Experimental method of determining Crystal structure.

X-ray diffraction and Bragg's Equation: Crystal structure has been obtained by studying on the diffraction of X-rays by solids. A crystal, having constituents particles arranged in planes at very small distances in three dimension array, acts as diffraction grating for X- rays which have wavelengths of the same order as the spacing in crystal.

When a beam of X-rays passes through a crystalline solid, each atom in the beam scatters some of the radiations. If waves are on same phase means if their peak and trough coincides they add together to give a wave of greater amplitude. This enhancement of intensity is called constructive interference. If waves are out of phase, they cancel. This cancellation is called destructive interference.

Thus X- ray diffraction results from the scattering of X-rays by a regular arrangement of atoms or ions.

Bragg's equation: Study of internal structure of crystal can be done with the help of X-rays. The distance of the constituent particles can be determined from diffraction value by Bragg's equation,

$n\lambda = 2d \sin\theta$ Where, λ = Wave length of X-rays, n = order of diffraction,

$\theta =$ Angle of reflection, d = Distance between two parallel surfaces

The above equation is known as Bragg's equation or Bragg's law. The reflection corresponding to n = 1 (for a given family of planes) is called first order reflection; the reflection corresponding to n = 2 is the second order reflection and so on. Thus by measuring n (the order of reflection of the X-rays) and the incidence angleθ, we can know d/λ.

$$\frac{d}{\lambda} = \frac{n}{2\sin\theta}$$

From this, d can be calculated if λ is known and vice versa. In X-ray reflections, n is generally set as equal to 1. Thus Bragg's equation may alternatively be written as

$$\lambda = 2\,d\,\sin\theta = 2\,d_{hkl}\sin\theta$$

Where dhkl denotes the perpendicular distance between adjacent planes with the indices hkl.