Application of Bragg's Law in Crystallography

- Wavelength of X-rays is nearly same order of magnitude as is the separation between two atoms in a given crystal
- So X-ray diffraction is best suited to study the structure and symmetry of crystals
- Bragg's law for diffraction of X-rays : $2d\sin\theta=n\lambda$
- Only those wavelengths can be diffracted from a crystal which will satisfy this equation
- Only a particular combination of d, θ and λ will satisfy this eqn.
- To check for various possible combinations, d, θ and λ are varied, one at a time so that Bragg's law is satisfied and diffraction occurs.
- Depending on which parameter is to varied, following three method are usually followed to study the crystal structure:
  1. **Laue Method:** Crystal is kept fixed and wavelength of X-rays (λ) is varied continuously. Crystal itself (based on Bragg's law) will select particular wavelength and diffract X rays made incident at specific value of θ.
  2. **Rotating Crystal Method:** In this method, instead of changing the value of wavelength, crystal itself is continuously rotated about a fixed vertical axis, which will change the orientation of the crystal regularly. When monochromatic X-rays are made incident on continuously rotating crystal, then X-rays will strike the particular atomic plane of crystal at a continuously changing value of angle θ. Only for a particular combination of θ and d, Bragg's equation will satisfy and hence diffraction will take place.
  3. **Powder Method:** in this method, specimen is used in the powdered form (polycrystalline). These crystallites and hence various sets of atomic planes are oriented randomly. When monochromatic X-rays are made incident on the sample, only a particular set of planes having specific value of d and θ will select wavelengths to be diffracted at an angle 2θ in accordance with Bragg's Law. The output of these diffracted rays will lie on a surface of cone with semi-vertical angle 2θ. Similarly other sets of planes with different values of d and θ will diffract X-rays and the output will lie on the surfaces of various cones.

     The analysis of the output thus obtained can lead to the determination of d and θ and thus crystal structure can be analyzed.