

## X – Ray Diffractometer

**Make:** Rigaku  
**Model:** ULTIMA IV

**Purpose:** Structural and phase analysis of powder as well as thin films (GI-XRD mode).

This instrument is used for

- Identification of single or multiple phases in materials
- Quantification of known phases of a mixture
- crystal structure information
- Surface and thin film analysis

### Working Principle:

When a crystalline sample is irradiated with X-rays, the constituent atoms scatter X-rays spatially in all directions. If the path difference of X-rays, scattered in a particular direction, from atoms in adjacent planes is integral multiple of the X-ray wavelength they interfere constructively and lead to a high intensity peak. This is expressed by a simple mathematical formulation which was enunciated by W.H Bragg and is given by

$$2d_{hkl} \cdot \sin \theta = n\lambda$$

Where  $d$  is the inter-planar spacing,  $(hkl)$  are miller indices,  $\lambda$  is the X-ray wave length,  $\theta$  is the angle between sample surface and incident X-rays and  $n$  is the order of reflection. The above expression imposes a condition that,  $\lambda \leq 2d$  i.e. the wave length of X-rays should be comparable to the interplanar spacing. X-ray diffraction data provides, phase information, basic crystal lattice information i.e. lattice parameters, atom positions in the crystal, crystallite size and strains present in the materials.

### Major Applications

Materials Science (Powder/Thin films)  
Pharmaceuticals  
Minerals  
Polymers

Metals  
Forensics  
Rocks  
Zeolites

