

DEPARTMENT OF PHYSICS AND NANOTECHNOLOGY SRM INSTITUTE OF SCIENCE AND TECHNOLOGY

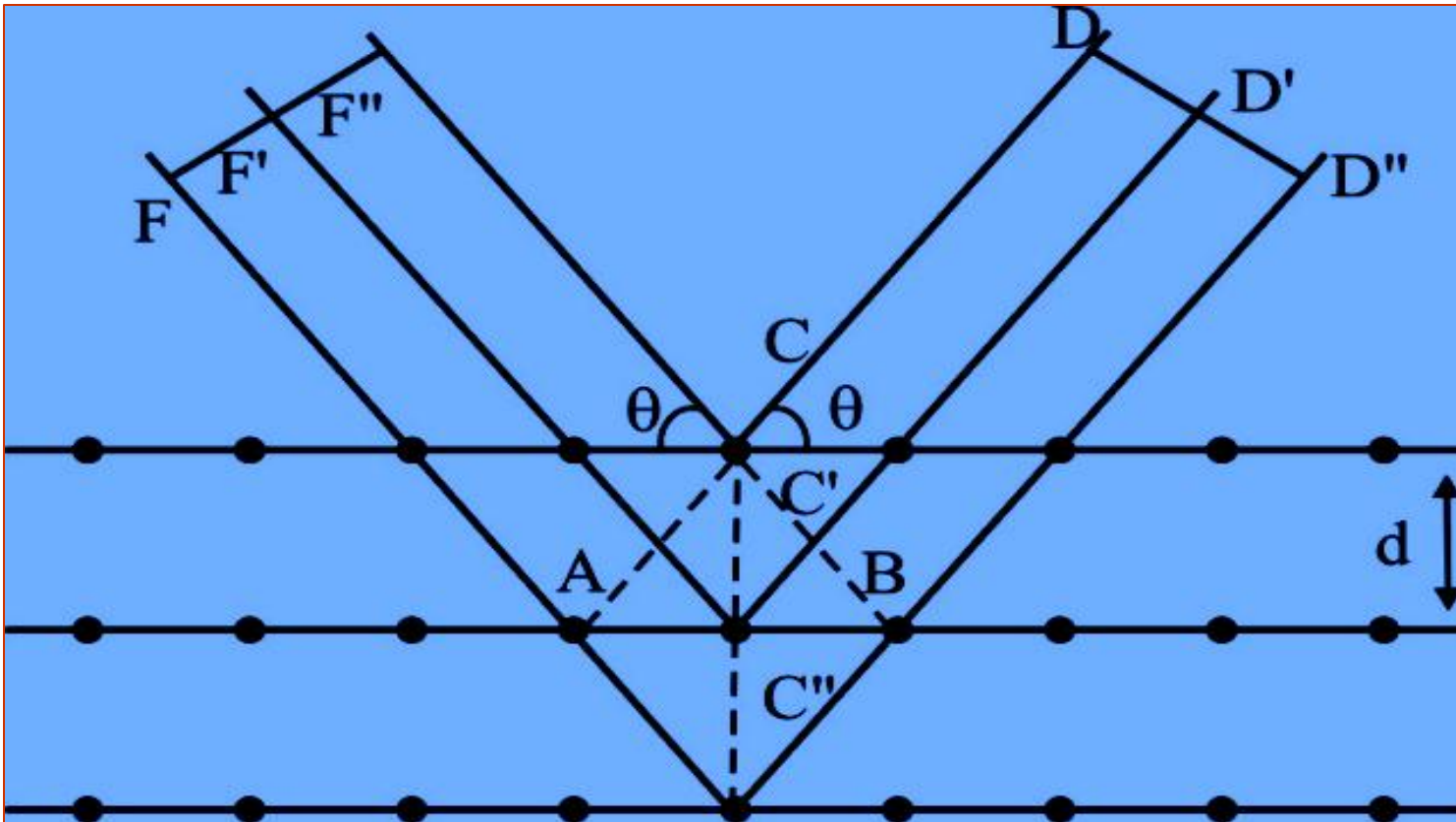
18PYB103J –Semiconductor Physics

Module-V Lecture-9

Characterization Techniques-X-Ray Diffraction-Powder Method

X-Ray Diffraction

- X-ray diffraction is used for the complete determination of molecular structure of crystals.
- Every lattice plane in a crystal behaves like diffraction grating, on the exposure of X-rays.
- The position of the spectral lines when diffracted depends on the distance between successive lines; similarly the nature of the X-ray diffracted by a crystal is determined by the spacing between successive planes.



If a beam of monochromatic X-rays is incident on a crystal at an angle θ , some of the rays will be diffracted by the layers of atoms in the crystal.

The path length $FC'D$ is larger than FCD by $AC'B$ which is equal to $2AC'$, and since $AC' = d\sin\theta$, the path difference is $2d\sin\theta$.

This difference in path length must be an integral number (n) of wavelengths (λ) for maximum diffraction of X-rays with destructive interference. Thus

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

which is the **Bragg's equation**.

With the help of the Bragg's equation it is possible to determine the spacing d between successive lattice planes, if λ is known and θ is measured.

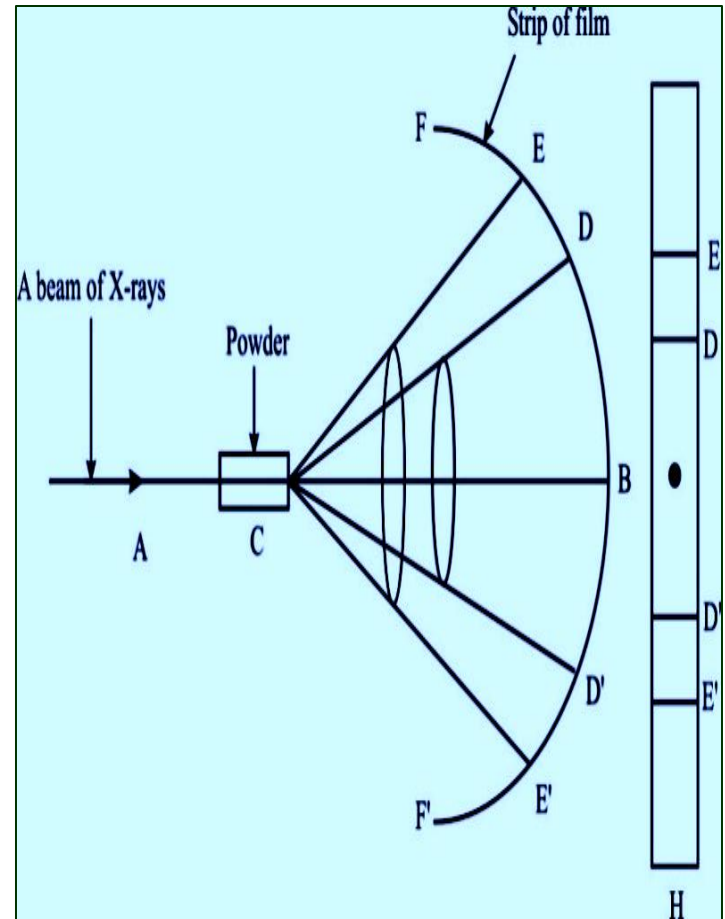
The powder method:

➤ A narrow beam of monochromatic X-rays fall on the finely powdered specimen to be examined, and the diffracted rays are passed on to a strip of film which almost completely surrounds the specimen.

➤ The random orientation of crystals produces diffraction rings.

➤ This method is commonly used for identification purposes by comparing the data with the standard files available.

➤ For a cubic crystal the identification of lines in the powder photograph is simple compared to other types.



Application of XRD

- ☀ XRD is a nondestructive technique
- ☀ To identify crystalline phases and orientation
- ☀ To determine structural properties: Lattice parameters (10-4Å), strain, grain size, phase composition.
- ☀ To measure thickness of thin films and multi-layers
- ☀ To determine atomic arrangement