incompressible	May be compressed to some extent.
5	Cooling with sharp edged tool	It break up into smaller crystals of same geometrical shape.	Broken pieces are not generally flats/have irregular surface.
6	Symmetry	They possess symmetry.	They do not possess any symmetry.
7	Volume change	Sudden change in volume when they melt.	No Sudden change in volume on melting.
8	Interfacial angles	They possess Interfacial angles.	They do not possess Interfacial angles.

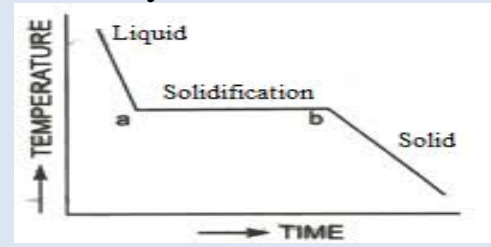
Sr.	Property	Crystalline solid	Amorphous solid
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9
Cooling curve

Cooling curve is smooth.

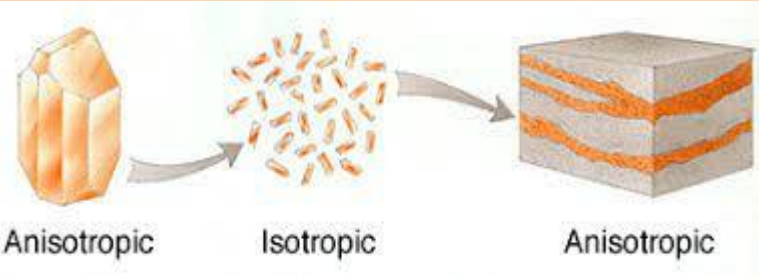
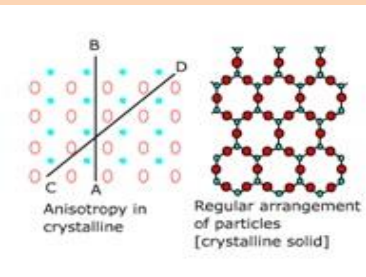


Cooling curve has two breaks ('a' and 'b') which corresponds to beginning and end of process of crystallization.

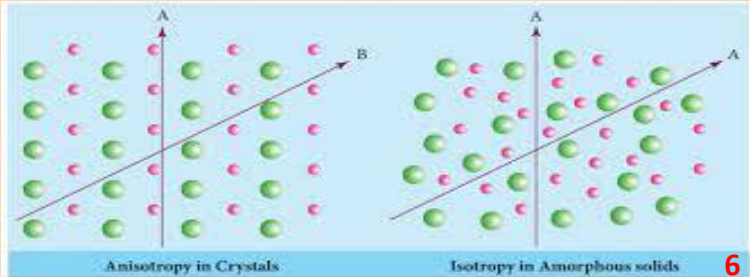
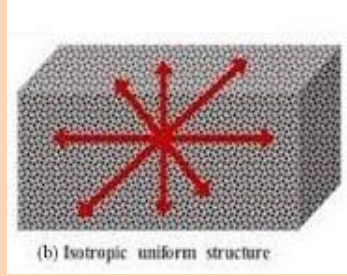


10
Isotropy and Anisotropy

They are anisotropic (Physical properties are different in different directions)



They are Isotropic (Physical properties are same in all directions)



Unit cell:

The smallest repeating unit of the crystal lattice is the unit cell, the building block of crystal.

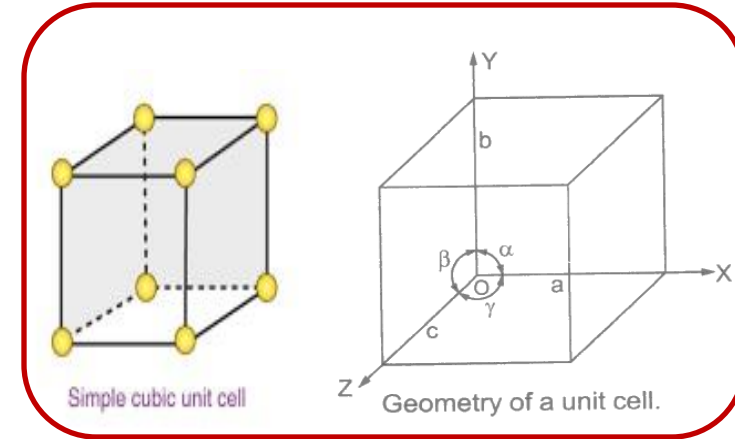
Or The smallest unit of the arrangement of atoms in a crystal is known as unit cell.

Example: Crystal of calcite (CaCO_3) can be broken into large number of small rhombus which have original shape; even if it again and again broken, a point would be reached at which the smallest crystal would exist.

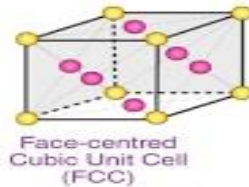
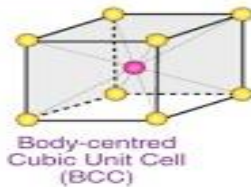
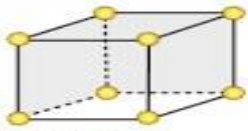
Three types: **1. Simple unit cell:** Atoms, ions or molecules are present only at the corner of the unit cell.

2. Face centered: Besides the corner, there is a point present in the center of each face.

3. Body centered: There is point at the center within the body of the unit cell.



TYPES OF UNIT CELL



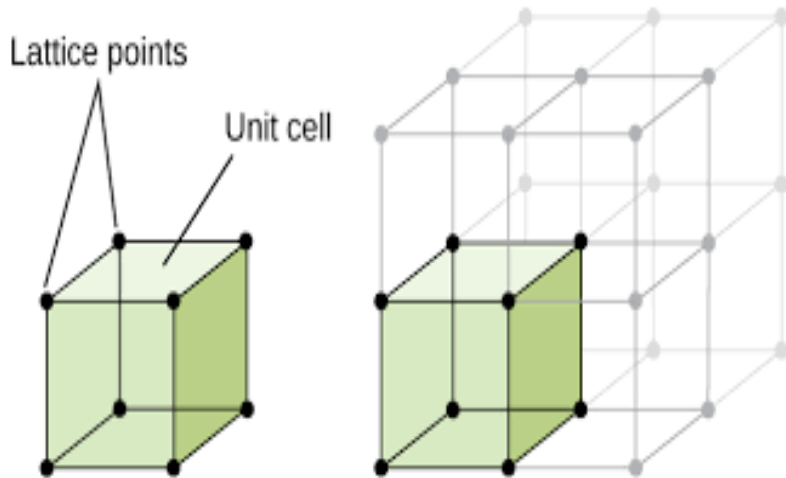
1. **a, b and c** are lengths of the edges of unit cell.
2. **α, β and γ** are angles between three imaginary axes.
3. **OX, OY and OZ** are three imaginary axes.
4. Unit cell has **8** corners & at each corner eight cells meet.

Crystal lattice:

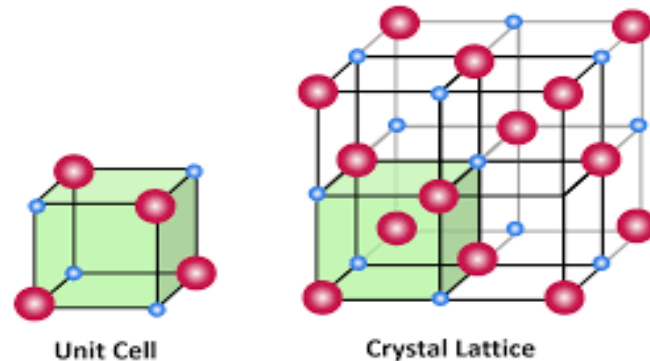
The unit cells which are all identical are defined in such a way that they fill space without overlapping. The 3D arrangement of atoms, molecules or ions inside a crystal is called a *crystal lattice or space lattice*. *Crystal lattice* is made up of numerous unit cells.

Lattice point:

A **lattice point** is a **point** at the intersection of two or more grid lines in a regularly spaced array of **points**, which is a **point lattice**.

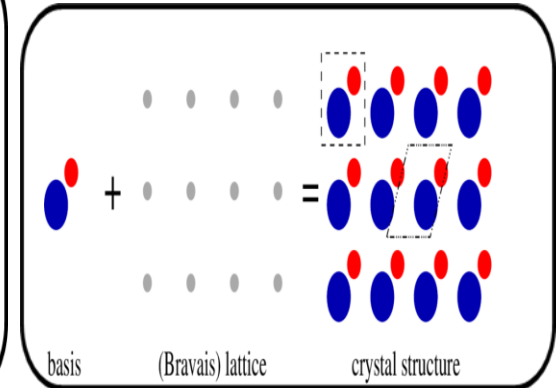
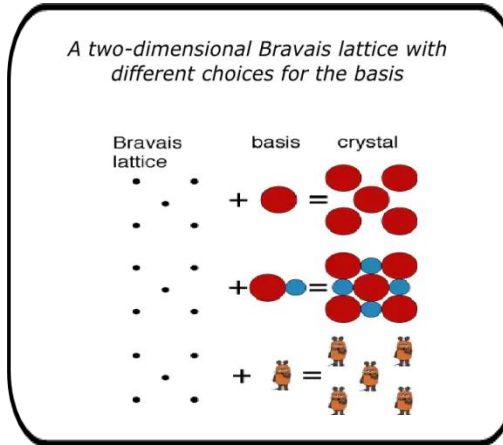
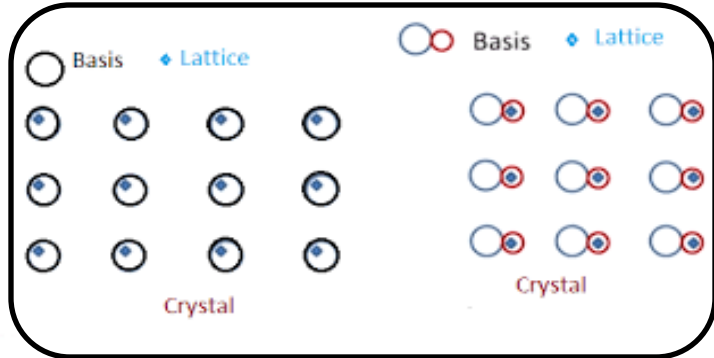


Crystal Lattice and Unit Cell



Basis and lattice:

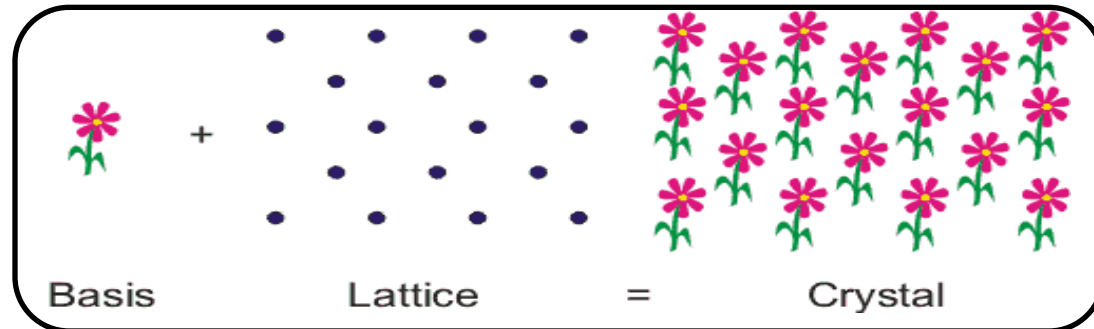
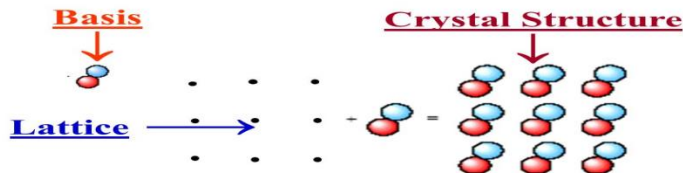
- A **lattice** is a hypothetical regular and periodic arrangement of points in space.
- A **basis** is a collection of atoms in particular fixed arrangement in space.
- We could have a **basis** of a single atom as well as a **basis** of a complicated but fixed arrangement of hundreds of atoms.



Crystalline Periodicity

Crystal Structure \equiv **Lattice** + **Basis**

For another example, see the figure.



Weiss indices and Miller indices

- Indices is nothing but **Indicator of crystal planes**.
- The Weiss parameters, introduced by **Christian Samuel Weiss in 1817**.
- It will help us to determine **the distance between the parallel planes** of the crystal or it characterizes and represents any plane of the crystal.
- Weiss indices are **ratio of intercept** on that axis to the unit length on that axis.
- Weiss indices = Intercept on the axis / Unit length on the same axis.
- Weiss indices are generally **small whole number** and may be **fractions of whole numbers** as well as **infinity**.

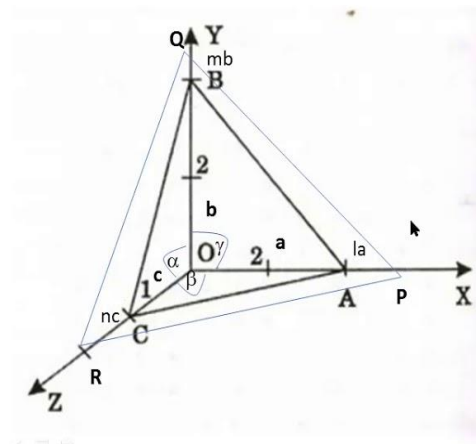
Conditions for Weiss indices:-

1. Three axis present namely **a,b,c values** (Weiss indices value) may be **fraction, integrals, positive, negative, infinite, but never be zero**.

Conditions for positive and negative in Weiss indices:-

- 1.If origin **to right** then W.I.is **positive** and origin to **left** W.I. will be **negative**.
2. If origin **to front** then W.I.is **positive** and origin to **back** W.I. will be **negative**.
3. If origin **to up** then W.I.is **positive** and origin **to down** W.I. will be **negative**.Origin **cannot** be present **along with the plane**.

Weiss indices/ Miller indices



Intercepts of **Unit plane** ABC

OA = a at x-axis

OB = b at y-axis

OC = c at z-axis

Intercepts of **any plane** PQR parallel to

ABC on three axis

OP = la on x-axis

OQ = mb on y-axis

OR = nc on z-axis

Ratio

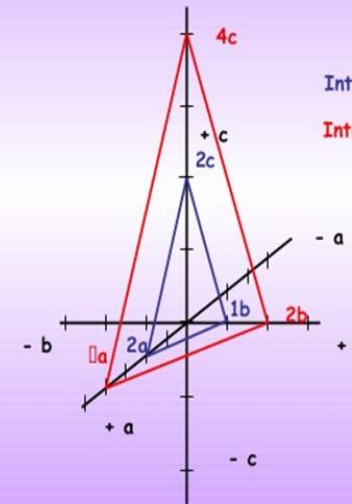
$x : y : z = la : mb : nc$

a, b, c are unit intercepts

l, m, n are small whole numbers but may be in fraction

Face intercepts III

Intercepts are always given as relative values, e.g. they are divided until they have no common factor. Parallel faces in the same quadrant have, therefore, the same indices



Intercepts: $2a : 1b : 2c = 2 : 1 : 2$

Intercepts: $4a : 2b : 4c = 4 : 2 : 4$
div. by 2

$\Rightarrow 2 : 1 : 2$

Intercept ratios are called **Weiss indices**

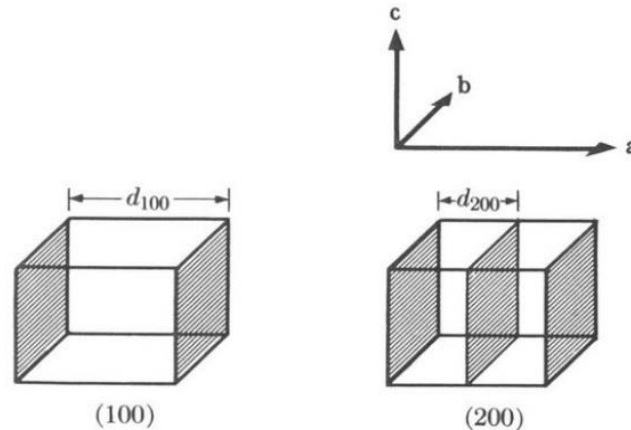
Miller indices:- (William Hallowes Miller 1839)

- It is **mathematical notation** to **represent crystal plane and its direction** in crystal structure.
- Miller indices of a plane are **the reciprocals of the distances from the origin** at which a given face intersects ,the three axes.
- In Miller indices (M.I.) **h,k,l** is used for different axis instead of ‘x’, ‘y’ and ‘z’ axis. That is ‘x’ is replaced by ‘h’, ‘y’ is replaced by ‘k’ and ‘z’ is replaced by ‘l’.
- M.I. obtained by taking the **reciprocals** of Weiss coefficients and **multiplying by the smallest number** that will express all the reciprocals as integers.

$$h = \frac{a}{\text{Intercept of plane along } x \text{ axis.}}, \quad h = \frac{b}{\text{Intercept of plane along } y \text{ axis.}}$$

$$\text{and } h = \frac{c}{\text{Intercept of plane along } z \text{ axis.}}$$

- Larger the value of M.I., smaller will be the value of the intercept of that plane along the given axis and when it is zero (The intercept is infinity), plane is parallel to that axis.
- Two parallel planes in a crystals have same miller indices, because they are equally spaced parallel planes.



How to calculate M.I ?

Selection of origin:- Rule I: As per definition of origin, origin should be left, down and back.

Rule II: Origin can't be present along with the plane x and y cannot taken as origin.

- Find the intercept on the respective axis (h,k,l)
- Obtain the reciprocal of Weiss indices.
- Eliminate on of fractions to make them integrals (Whole numbers).
- Miller indices of the plane are (h,k,l)
- Origin is never considered on the plane because if considered intercept will become zero and thus M.I. will become infinite but we know that M.I. is never infinite.
- Origin is considered/fixed on such a point for which point in one step we should reach /move to it from plane. or in other words we may say that distance of plane from origin should be one unit.

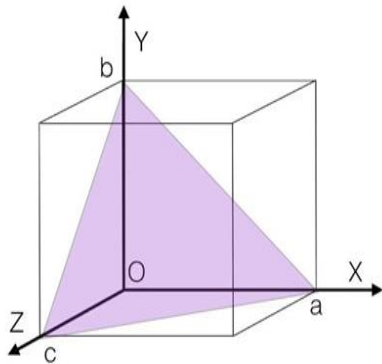
Condition for Miller indices: It can be integer, positive, negative or zero but never be infinite or fraction. If negative then it is denoted by 1^- (Bar-).

Rules for Miller Indices:

1. Determine the intercepts of the face along the crystallographic axes, in terms of unit cell dimensions.
2. Take the reciprocals.
3. Clear fractions.
4. Reduce to lowest terms.

Some General Principles:

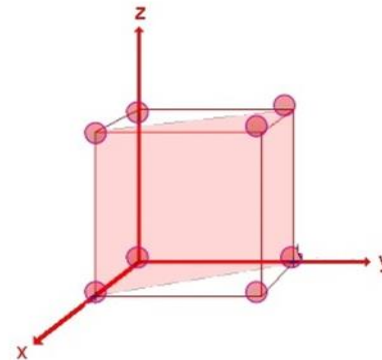
- If a Miller index is zero, the plane is parallel to that axis.
- The smaller a Miller index, the more nearly parallel the plane is to the axis.
- The larger a Miller index, the more nearly perpendicular a plane is to that axis.
- Multiplying or dividing a Miller index by a constant has no effect on the orientation of the plane.
- Miller indices are almost always small.



Here the plane intersects x axis at **a**, y axis at **b** and z axis at **c**..
Therefore,

$$\frac{a}{h} : \frac{b}{k} : \frac{c}{l} = \frac{1}{1} : \frac{1}{1} : \frac{1}{1} = (111)$$

Miller Indices of plane is (111).

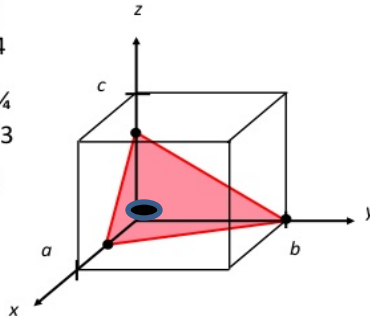


Axis	x	y	z
Intercept points	1	1	∞
Reciprocals	1/1	1/1	1/ ∞
Smallest Ratio	1	1	0
Miller Indices (110)			

Crystallographic Planes

example

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

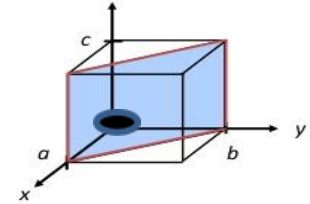


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Crystallographic Planes

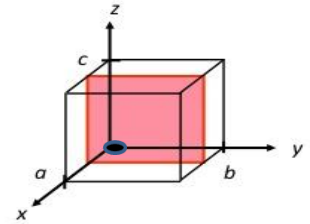
example

	<i>a</i>	<i>b</i>	<i>c</i>
1. Intercepts	1	1	∞
2. Reciprocals	1/1	1/1	1/ ∞
3. Reduction	1	1	0
4. Miller Indices	(110)		

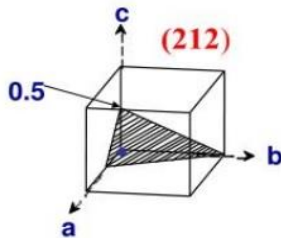
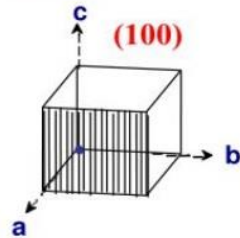
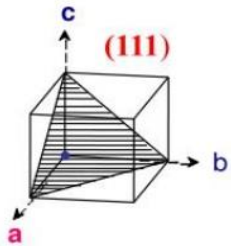


example

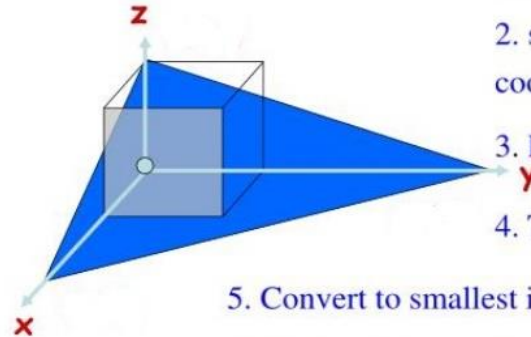
	<i>a</i>	<i>b</i>	<i>c</i>
1. Intercepts	1/2	∞	∞
2. Reciprocals	1/1/2	1/ ∞	1/ ∞
3. Reduction	2	0	0
4. Miller Indices	(200)		



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Miller Indices for planes

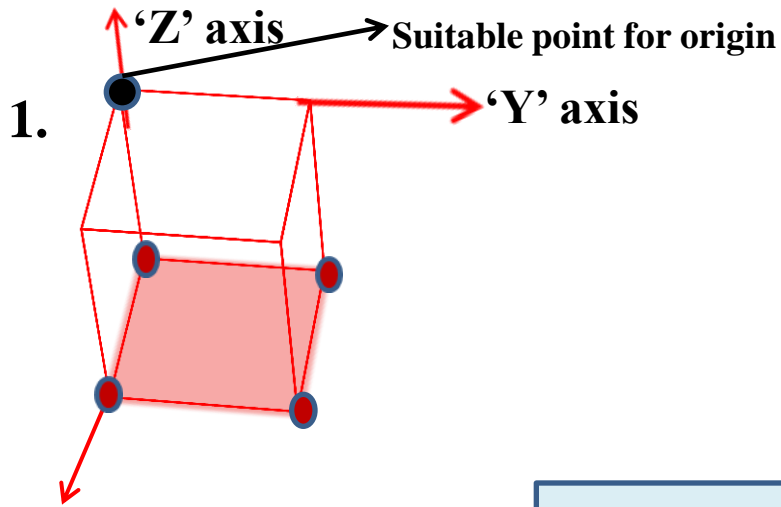


1. Select an origin not on the plane
2. select a crystallographic coordinate system
3. Find intercepts along axes **2 3 1**
4. Take reciprocal **1/2 1/3 1/1**

5. Convert to smallest integers in the same ratio: **3,2,6**

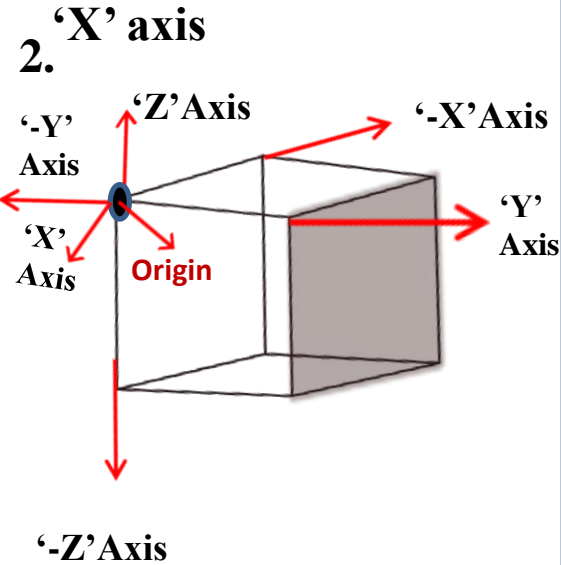
6. Enclose in parenthesis: **(3,2,6)**

16



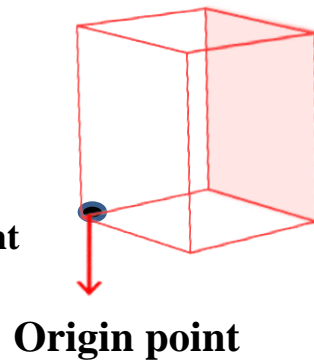
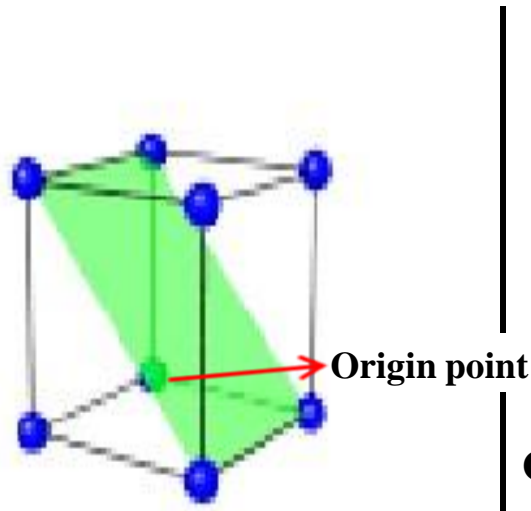
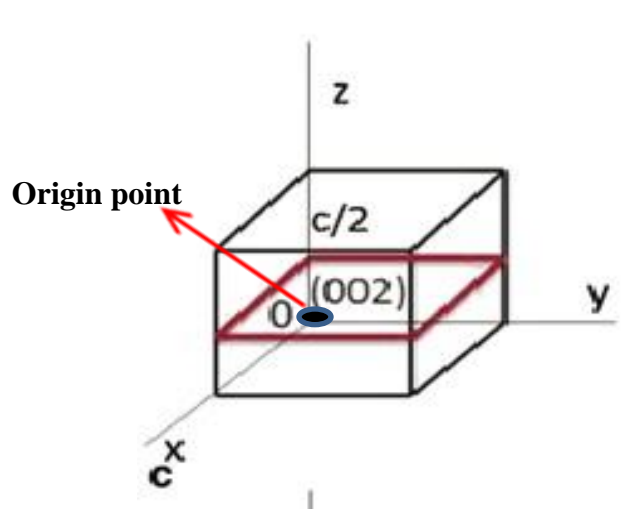
● On these points origin cannot be considered.

Axis	X or 'a'	Y or 'b'	Z or 'c'
Intercept points	∞	∞	-1
Reciprocals	$1/\infty$	$1/\infty$	$1/-1$
Smallest ratio	0	0	-1
Miller Indices	$(0\ 0\ 1^-)$ (Bar-)		



Note: 1.If we move towards 'Y' then we found the plane at one unit so intercept = 1.
 2.Similarly, along 'X' axis on infinite so Intercept = ∞ .
 3. Along 'Z' axis on infinite so intercept = ∞ .
 4. When plane is parallel to 'Z' axis then intercept is always ' ∞ '.

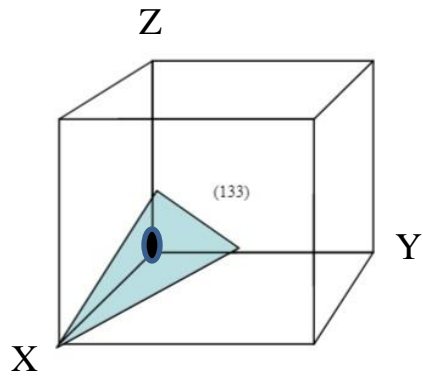
Axis	X or 'a'	Y or 'b'	Z or 'c'
Intercept points	∞	1	∞
Reciprocals	$1/\infty$	1/1	$1/\infty$
Smallest ratio	0	1	0
Miller Indices	$(0\ 1\ 0)$		



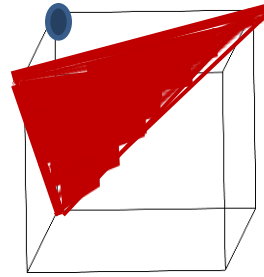
Axis	X	Y	Z
Intercept points	∞ parallel to plane	∞ parallel to plane	1/2
Reciprocals	1/ ∞	1/ ∞	2
Smallest ratio	-1	0	0
Miller Indices	(0 0 2)		

Axis	X	Y	Z
Intercept points	∞ parallel to plane	1	1
Reciprocals	1/ ∞	1/1	1/1
Smallest ratio	0	1	1
Miller Indices	(0 1 1)		

Axis	X	Y	Z
Intercept points	-1 Back to meet origin hence -1	∞ parallel to plane	∞ parallel to plane
Reciprocals	1/-1	1/ ∞	1/ ∞
Smallest ratio	-1	0	0
Miller Indices	(1 ⁻ 0 0)		



The (133) plane intersects the y and Z axes at 1/3.



Qu. Draw correct crystal plane if the following Miller indices are given

Qu.1. M.I.(0 0 1)

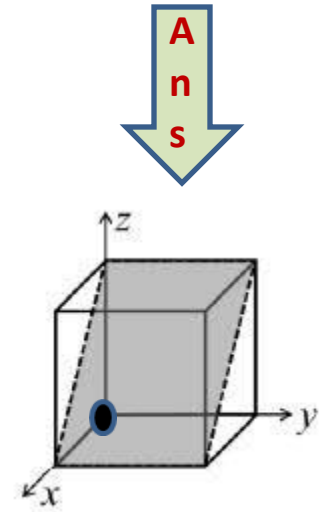
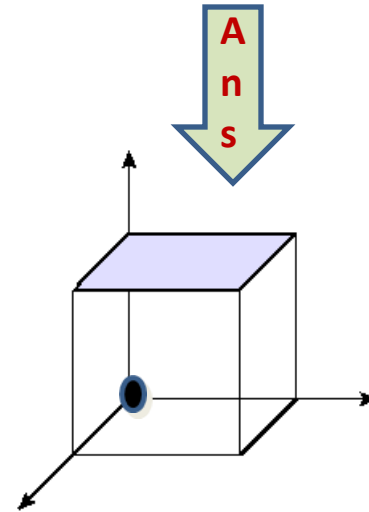
Miller Indices	0	0	1
Intercept	1/0	1/0	1/1
Intercept	∞	∞	1

Qu.2.M.I.(1 0 1)

Miller Indices	1	0	1
Intercept	1/1	1/0	1/1
Intercept	1	∞	1

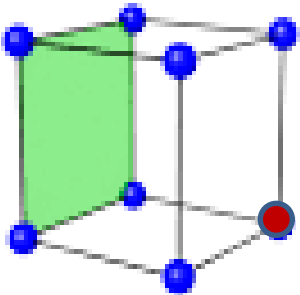
Axis	X	Y	Z
Intercept points	1	1/3	1/3
Reciprocals	1/1	1/1/3	1/1/3
Smallest ratio	1	3	3
Miller Indices	(1 3 3)		

Axis	X	Y	Z
Intercept points	1	1	-1
Reciprocals	1/1	1/1	1/-1
Smallest ratio	1	1	1 ⁻
Miller Indices	(1 1 1 ⁻)		



Qu.3. M.I.(0 1̄ 1)

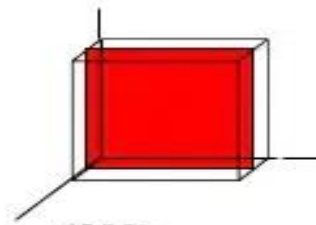
Miller Indices	0	1̄	0
Intercept	1/0	1/1̄	1/0
Intercept	∞	1̄	∞



(01̄0)

Qu.4. M.I.(200)

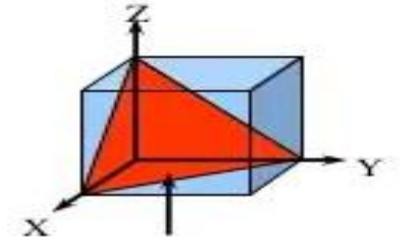
Miller Indices	2	0	0
Intercept	1/2	1/0	1/0
Intercept	1/2	∞	∞

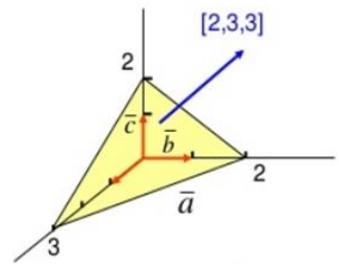


(200)

Qu.5. M.I.(111)

Miller Indices	0	0	1
Intercept	1/0	1/0	1/1
Intercept	∞	∞	1



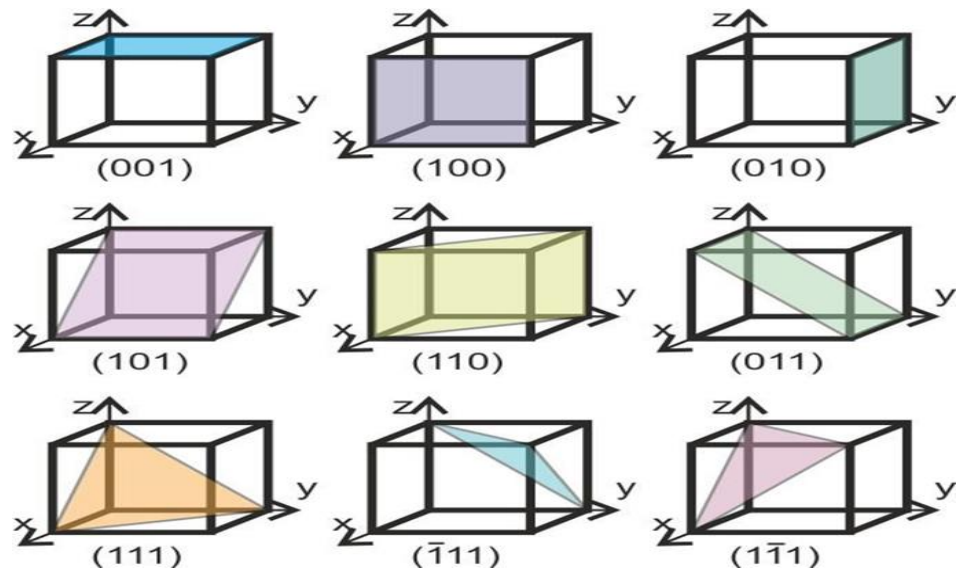
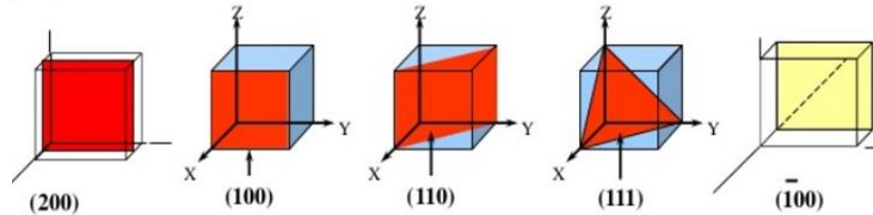


Plane intercepts axes at $3\bar{a}, 2\bar{b}, 2\bar{c}$

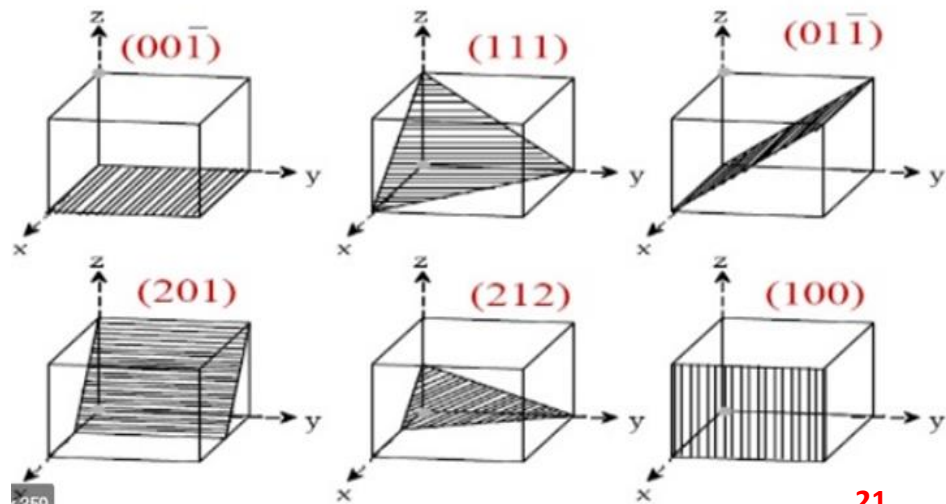
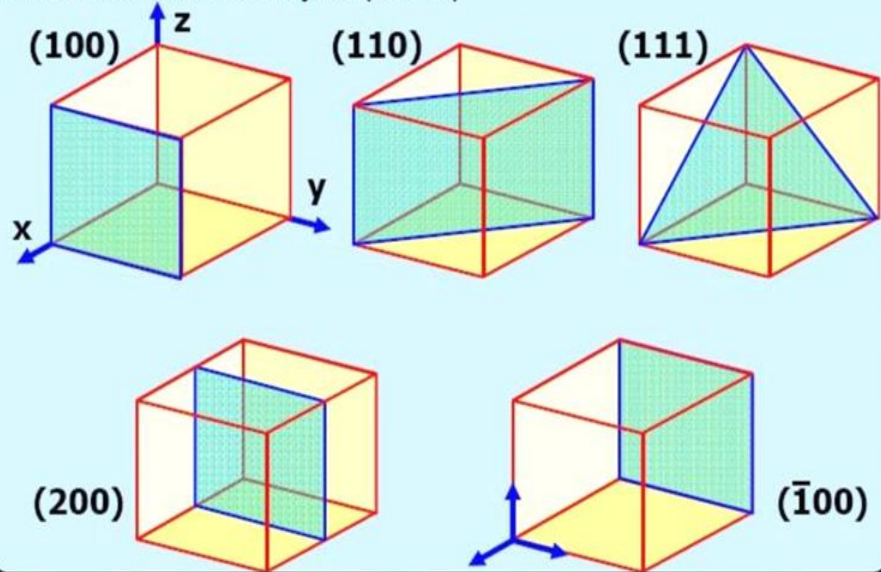
Reciprocal numbers are: $\frac{1}{3}, \frac{1}{2}, \frac{1}{2}$

Indices of the plane (Miller): $(2,3,3)$

Indices of the direction: $[2,3,3]$



Miller's indices in cubic crystal (Silicon)

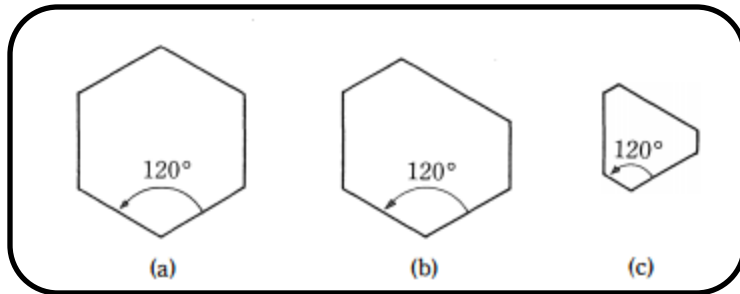


Laws of Crystallography:

The geometric crystallography is based on three fundamental laws;

1. Law of constancy of interfacial angles: Angle between adjacent corresponding faces is inter facial angles of the crystal of a particular substance is always constant in spite of different shapes and sizes and mode of growth of crystal. The size and shape of crystal depend upon the conditions of crystallization.

This law is also called as First law of crystallography.



In short, that the size and shape of a crystal of a compound varies with conditions of crystallization, but the angle between the faces (Interfacial angle) remains constant.

❖ The crystals of the same substance can have different shapes, it depends on number and sizes of faces but the angle between the corresponding faces remains always equal.

2.Law of Symmetry:

It states that, all crystals of the same substance possess the same elements of symmetry.

➤ Symmetry in the crystals may be due to a plane, a line or a point, on the basis of this law there are three types of symmetry.

1. Plane of symmetry

2.Axis of symmetry

3.Centre of symmetry.

3.Law of rational indices (Havy law):

The ratio between the intercepts on the axes for the different faces of the crystal can be expressed by rational numbers.

Example $la: mb: nc$ where l, m and n are small whole numbers and a, b and c are the intercepts made by unit plane along the crystallographic axes.

Elements of symmetry:

- The large number of crystals are formed by different substances, depending on the condition of crystallization, each substance having a characteristic crystalline form(s).
- There are more than 200 crystal forms, so that there is a problem to classify them, but on the basis of elements of symmetry they can be grouped into a small number of different classes.

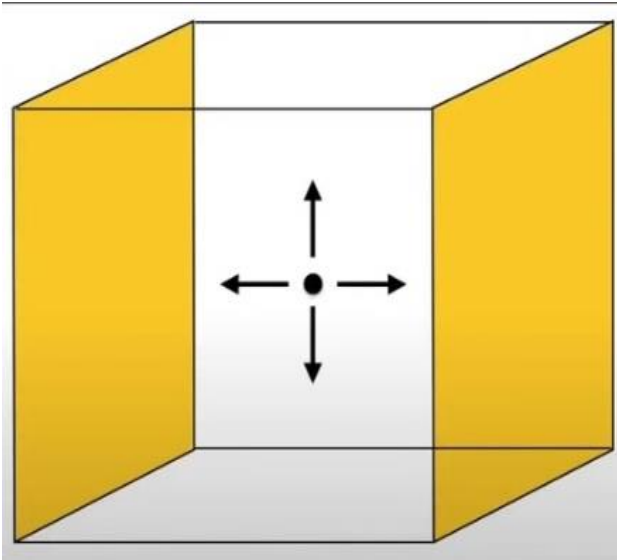
1. Centre of symmetry

2. Plane of symmetry

3. Axis of symmetry

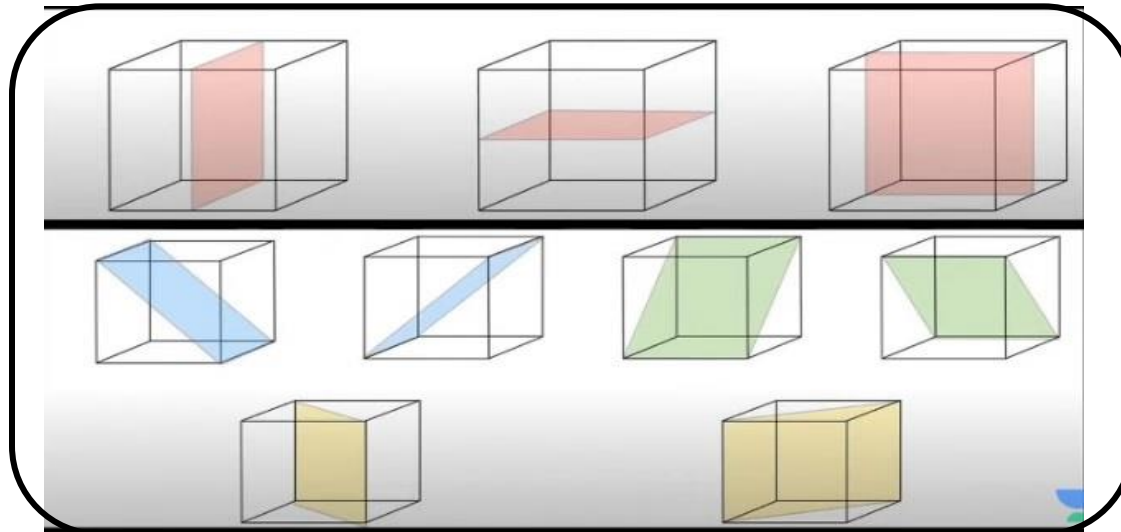
Centre of symmetry:

- It is defined as an imaginary point within the crystal such that any line passing through this point intersects the opposite face of the crystal at equal distances.
- In other words, any line drawn through this point will intersect surface at equal distance in both the directions.



Plane of symmetry:

- It is an imaginary plane which divides the crystal into two equal parts such that one is the mirror image of the other.
- For example Regular cubic structure can have **9** planes of symmetry.
- Three planes of symmetry are parallel to the cube faces and six diagonal planes are passing through opposite cube edges.



Axis of symmetry:

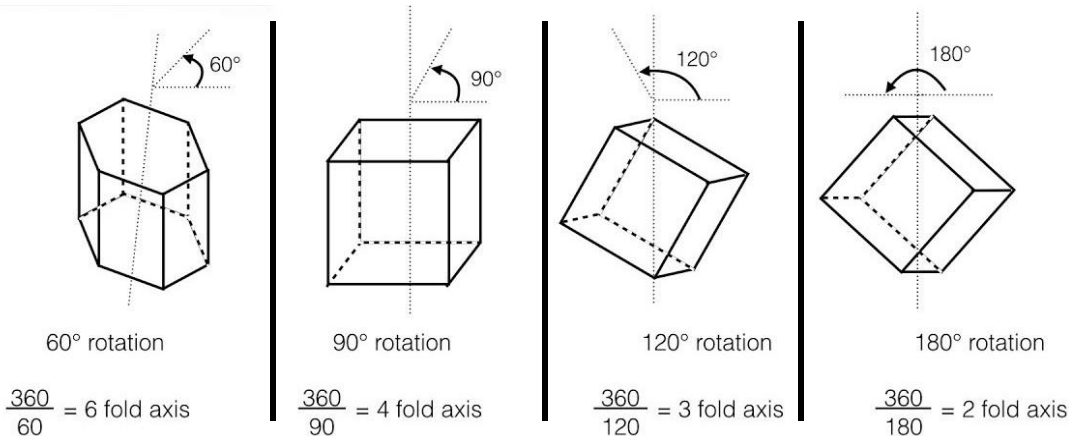
Axis of symmetry is a line about which the crystal may be rotated such that it presents the same appearance more than once during the complete revolution through 360 deg.

- If a crystal presents the same appearance 'n' times in complete revolution, the axis is said to be 'n' fold symmetry. The cube contains **three different types** of symmetry axes.

A) Three-4 fold axes, each of which passes through the centers of two opposite faces.


B) Four- 3 fold axes, each of which passes through two opposite vertices and

C) Six-2 fold axes, such of which passes through the midpoints of two opposite edges.



Symmetry elements of Cube = 23

Axis of Symmetry
2-fold or dyad axis of symmetry
 180° $360/180 =$
2 times same appearance



2 edges = 1
12 edges = 6

27

Symmetry elements of cube:

(a) Centre of symmetry		1	
(b) Planes of symmetry		9	
(Straight planes -3, Diagonal planes -6)			
(c) Diad axes		6	
(d) Triad axes		Axis of symmetry(c)	4
(e) Tetrad axes		6+4+3	3

Total number of symmetry elements =		23	

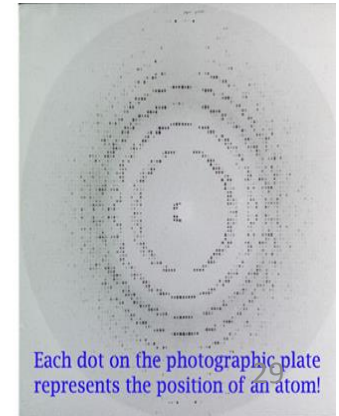
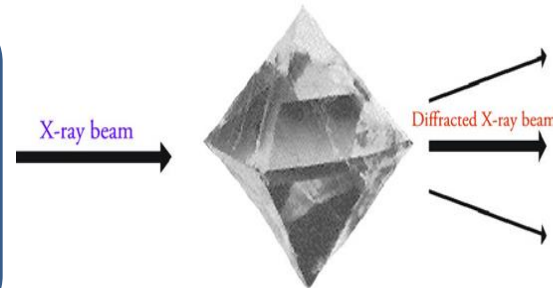
Thus the total number of symmetry elements of a cubic structure is 23.

X-ray diffraction from crystals:

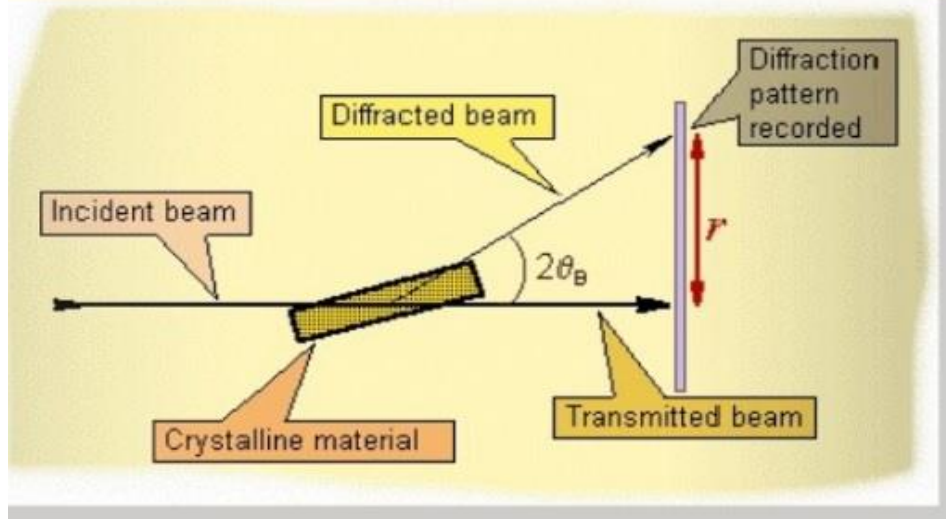
- X-ray diffraction or X-ray crystallography is used to **determine crystal structures/atomic and molecular structure** by **interpreting the diffraction patterns** formed when x-rays are scattered (diffraction in many specific directions) **by the electrons** of atoms in crystalline solids.
- X-ray are sent through a crystal to **reveal the pattern** in which the molecules and atoms.

- ❑ X-ray crystallography works based on **X-ray diffraction principle**; it means that scattering of x-ray by crystal.
- ❑ X-ray **diffraction is based on constructive interference** of monochromatic x-rays and crystalline sample.

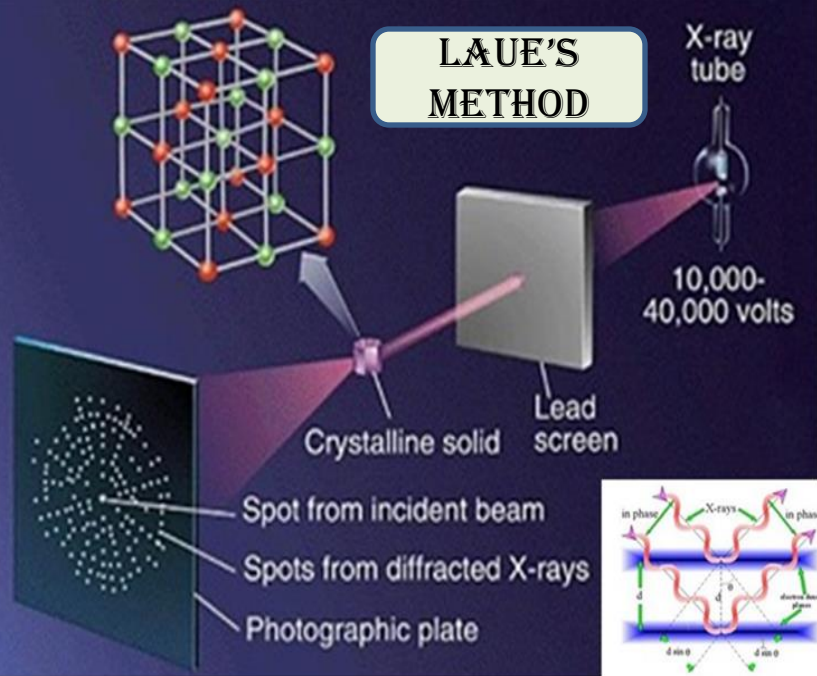
“Every crystalline substance gives a patterns; **the** same substance **always** gives **the** same pattern; and in a mixture of substances **each** produces **its** pattern independently **of the others**”



What is X-ray Diffraction ?



LAUE'S METHOD



➤ **Laue's photographic method:** Max Von Laue (1912) passed continuous beam of X-rays with different wavelength through a crystal to get a diffraction pattern to get positions of ions or molecules in crystals.

- The fine beam coming out of the slit (Lead) passed through crystal placed on the holder.
- The beam emerging from the crystal was made to fall on a photographic plate, kept few Cm from crystals

- Photograph is obtained, it consist of a **central spot** which arises due to the **un- diffracted beam**, the central spot is **surrounded by spots** which arise from different **diffracted beam**. Thus pattern of spots gives idea about the crystal structure.
- The maths involved in this method for calculations are **highly complex**.
- The reason for use of X-ray that, the wavelength of X-ray was of about the same order as the interatomic distances in a crystal. X-ray **penetrates more** than the cathode rays.
- X- ray has **High frequency** (3×10^{16} Hz to 3×10^{19} Hz) and **high energy** but **low wavelength** (10^{-8} to 10^{-11} m) than visible light.
- Electric and magnetic field have no influence on X-rays and so they evidently do not consist of charged particles.

Diffraction:

- ❖ The process by which a beam of light or other system of waves is spread out or bending of EMR as a result of passing through a narrow aperture or across an edge, typically accompanied by interference between the wave forms produced. Dark band observes due to constructive interference.
- ❖ Diffraction takes place with electromagnetic radiation like light, X-ray, and gamma rays and with very small particles such as atoms, neutrons and electrons which show wave like properties.

Interference of light:

- It is the phenomenon in which **two waves superpose** to form the **resultant** wave of **lower, higher or same amplitude**.
- The most commonly seen interference is the **optical interference** or **light interference**.

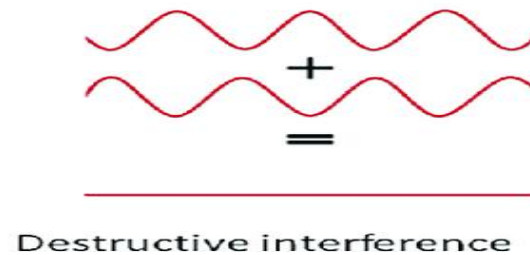
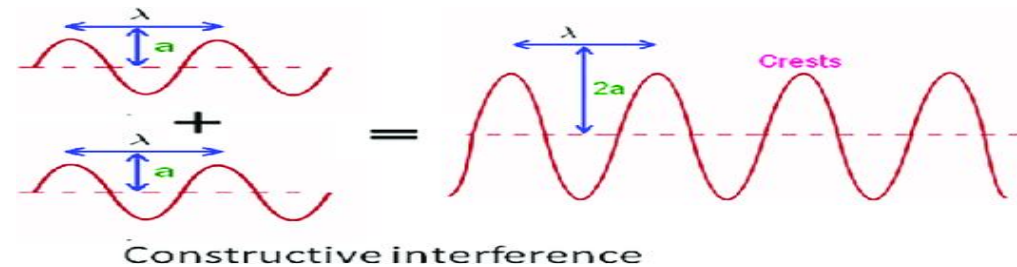
1. Constructive interference:

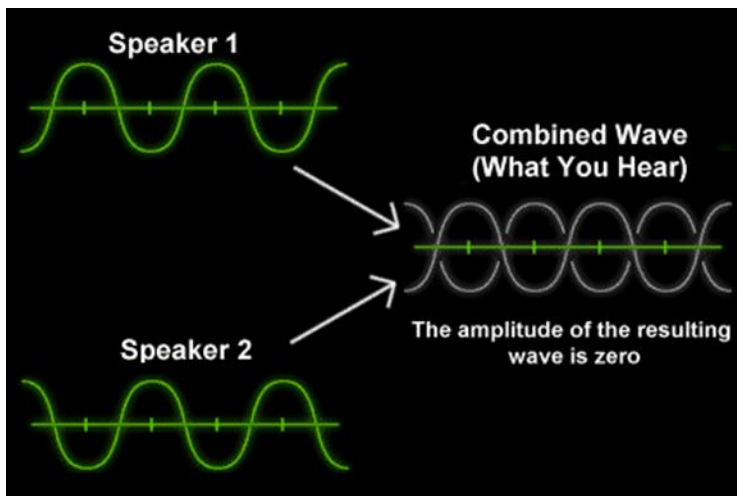
It occurs when the **maxima or minima of two waves add together** (the two waves are in phase), so that the amplitude of the resulting wave is equal to the sum of the individual amplitudes. (**Higher amplitude**).

For example: Two speakers playing same music while facing each other. At this time, music will appear louder and powerful as compared to music played by single speaker.

2. Destructive interference: when the **maxima** of two waves are **180 degrees out of phase**: a positive displacement of one wave is cancelled exactly by a negative displacement of the other wave. The **amplitude** of the resulting wave **is zero**.

The **dark regions occur** whenever the waves destructively interfere.

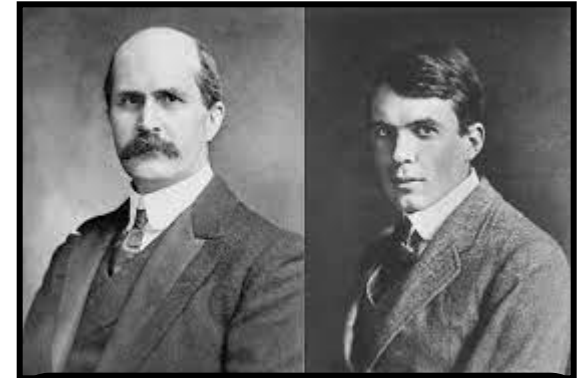




If the **speakers** are at the same position, there will be constructive **interference** at all points directly in front of the **speaker**. If the **speakers** are separated by half a wavelength, then there is **destructive interference**, regardless of how far or close you are to the **speakers**.

Bragg's Equation:

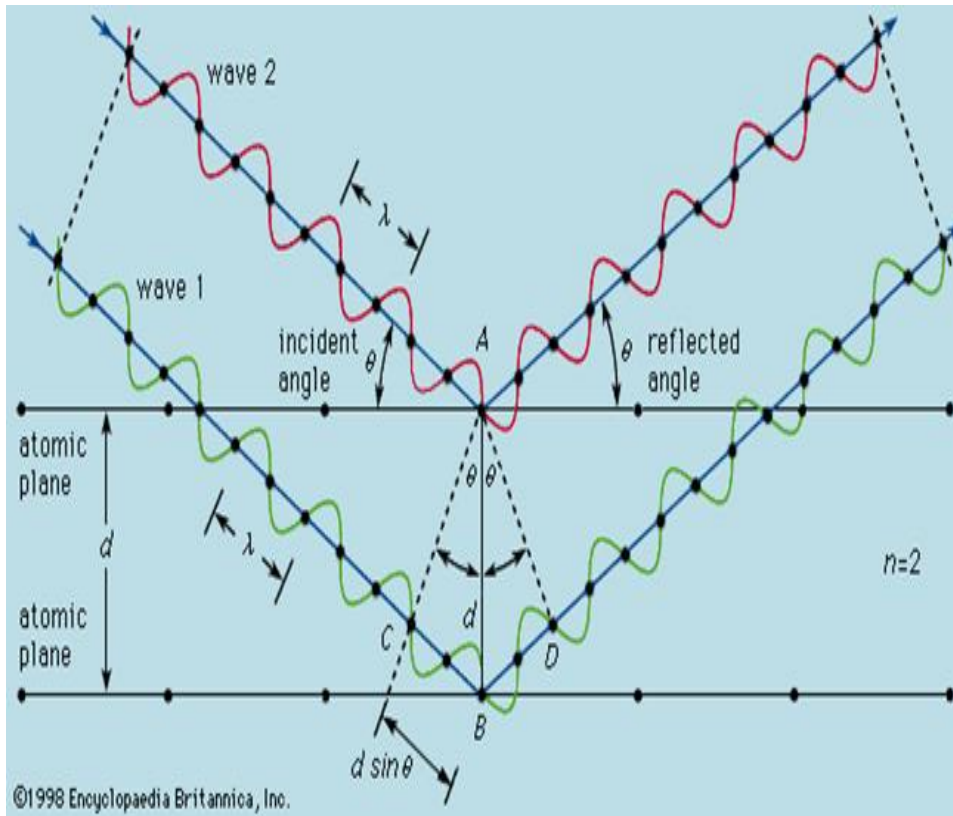
- W.Henry and W.L.Bragg devised and studied that each crystal plane reflects radiation as a mirror and analyzed this situation for cases of constructive and destructive interference.
- When a beam of X-rays is passed through a crystal each atom in the path acts as scattering centre and thus emits secondary radiations.



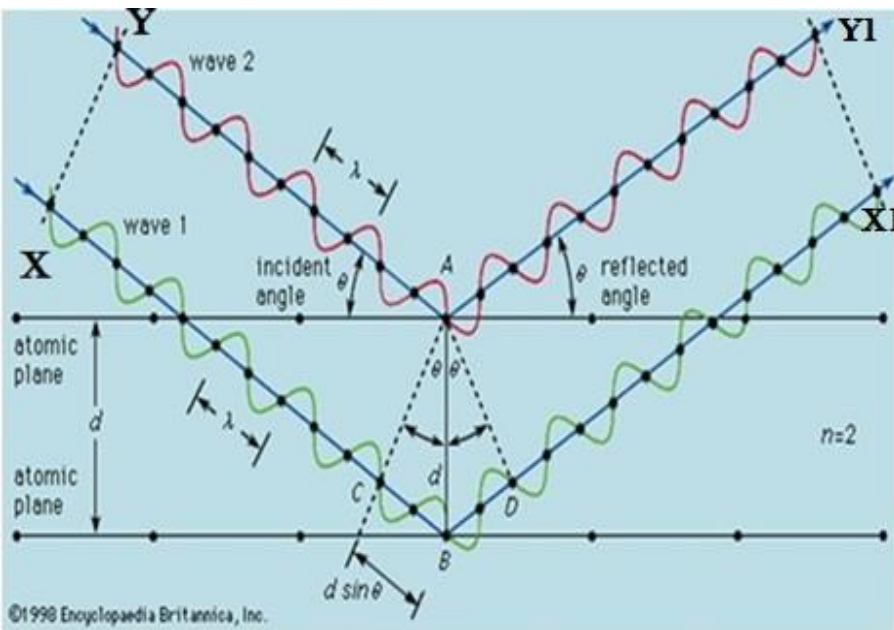
William Henry and
William Lawrence Bragg
(Father and Son)

Nobel prize winner 1915

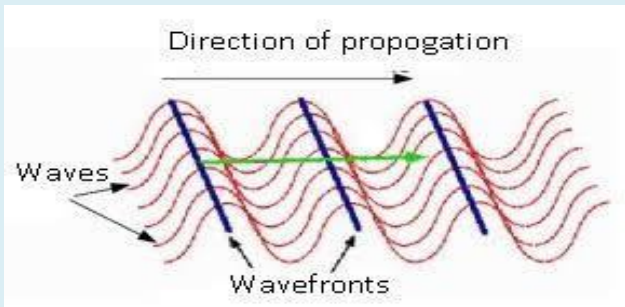
- However, reflection of X-rays can take place at certain angles when the path difference of emitted ray from the successive planes is a whole number multiple of the wavelength.



- Consider a set of parallel atomic planes whose spacing is 'd' and let a narrow monochromatic beam of X-rays fall upon these parallel planes at a glancing angle ' θ '
- Each atom in a given layer, according to Huygens's principle, becomes the centre of expanding wavelets whose envelope gives rise to reflected wave front.



Wave fronts: Time-varying field is the set (locus) of all points where the wave has the same phase.



- As in the case of optical reflection, the reflected wave front will have maximum intensity at angle 'θ' to this plane, which is equal to the glancing angle.
- Each parallel layer/planes (third, fourth, fifth etc.) in the given set gives rise to the reflected wave front (for I and II, X_1Y_1).

Condition for constructive interference:

Path difference between reflected wave fronts from one layer and that from the next must be equal to an exact wavelength or an integral multiple of wavelength ($n \lambda$), where 'n' is an integer and 'λ' is wavelength.

- Each crystal diffracts to X-ray because interplanary spacing in a crystal lattice is of the same order as that of wavelength of X-rays.(X-rays can penetrates to crystal lattice).
- Draw a perpendicular line from A to B, similarly draw AC and AD perpendicular to the direction of the incident and reflected rays.
- The rays reflected from B travels a longer distance than that reflected from A.(path-II > path-I).
- Each of these lines makes an angle θ with AB whose length is equal to the spacing d .
- Path difference = $BC + BD$ (path diff.= $BC + BD$) should be equal to $(n.\lambda)$ (1) **that is,**

$$BC+BD=n\lambda$$

$$BC + BD = n.\lambda \text{ or path difference} = n.\lambda \text{(2)}$$

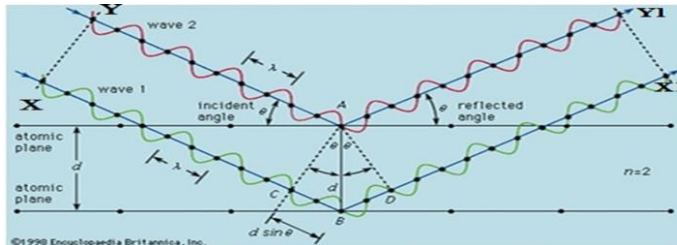
$$\text{In triangle ACB, } \sin\theta = \frac{BC}{AB}$$

$$\text{It may written as, } \frac{BC}{d \text{ (diagonal)}} \text{ Or } \boxed{BC = d \sin \theta}$$

Similarly in triangle ABD,

$$\sin\theta = \frac{BD}{AB} \text{ or it may be written as,}$$

$$\frac{BD}{d \text{ (diagonal)}} \text{ or } \boxed{BD = d \sin \theta}$$



$$\begin{aligned} \text{Path difference} &= BC + BD = d \sin \theta + d \sin \theta \\ &= BC + BD = 2 d \sin \theta \text{(3)} \end{aligned}$$

$$\begin{aligned} \text{Path difference} &= BC + BD = d \sin \theta + d \sin \theta \\ &= BC + BD = 2 d \sin \theta \dots\dots\dots(3) \end{aligned}$$

Note that :
BC+BD=nλ..... (1)

Equating equation 1 and 3 we get, $n \cdot \lambda = 2d \sin \theta$ or $d = \frac{n \cdot \lambda}{2 \sin \theta}$

Where,

θ - is angle on which x-rays falls.

d - is interplanar separation.

n – is order of refraction (integer 1,2,3,4....& so on)

d, n, λ and θ are variables, if any three can known we calculate forth.

Braggs Law:
Constructive interference of the radiation from successive planes occurs when the path difference is an integral number of wavelength.

Problem: Calculate the distance between two layers/scattering planes if $n=2$ (Second order), $\lambda= 1$ Angstrom, θ is 60 degree ?

Ans: We know that, $d = \frac{n \lambda}{2 \sin \theta} = \frac{2 \times 1}{2 \sin 60} = \frac{2}{2 \cdot \sin 60} = \frac{2}{2 \sin \theta} = \mathbf{1.15 \text{ AU}}$ is the distance between two layers of crystal.

Application of XRD / Why XRD ?

- ✓ By measuring the **angles and intensities** of these diffracted beams, a crystallographer can produce a **3D of electron density** within the crystal.
- ✓ Measures the **average spacing** between layers or rows of atoms.
- ✓ Determines the **orientation** of a single crystal or grain.
- ✓ Finds the **crystal structure** of an unknown material.
- ✓ Measures the **size, shape and internal stress** of small crystalline regions.
- ✓ Electron density and accordingly position of the atoms in **complex structures (position of atoms, chemical bonds, their disorder** etc. can be determined.
- ✓ Useful to determine whether the compound is **solvated or not**.
- ✓ Useful to determine **cis-trans isomerization** and state of **anneal in metals**.
- ✓ It is novel and **non destructive** method of chemical analysis.

Thank



you

