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# Al-Mustaqbal University College

## Medical Physics Department

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DR. Aiyah Sabah Noori

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Out lines

Bragg's law

X-ray Diffraction

The method of x-ray diffraction

Electron diffraction

Neutron diffraction

## INTRODUCTION:

♣ On 8 Nov, 1895, Wilhelm Conrad Röntgen (accidentally) discovered an image cast from his cathode ray generator, projected far beyond the possible range of the cathode rays (now known as an electron beam).

♣ In 1912, Max Von Laue, showed that if a beam of X rays passed through a crystal, diffraction would take place and a pattern would be formed on a photographic plate placed at a right angle to the direction of the rays. This discovery provided a new method for investigating the fine structure of matter.

## BRAGG'S LAW:

♣ After few months, In 1913, English physicists Sir William Henry Bragg and his son Sir William Lawrence Bragg developed a relationship to explain why the cleavage faces of crystals appear to reflect X-ray beams at certain angles of incidence ( $\theta$ ).

♣ The variable  $d$  is the distance between atomic layers in a crystal, and the variable  $\lambda$  is the wavelength of the incident X-ray beam;  $n$  is an integer

♣ Although Bragg's law was used to explain the interference pattern of X-rays scattered by crystals, diffraction has been developed to study the structure of all states of matter with any beam.

♣ Bragg carried out a series of experiments, the result of which he published the Bragg equation

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

where, assume

$n = 1$  for the first order reflection

$\lambda$  = wavelength

$\theta$  = X-ray incidence angle

$d$  = distance between atomic layer

## Types of diffraction

1- X-ray diffraction

2- Electron diffraction

3- Neutron diffraction

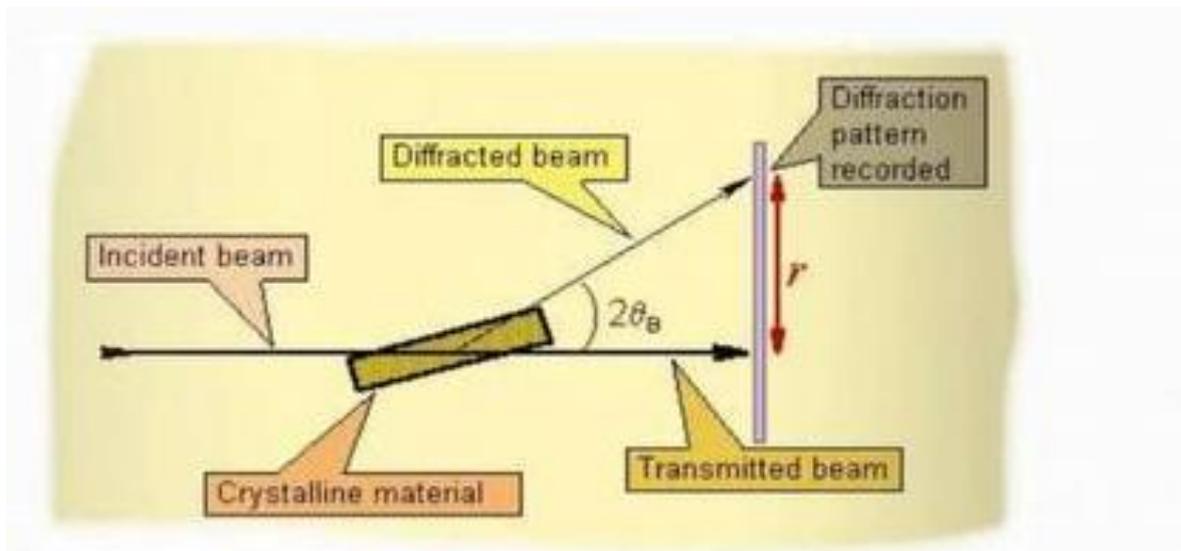
### **X-RAY DIFFRACTION:**

♣ X-ray powder diffraction (XRD) is a rapid analytical technique primarily used for phase identification of a crystalline material and can provide information on unit cell dimensions.

♣ To get the diffraction pattern from all parts of crystal, the primary beam must strike the crystal from many different directions. This is achieved by rotating the crystal in the beam during the experiment.

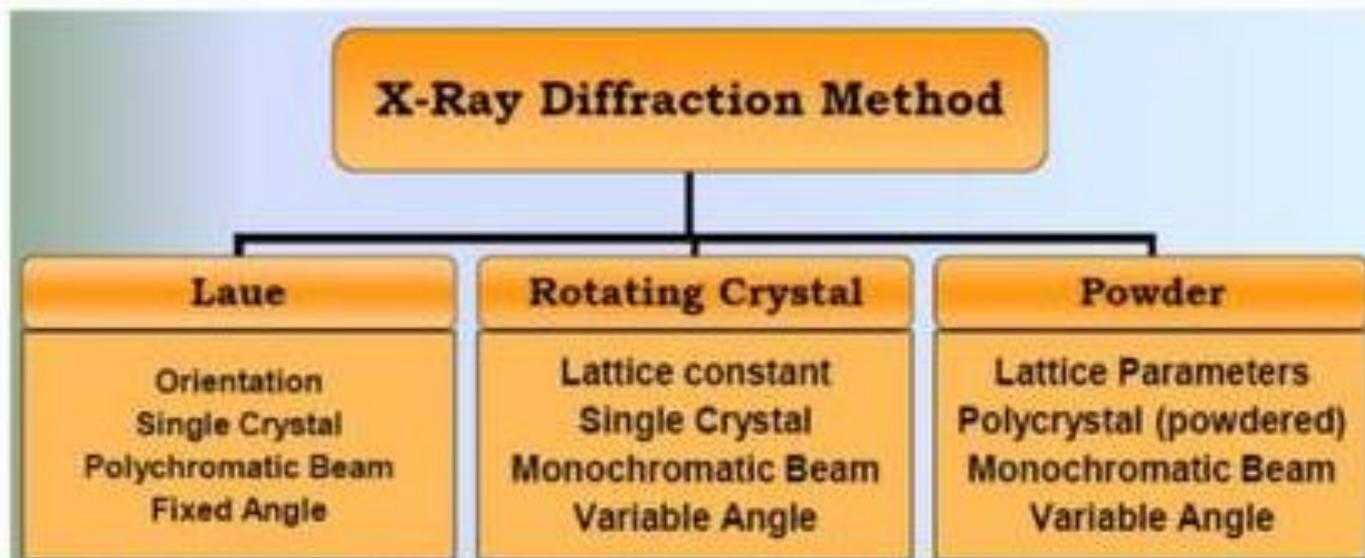
♣ The diffracted spots are recorded either on a film or by an electronic detector feed the signals directly in a digitized form into a computer. Several thousand diffraction spots are collected.

♣ All diffraction methods are based on generation of X-rays in an X-ray tube. These X-rays are directed at the sample, and the diffracted rays are collected



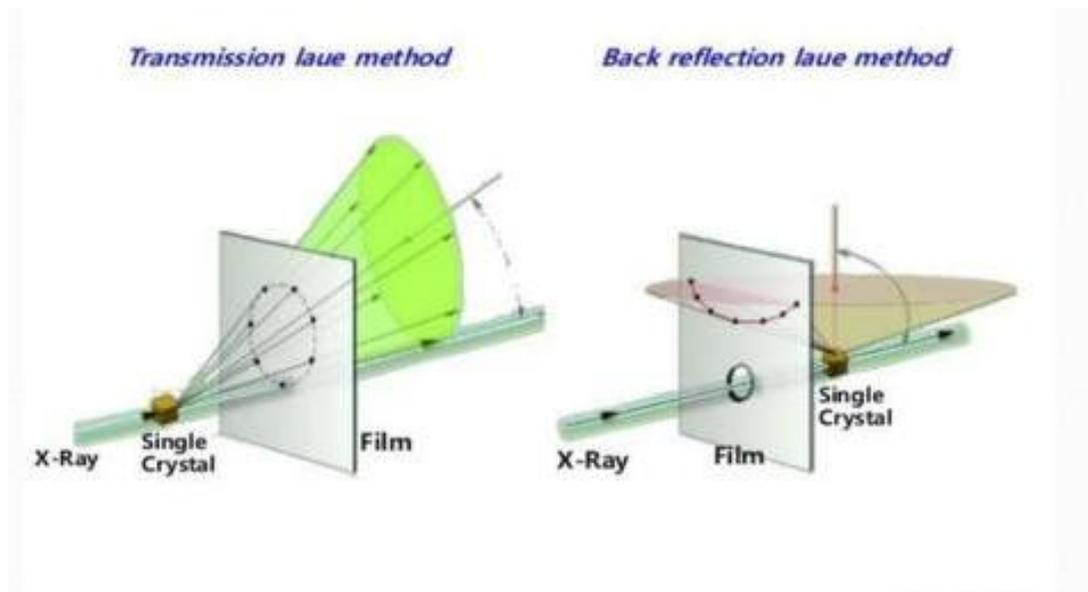
## X-RAY DIFFRACTION METHODS:

♣ Generally, there are three methods which is used for diffraction of X-ray. I. Laue method II. Rotating crystal method III. Powder method



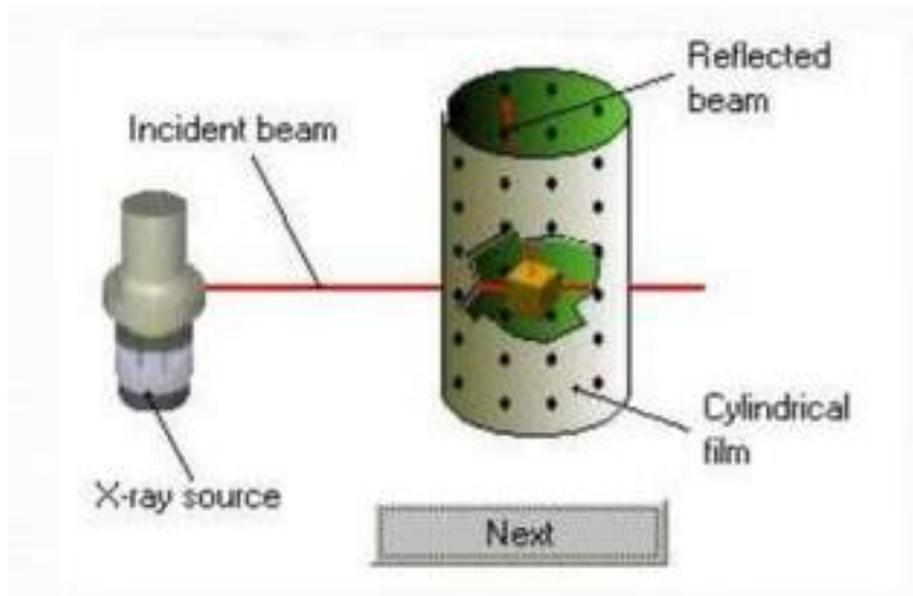
## 1) LAUE METHOD:

The Laue method is mainly used to determine the orientation of large single crystals while radiation is reflected from, or transmitted through a fixed crystal. The Bragg angle is fixed for every set of planes in the crystal. Each set of planes picks out and diffracts the particular wavelength from the white radiation that satisfies the Bragg law for the values of  $n$  and  $\theta$  involved.



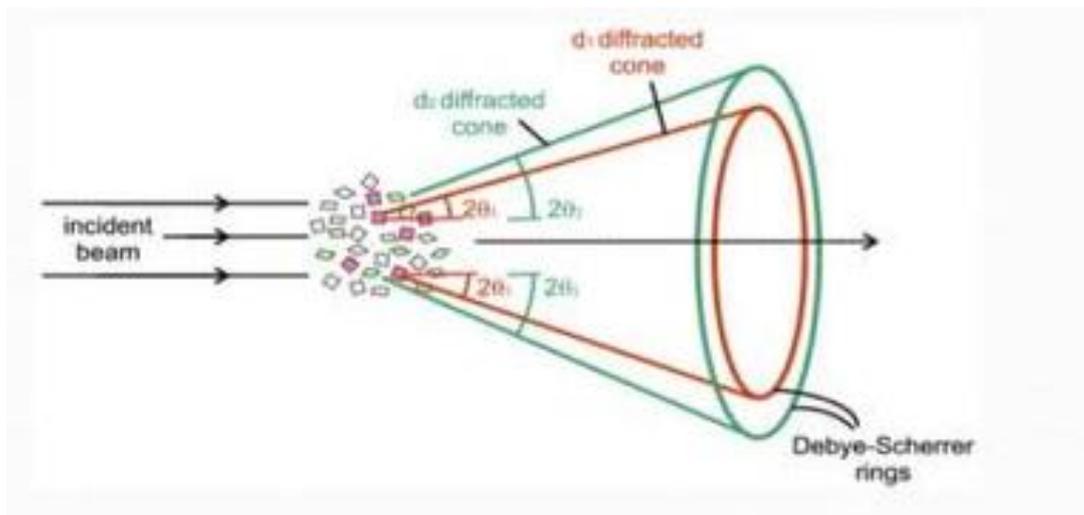
## 2) ROTATING CRYSTAL METHOD:

- ♣ In a rotating crystal method, a single crystal is mounted with an axis normal to a monochromatic X-ray beam. A cylindrical film is placed around it and the crystal is rotated about the chosen axis.
- ♣ As a crystal rotates, sets of lattice will at some point make the correct Bragg angle for the monochromatic incident beam, and at that point a diffracted beam will be formed.
- ♣ Lattice constant of the crystal can be determined by means of this method; for a given wavelength if the angle at which reflection occurs is known, can be determined.



### 3) POWDER METHOD:

If a powdered specimen is used, instead of a single crystal, then there is the specimen, because there will always be some crystals at an orientation for which diffraction is permitted. Here a monochromatic X-ray beam is incident on a powdered or polycrystalline sample. This method is useful for samples that are difficult to obtaining single crystal form.



## APPLICATIONS OF X-RAY DIFFRACTION:

- ♣ In material sciences, many complicated inorganic and organometallic systems have been analyzed using single-crystal and powder methods.
- ♣ In mineralogy and metallurgy, X-ray diffraction has been used for determining the arrangement of atoms in minerals and metals.
- ♣ X-ray diffraction is used to study the larger molecules, such as chlorophyll.
- ♣ XRD is used to solving the structures of various biological molecules, e.g., penicillin, insulin, cholesterol.

### The difference between the three types of diffraction

In X ray diffraction, diffraction takes place from the atomic planes of the interacting crystalline substance.

In electron diffraction, a beam of electrons interact with the atoms and molecules and this technique is primarily used especially the study of crystal structure.

In neutron diffraction, the beam of neutrons interact with the nucleus of the substances and help in the determination of atomic and magnetic structure.