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Subject : Physics

B.SC – Second Year Semester IV
Paper – I

Unit - 2

Topic : X-ray Diffraction

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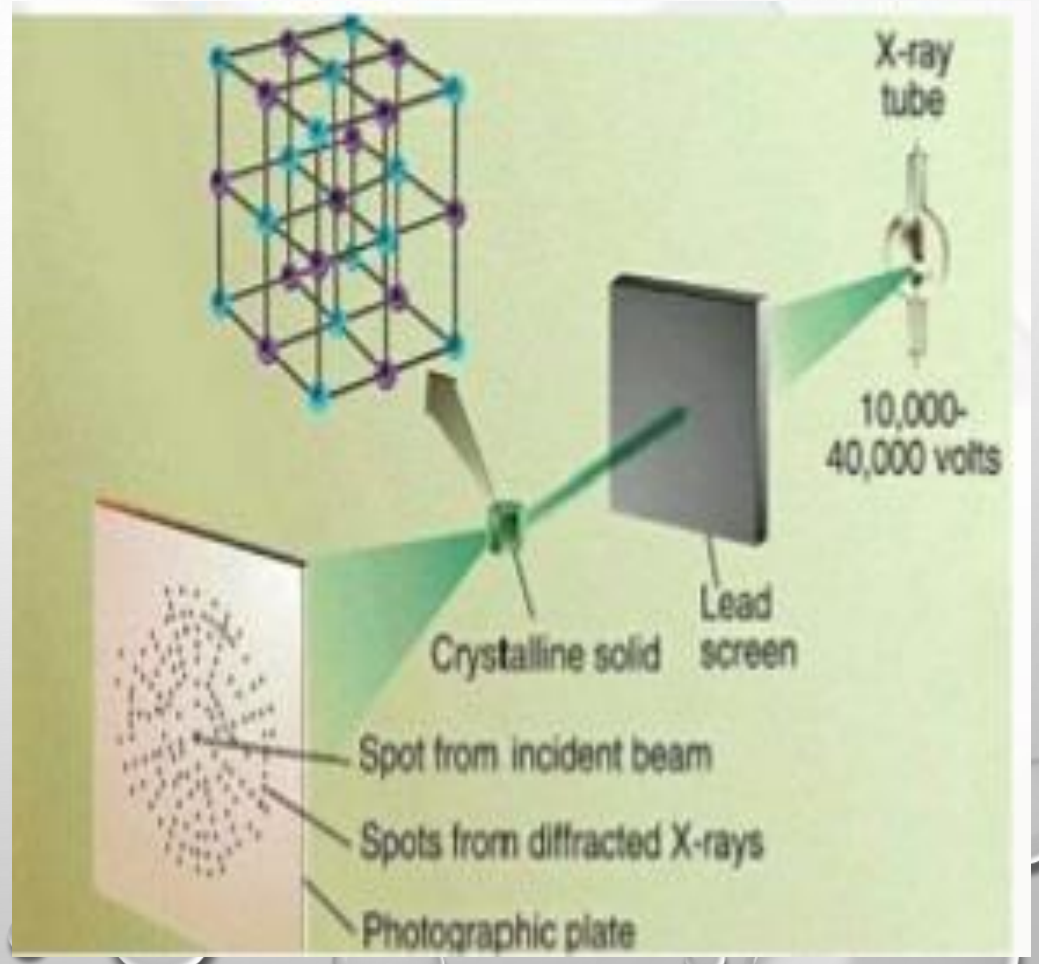
X-RAY DIFFRACTION

A TECHNIQUE USED TO DETERMINE THE ATOMIC AND MOLECULAR STRUCTURE OF A CRYSTAL, IN WHICH THE CRYSTALLINE ATOMS CAUSE A BEAM OF INCIDENT X-RAYS TO DIFFRACT INTO MANY SPECIFIC DIRECTIONS.

MAX VON LAUE (1912) SUGGESTED THAT X-RAY MIGHT BE DIFFRACTED WHILE PASSING THROUGH A CRYSTAL WHERE IT ACTS AS A THREE DIMENSIONAL DIFFRACTION GRATING AND PRODUCE INTERFERENCE EFFECT. HE REALIZE THAT THE WAVELENGTH OF THE X-RAY ARE COMPARABLE TO THE SEPARATION OF LATTICE PLANES.



ORIGIN OF XRAY

1895	X-rays discovered by Roentgen
1914	First diffraction pattern of a crystal made by Knipping and von Laue
1915	Theory to determine crystal structure from diffraction pattern developed by Bragg.
1953	DNA structure solved by Watson and Crick
Now	Diffraction improved by computer technology; methods used to determine atomic structures and in medical applications

BRAGG'S LAW

➢ BRAGG'S LAW :

Bragg's law states that the x-rays reflected from different parallel planes of a crystal interfere constructively when the path difference is integral multiple of the wavelength of x-rays.

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

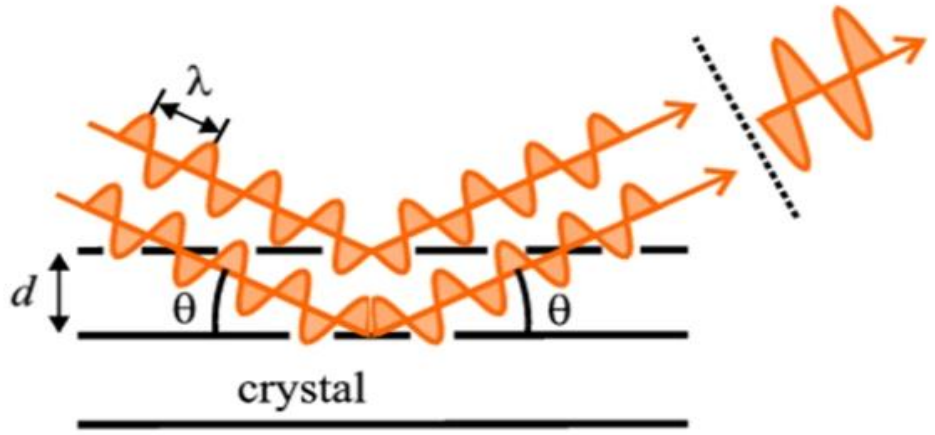
Where,

λ = wavelength of x-ray

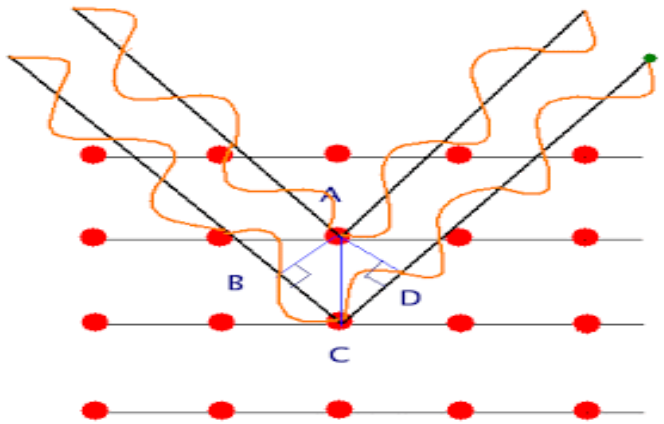
d = interplanar spacing

θ = incident angle

n = integer



Explanation of Bragg's Law



FORMULA

Formula: **1. $n\lambda = 2d\sin\theta$**

Where,

λ = wavelength of x-ray

d = interplanar spacing

θ = incident angle

n = integer

2. $\theta = \frac{1}{2} \tan^{-1} (r/D)$

Where,

D = distance between the specimen and the film.

r = distance of Laue's spot from centre of film.

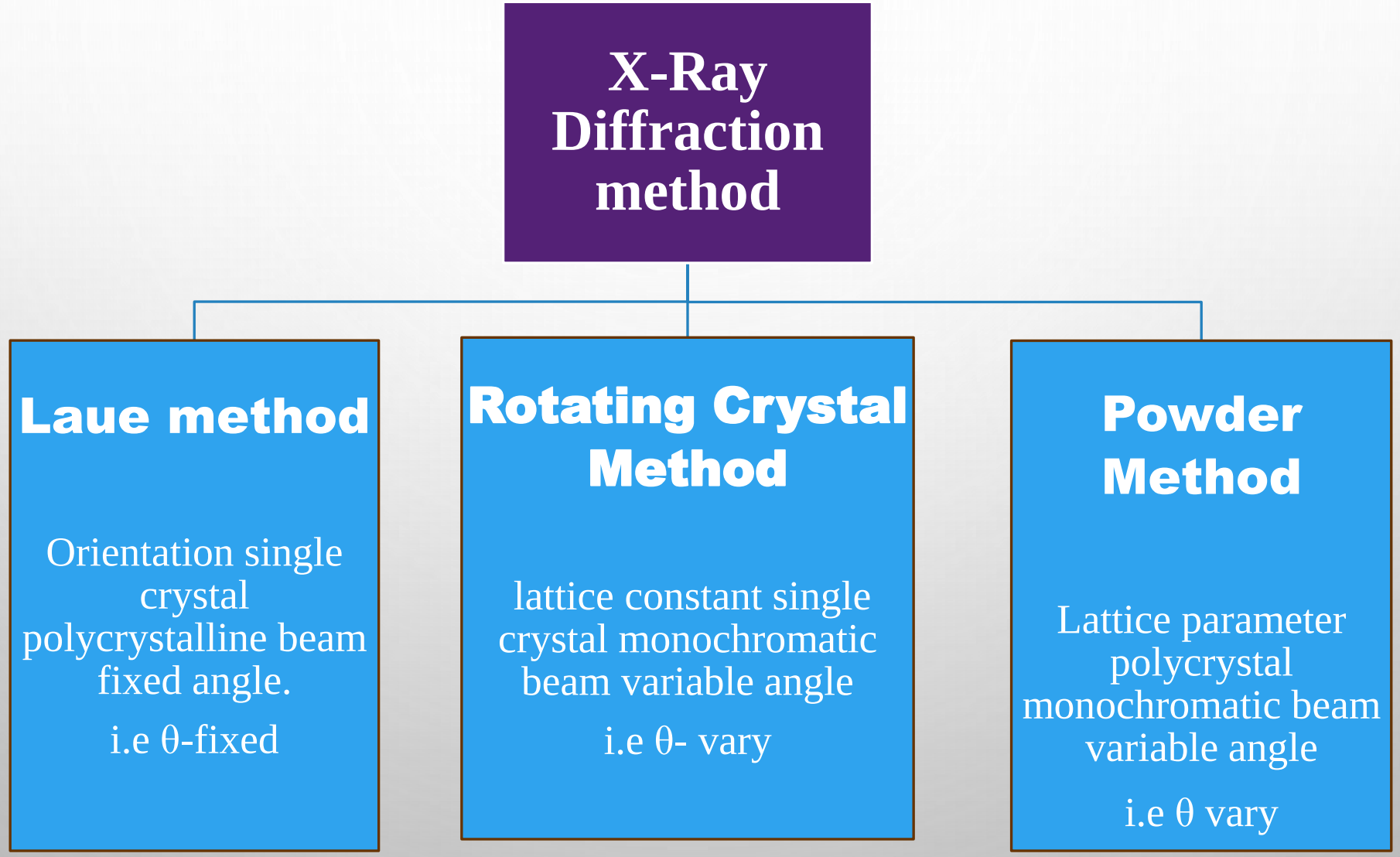
APPLICATIONS OF BRAGG'S LAW

- It is used in the construction of instrument such as Bragg's spectrometer.

- Lattice parameters can be determine using Bragg's law.

- In X-ray diffraction:
  - The interplanar spacing of a crystal is used for characterization and identification purpose.
  - Also it is used to determine the intermolecular distance between the liquid.

X-RAY DIFFRACTION METHOD

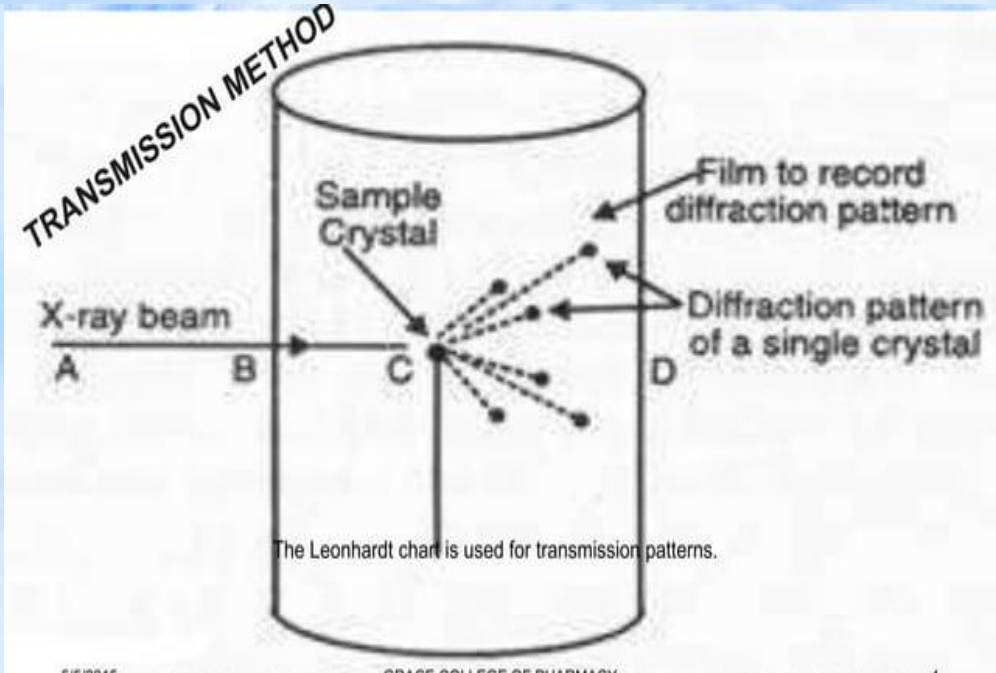


LAUE PHOTOGRAPHIC METHOD

- The Laue method is mainly used to determine the orientation of large single crystals
- White radiation is reflected from, or transmitted through, a fixed crystal
- Two Types:-

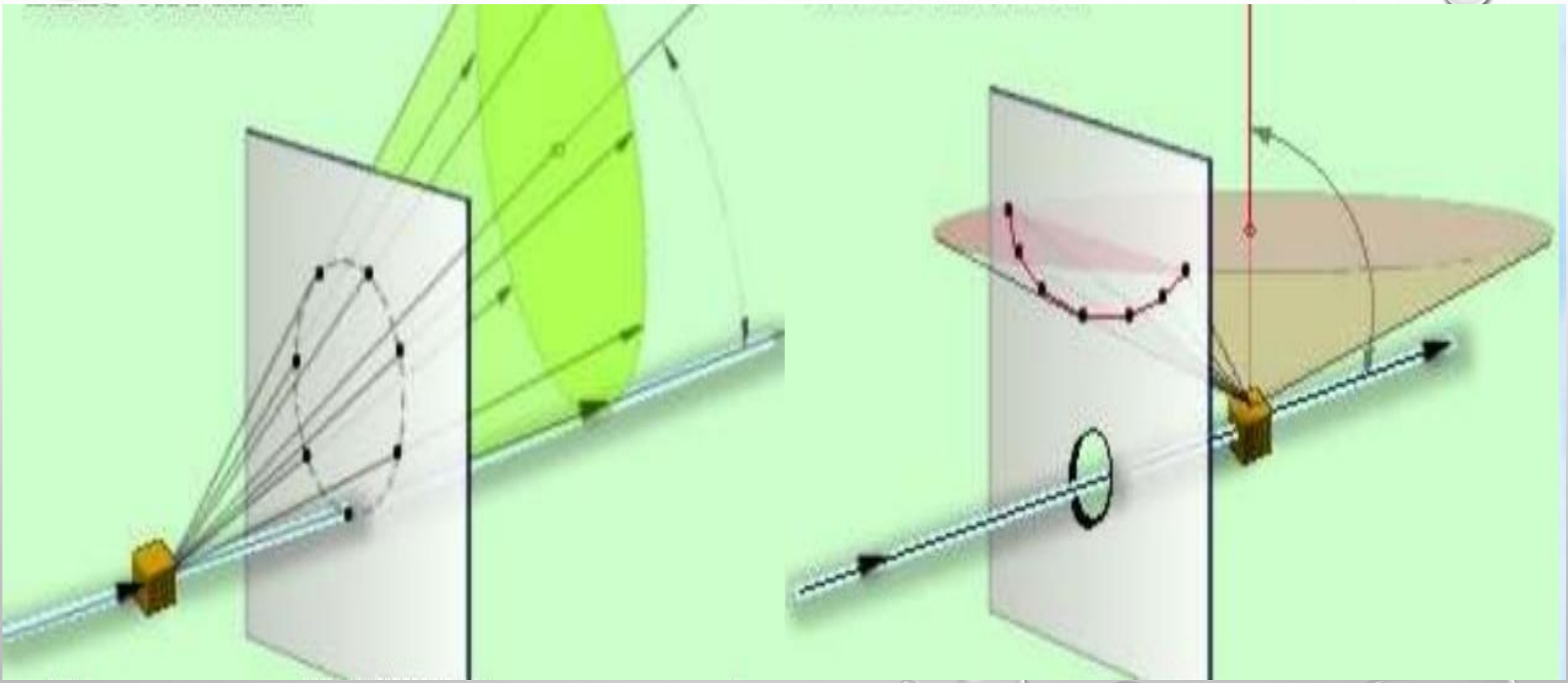
a. **Transmission Method**: In the transmission Laue method, the film is placed **behind** the crystal to record beams which are transmitted through the crystal. Leonhardt chart is used.

a. **Back Reflection Method**: In the back-reflection method, the film is placed **between** the x-ray source and the crystal. The beams which are diffracted in a backward direction are recorded.



Equipment for Laue's transmission method.

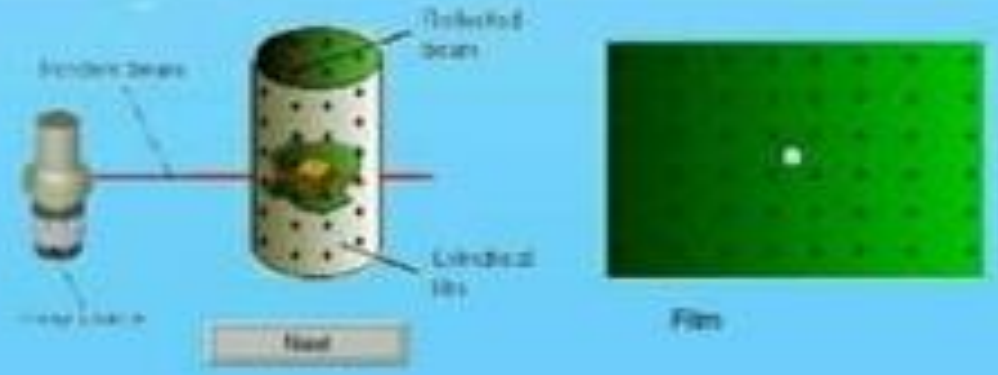
LAUE DIFFRACTION



ROTATING CRYSTAL METHOD

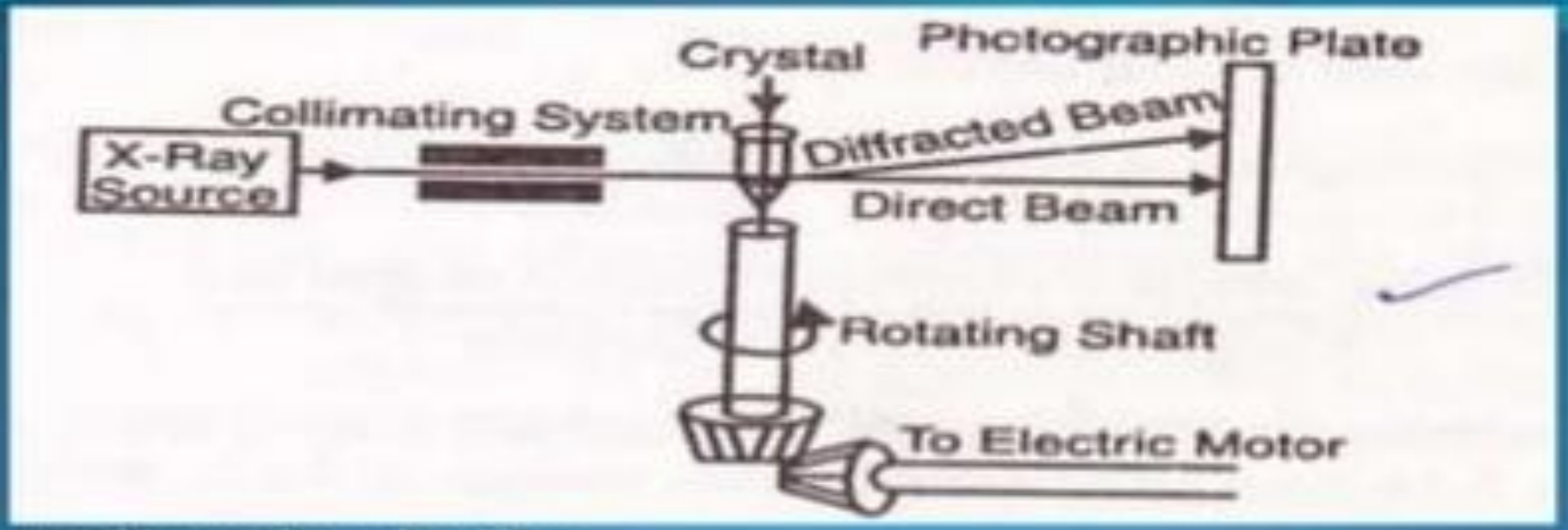
Rotating Crystal Method

The reflected beams are located on the surface of imaginary cones. By recording the diffraction patterns (both angles and intensities) for various crystal orientations, one can determine the shape and size of unit cell as well as arrangement of atoms inside the cell.



The **rotation method** is the most common **method** to determine steady state **crystal** structures. The orientation of the **rotation** axis and the **rotation** range can be chosen to select a subset of diffraction peaks fulfilling the Bragg condition $\Delta k = k - k = Hhkl(r,\varphi)$

ROTATING CRYSTAL METHOD:



Photographs can be taken by :

- 1.Complete rotation method:in this method series of complete revolutions occur
- Each set of a plane in a crystal diffracts four times during rotation
- Four diffracted beams are distributed into a rectangular pattern in the central point of photograph
- 2.Oscillation method:the crystal is oscillated at an angle of 15° or 20°
- The photographic plate is also moved vack and forth with the crystal
- The position of the spot on the plate indicates the orientation of the crystal at which the spot wasformed

POWDER DIFFRACTION METHOD

X-ray Powder Diffraction

- Diffraction is defined as the bending of light around or into the geometrical shadow of the obstacle.
- In powder X-ray diffraction, the diffraction pattern is obtained from a powder of the material, rather than an individual crystal.
- Powder diffraction is often easier and more convenient than single crystal diffraction as about 1 mg of material is sufficient for the study.

APPLICATIONS OF X-RAY DIFFRACTION

X-RAY DIFFRACTION IS USE FOR

- X-ray diffraction is used to obtain structural information about crystalline solids.
- Useful in biochemistry to solve the 3D structures of complex biomolecules.
- Bridge the gaps between physics, chemistry, and biology.

X-ray diffraction is important for:

- Solid-state physics
- Biophysics
- Medical physics
- Chemistry and Biochemistry