X-ray Diffraction

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1 Bragg's Law

X-rays like other electromagnetic waves, interact with the electron cloud of the atoms. Because of their shorter wavelengths, X-rays are scattered by adjacent atoms in the crystal which can interfere and give rise to diffraction effects. When X-rays enter into a crystal each atom acts as a diffraction center and crystal as a whole acts like a three dimensional diffraction grating. The diffraction pattern so obtained can tell us about the internal arrangement of atoms in the crystal.

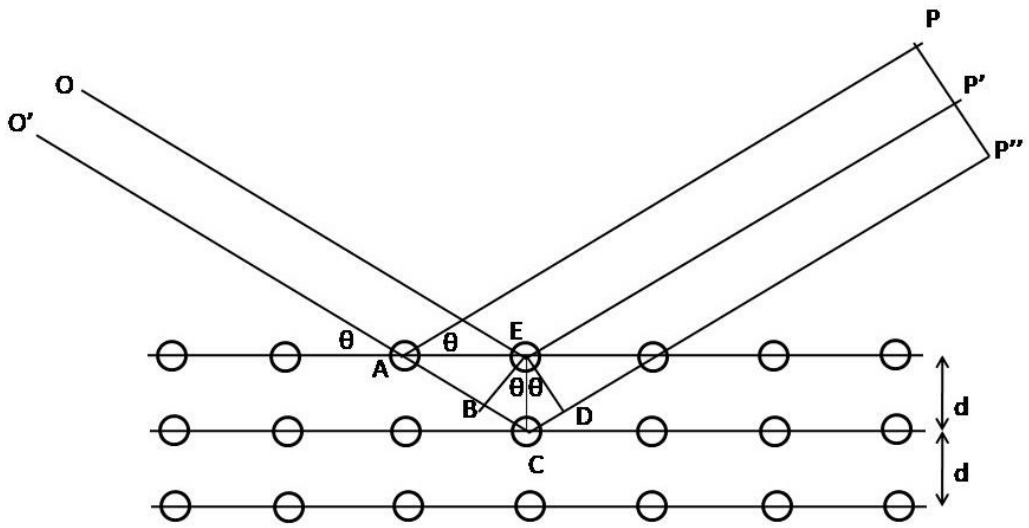

Figure 1: Beams reflected from successive planes interfere constructively only if BC+CD is an integral multiple of wavelength

Consider a crystal made of equidistant parallel planes of atoms with inter-planar spacing ‘d’. Consider a monochromatic X-ray beam of wavelength λ having a common wavefront, falls at an angle θ on these planes. Each atom scatters the X-rays more or less uniformly in all directions, but because of the periodic arrangement of atoms, the scattered radiation from all atoms in a set of planes is in phase in certain directions only where they interfere constructively. In all other directions they interfere destructively.

Consider two of incoming X-rays OE and O′A inclined at an angle θ with the topmost plane of the crystal and are scattered in the directions AP and EP’, also at an angle θ with that plane. Since the path lengths OEP′ and O′AP are the same, they arrive at P and P′ respectively in phase with each other and again form a common wavefront.

In order to see the effect of adjacent plane, consider incoming beam O′C and scattered ray CP″. If EB and ED are parallel to incident and scattered wavefront respectively, then the total pat O′CP″ is larger than the path OEP′ or O′AP by an amount

$\triangle = BCD = 2BC$

From right $\triangle BCE$, we have $BC = d\sin\theta$

$$\therefore \triangle = 2BC = 2d\sin\theta \tag{1}$$

If the two consecutive planes scatter in phase with each other then the path difference $\triangle$ must be equal to an integral multiple of wavelength.

i.e. $\triangle = n\lambda$ where n=0,1,2,3,. . . gives the order of reflection.

Thus the condition for in phase scattering by a set of equidistant parallel planes in a crystal is given by

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

This equation is known as Bragg’s law after W.L. Bragg who first derived it. The Bragg’s equation can be used to find the wavelength of an X-ray beam if we observe the diffraction pattern from any known crystal. If the interplanar spacing of the crystal is known, observing the angle of diffraction, and substituting the values in Bragg’s equation gives us the value of the wavelength of X-ray beam used in the diffraction.

A further note from the above equation $(\sin\theta)_{max} = 1$

$$\therefore \frac{n\lambda}{2\theta} \leq 1 \tag{3}$$

This indicates that λ must not be greater than twice the interplanar spacing, otherwise no diffraction will occur.

2 Diffraction of X-rays according to von Laue

When an electron is subjected to a monochromatic beam of X-rays, the electric field vector of the radiation forces it to carry out vibrations of a frequency equal to that of the incident beam. As a consequence of the acceleration of the electron, it in turn emits radiations of the same wavelength in all directions. Thus in an atom all electrons contribute to the scattering of X-rays in this manner.

Consider a one dimensional row of atoms with interatomic distance 'a'. Even though the individual atoms scatter radiation in all directions, there are only few directions in which these wavelets reinforce each other.

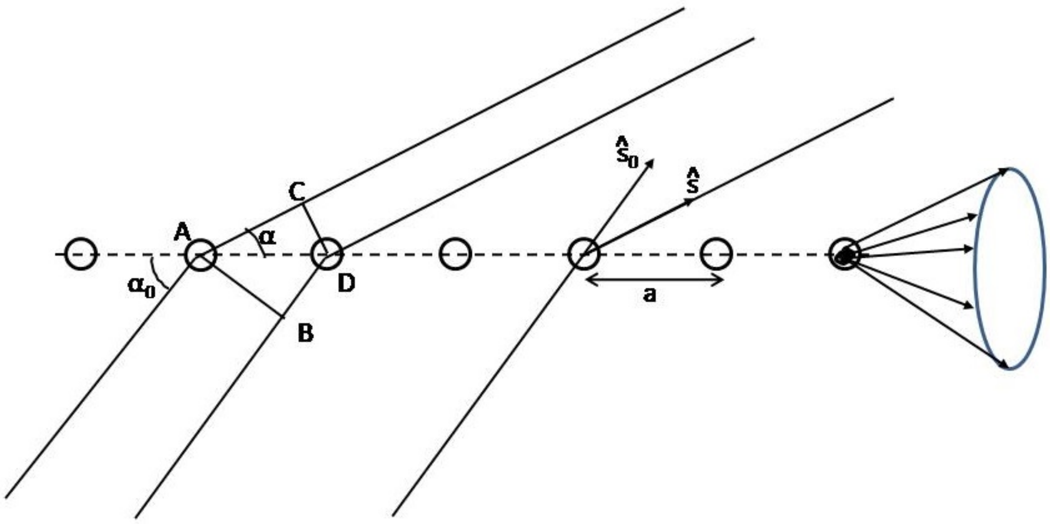

Figure 2: For reinforcement AC-BD should be integer times wavelength, $\hat{s_0}$ and $\hat{s}$ are unit vectors in the direction of incident and diffracted beams respectively

Suppose AB is a wave crest of incident beam and CD is a wave crest of diffracted beam. Diffracted beam is observed only if the path difference (AC-BD) shall be an integer times the wavelength of the beam. Thus a diffracted beam is observed only if

$$a(\cos\alpha - \cos\alpha_0) = e\lambda \text{ with } e = 0, 1, 2, 3\ldots \tag{4}$$

For a given value of α_0, a, λ and e there is only one possible value of α. Such a value exists only if at the same time $\cos\alpha \leq 1$.

Suppose then that to a certain value of e there corresponds a value α. The direction of diffracted beam then forms a cone of directions with the row of atoms as its axis. Thus a monochromatic X-ray beam falling on a row of atoms gives rise to a family of cones representing the direction of diffracted beams. Above equation can also be written in vector notation; if $\overrightarrow{S_0}$ and $\overrightarrow{S}$ represent unit vectors, respectively in the direction of incident and scattered beam and if $\overrightarrow{a}$ represents the translation from A to D, then

$$\overrightarrow{a}.(\overrightarrow{S} - \overrightarrow{S_0}) = e\lambda \tag{5}$$

For a two dimensional lattice two equations of the type of equation 5 are required to be satisfied giving rise to a set of two cones and diffracted beam will occur only in the directions in which the two cones superpose which will be the direction in which both conditions are satisfied.

The conditions become more stringent in the three dimensional lattice, which requires the satisfaction of three equations of the type of equation 5, giving rise to a set of three cones. The diffracted beam can be observed only along the directions in which all the three cones meet simultaneously. Consider a simple space lattice with unit cells defined by the primitive translation vectors $\overrightarrow{a}, \overrightarrow{b}$ and $\overrightarrow{c}$. Then for the diffraction to occur, the following equations for the path differences must be satisfied:

$$\begin{aligned} a(\cos\alpha - cos\alpha_0) &= \overrightarrow{a}.(\hat{s} - \hat{s_0}) = e\lambda \\ b(\cos\beta - \cos\beta_0) &= \overrightarrow{b}.(\hat{s} - \hat{s_0}) = f\lambda \\ c(\cos\gamma - \cos\gamma_0) &= \overrightarrow{c}.(\hat{s} - \hat{s_0}) = g\lambda \end{aligned} \tag{6}$$

where e,f and g are integers; α_0, β_0, γ_0 and α, β and γ represent the angles between the incident and scattered beams with the axes $\overrightarrow{a}$, $\overrightarrow{b}$ and $\overrightarrow{c}$. These are known as **von Laue** equations. It is to be noted that for a monochromatic X-ray beam,it is not possible to get diffraction pattern in general for a any direction of incidence due to the restrictions made by the three Laue equations (eqn. 6).