XRD(X- RAY DIFFRACTION)

XRD : XRD is a technique that uses X-rays to determine the structure of a material.

- It is a powerful technique to identify the crystalline phase present in a material and to measure the phase composition, preferred orientation, grain size, strain size, and defect structure of these phases.
- Some fundamental techniques like Bragg's law, Powder method, Sherrer's formula are used to determining crystal structure and size of crystal based XRD.

Principle:

- The principle of XRD is based on constructive interference by X-rays and the crystalline structure of a material & Bragg's law.

Construction / Experimental arrangement:

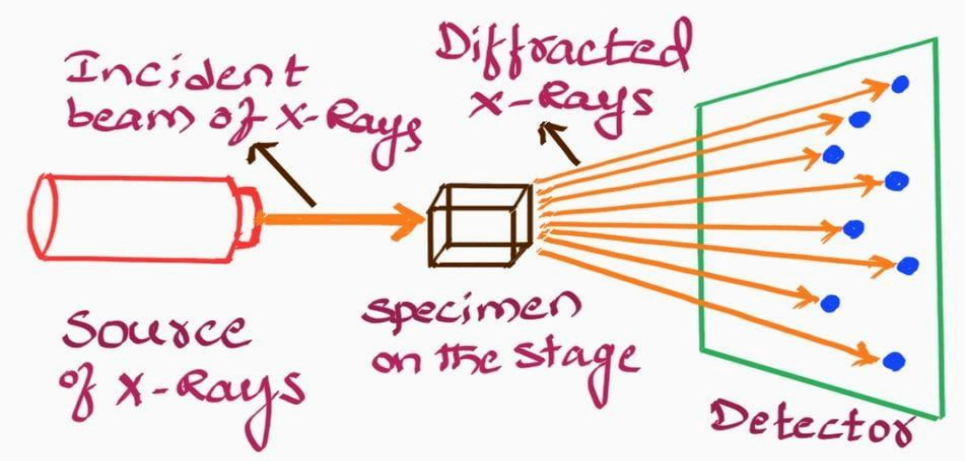
- XRD instrumentation consists of 4 main components such as

  (i) Source of X-rays

  (ii) Specimen stage (crystal)

  (iii) Diffracted X-rays and

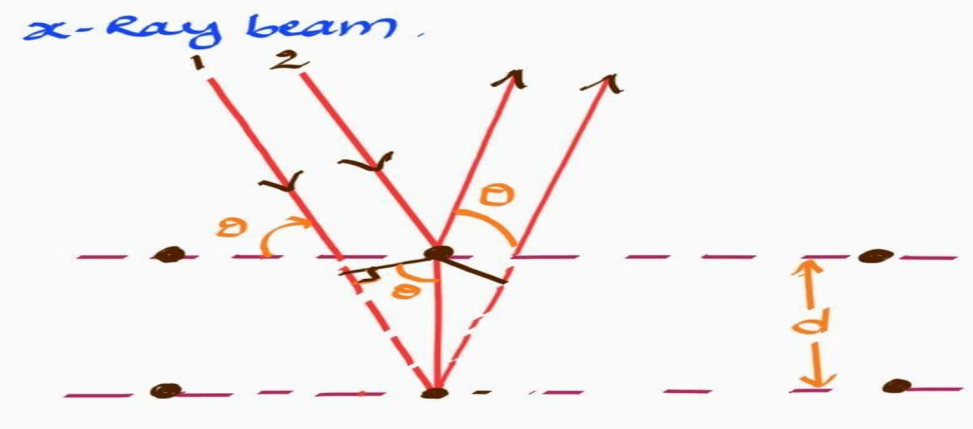
  (iv) Detector.



Working process:

- A beam of X-rays of wavelength λ is directed to the crystal by the source, at an angle θ to the atomic planes.

- The interaction between X-rays and the electrons of the atoms is visualized as a process of X-rays reflections by the atomic planes.
- The atomic planes allow a part of the X-rays to pass through and reflect the other part, the incident angle θ being equal to the reflected angle called Bragg's angle. There is a path difference between rays reflected from plane 1 and the adjacent plane 2 in the crystal.
- The two reflected rays will reinforce each other only when this path difference is equal to an integral multiple of the wavelength λ.
- If d is the interplanar spacing, the path difference is twice the distance dsinθ.



Analysis: XRD analysis is based on Bragg's Law and Bragg's angle.

- Bragg's Law given by $n\lambda=2d\sin\theta$

Where: n→ An integer

λ→ wavelength of X-rays

θ→ The diffraction angle

APPLICATIONS:

- Phase Identification in nanomaterials, nanoparticles, nanowires and thin films by XRD
- Crystal structure analysis is used to understand the physical, chemical properties of nanomaterials and their behaviour by XRD
- Grain size & Strain analysis of nanomaterials by XRD
- Texture analysis & Preferred orientation of crystalline grains in nanomaterials by XRD
- Quantitative phase analysis of phase abundance in nanomaterials is valuable for assessing phase purity, phase transformation etc by XRD
- Stress & Texture mapping done by XRD techniques, provides local structure property relationships and investigate defects etc
- Catalysis & Energy materials are developed by XRD, in battery electrodes, photovoltaic devices, catalyst nanoparticles etc.