X-RAY DIFFRACTION

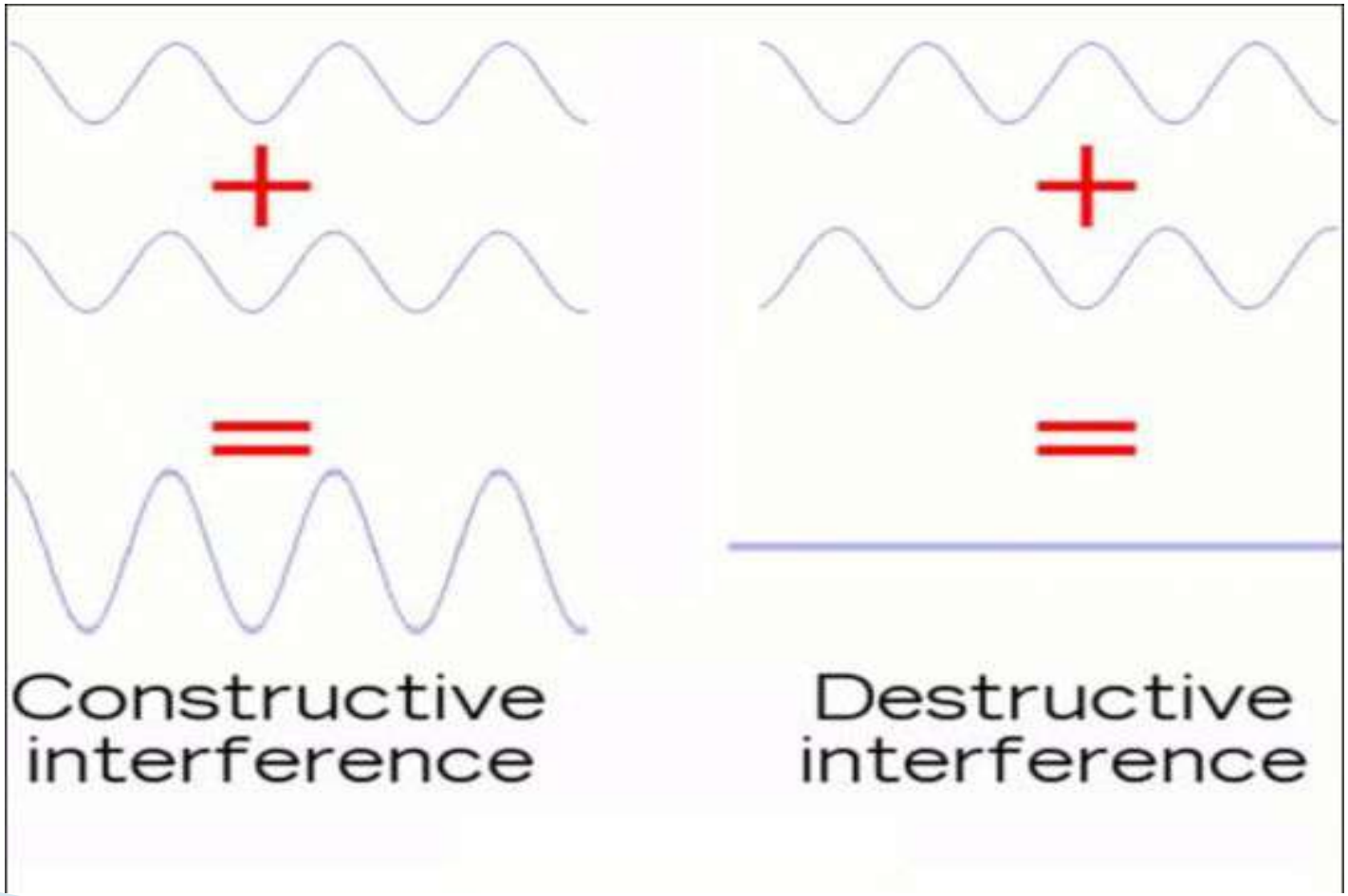
- Diffraction is when light bends slightly as it passes around the edge of an object or encounters an obstacle .
- X-Ray Diffraction is the scattering of X-Rays by atoms of a crystal that produces an interference effect so that the diffraction pattern gives information on structure of crystal and identifying of a crystalline substance.

HISTORY

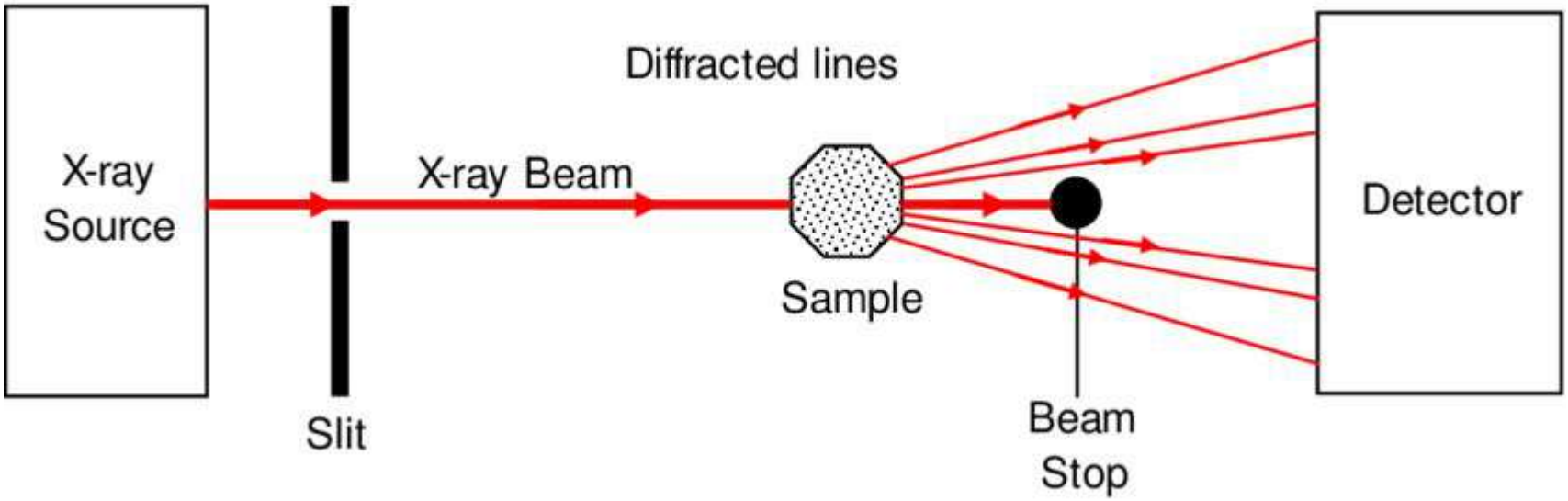
- 1895- X-Ray discovered by Roentgen
- 1912-First diffraction pattern of crystal made by Knipping and Von Laue.
- 1913- Theory to determine crystal structure from diffraction pattern developed by W.C.Bragg.
- 1953-DNA structure solved by Watson & Crick.
- Now-Diffraction improved by computer technology, methods used to determine atomic structureand in medical application.

PRINCIPLE

- For X-Ray to be diffracted the size of obstacle should be few angstroms(approx 1 angstroms) which is approx the wavelength of X-Ray.
- Thus for diffraction size of obstacle should be nearly equal to wavelength of light used.
- It is based on constructive interference of monochromatic X-Ray and crystalline sample.


Constructive interference
Destructive interference

INSTRUMENTATION



WORKING

- X-Rays are generated by cathode ray tube, filtered to produce
- monochromatic radiation, collimated to concentrate and directed towards sample.
- When monochromatic ray incident occurs on crystal.
- Atomic electrons in crystal are sent into vibration, with same frequency as that of frequency of incident ray and are accelerated.

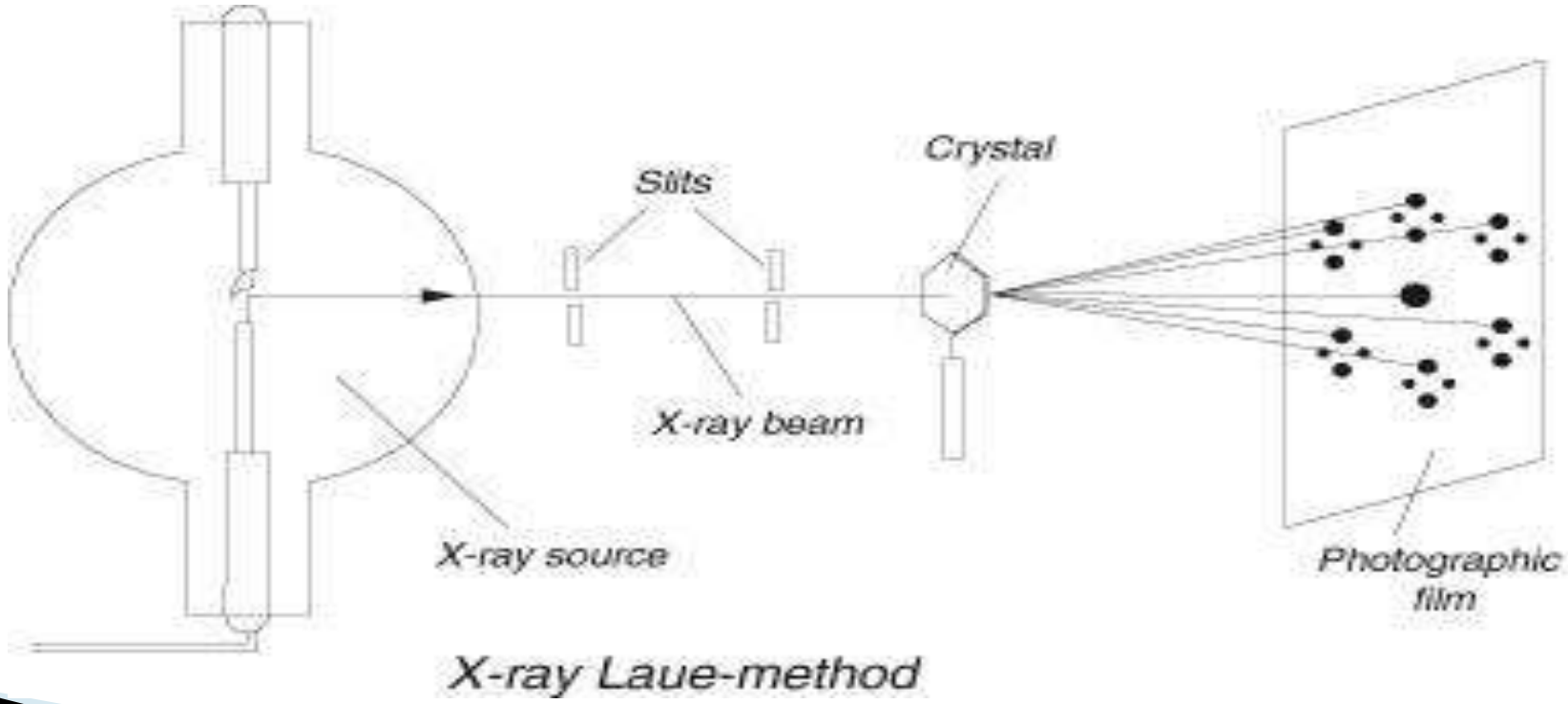
WORKING

- Accelerated electrons then emit the radiation of same frequency as that of incident X-Ray in all directions.
- If wavelength of incident radiation is large compared to the dimensions of crystal. Then the radiated X-Ray are in phase with each other.

- But since the atomic dimension are nearly equal to wavelength of X-Ray.
- The radiation emitted by electron is out of phase with each other.
- These radiation may interfere constructively or destructively producing a diffraction pattern (i.e. maxima and minima) in certain directions.

METHODS OF X-RAY DIFFRACTION

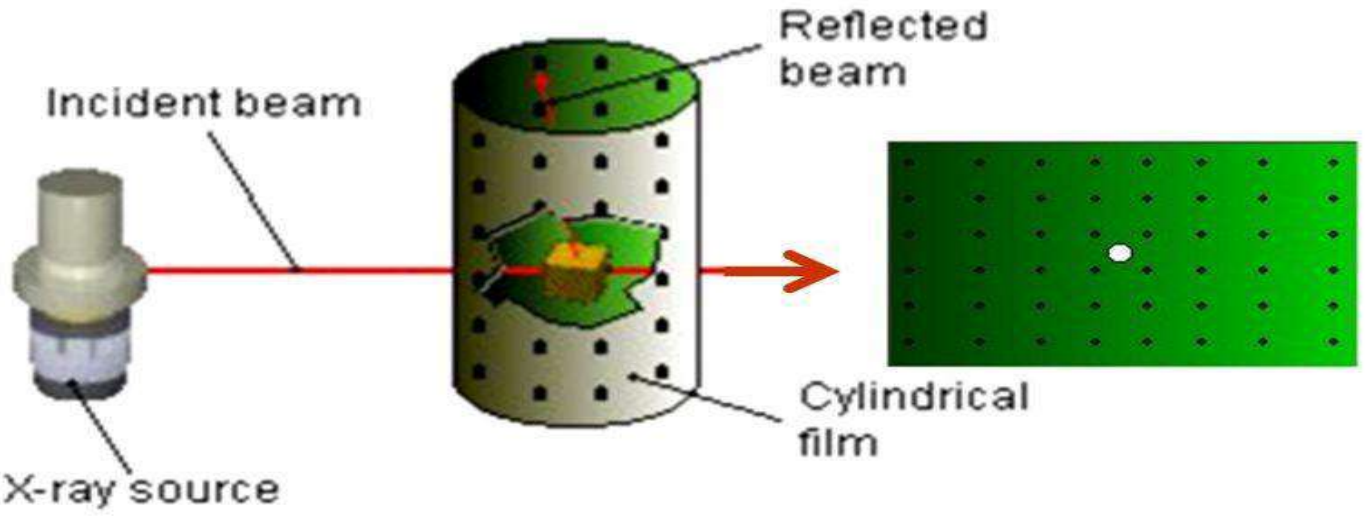
- LAUE METHOD



X-ray Laue-method

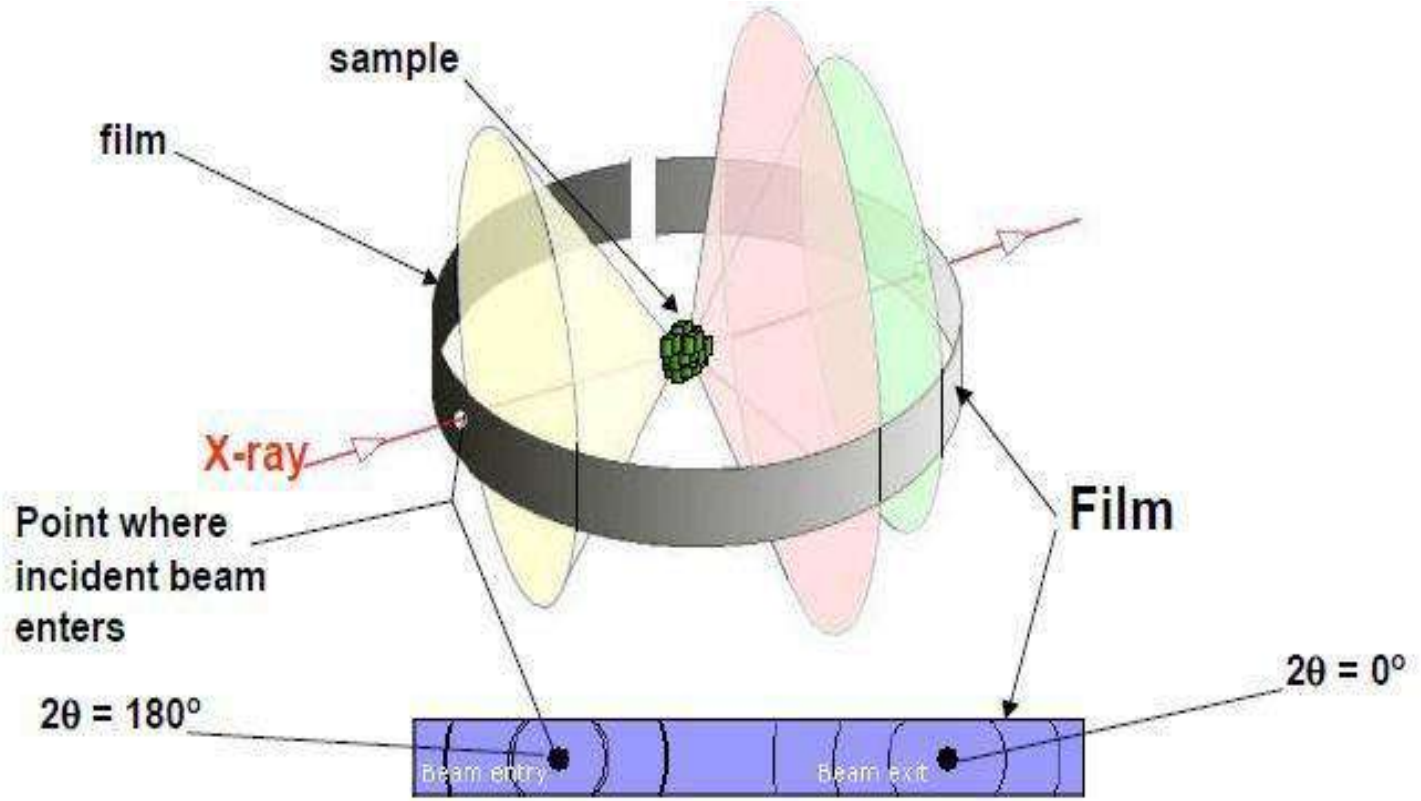
- ROTATING CRYSTAL METHOD

Rotating Crystal Method



- Determination of unknown crystal structures

- POWDER METHOD



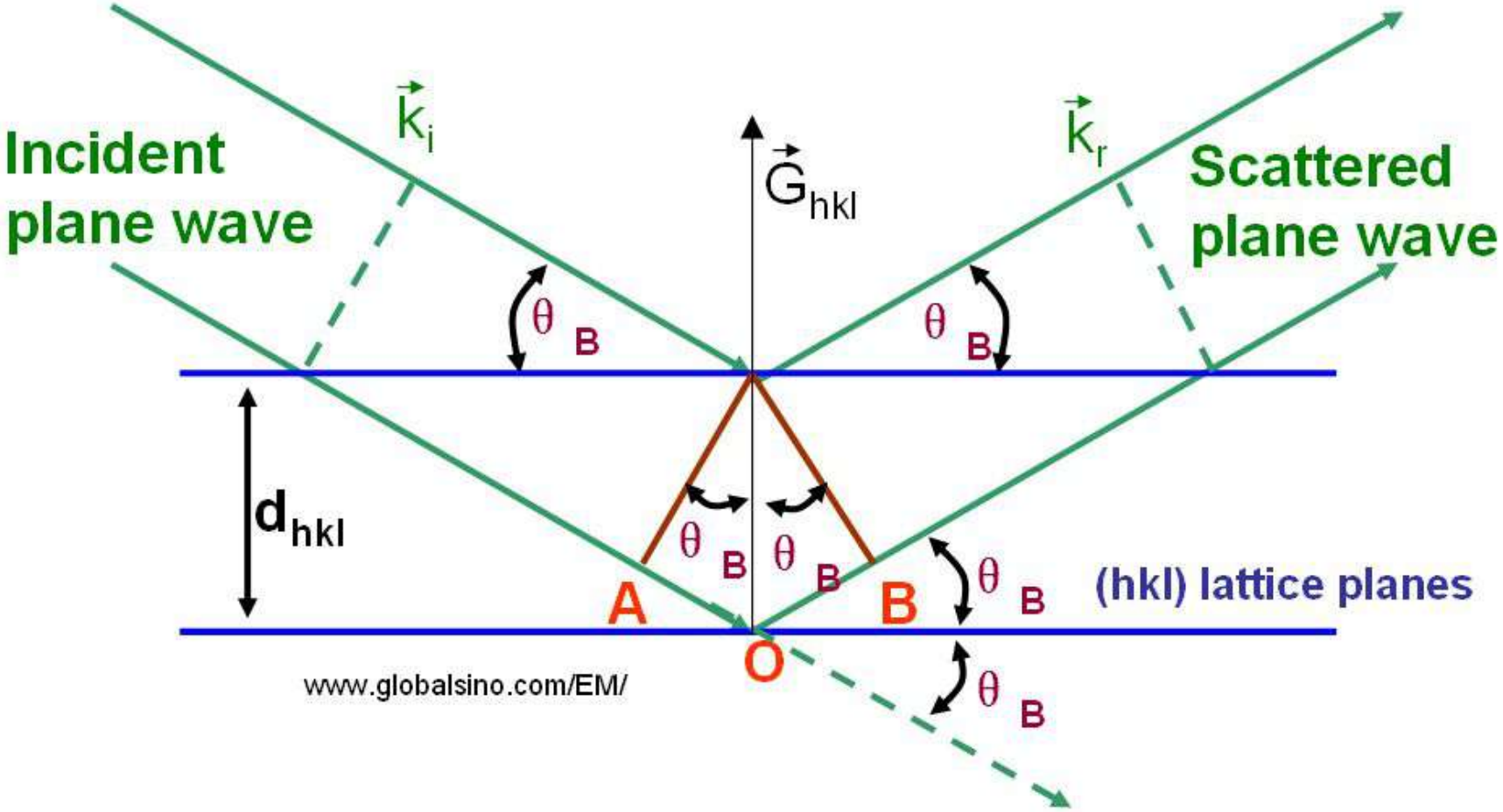
BRAGG'S LAW

- W.L. Bragg gives Bragg's law of diffraction i.e. **$2d\sin\theta = n\lambda$.**
- Diffraction will only occur if the way the x-Ray and substance interactaction meets the condition of Braggs law.

This require that

1. Angle of incidence = angle of scattering
2. The path length difference is equal to an integer no. of wavelength.

- This allows for a condition of max. Intensity which then enables a calculation about details of crystal structure concerned.


Incident
plane wave
$\vec{k}_i$
$\vec{G}_{hkl}$
$\vec{k}_r$
Scattered
plane wave
θ_B
θ_B
d_{hkl}
θ_B
θ_B
θ_B
θ_B
A
B
O
(hkl) lattice planes
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APPLICATIONS

- It helps in measuring avg. spacing between layers of rows of atoms in a substance.
- Identify crystal structure of an unknown substance.
- Measure size , shape and internal stress of small crystalline areas.

- For composition of material used in pharmaceuticals , industries.
- In forensic science use in trace analysis to detect very small amount substance.
- In glass production microelectronics, geological applications I.E. For identification of minerals in rock or soil and their proportion.

ADVANTAGES

- Rapid & powerful technique for identifying unknown minerals & materials.
- Only requires preparation of minimal sample for analysis.
- XRD measurements instruments are widely available.
- Interpreting the resulting data is relatively straight forward.

DISADVANTAGES

- To best identify an unknown powder material sample should be homogenous.
- XRD analysis requires access to standard reference data.
- Preparation of sample often require grinding them down to a powder.
- If crystal sample is non isometric then the indexing of patterns can be complex when determining unit cell.