2

Diffraction of X-rays by Crystals

X-rays can be diffracted by crystals just in the same way as the visible light is diffracted by a diffraction grating ; in other words, we can say that crystals can be used as diffraction gratings for the diffraction of X-rays. This important concept was first conceived by Von Laue in 1912, and subsequently tested by Freidrich and Knipping who demonstrated that an X-rays beam passing through a single crysta was indeed broken up into a collection of diffracted beams. Our immediate goal with the diffraction o these rays by crystals is only in connection with the direct exploration of the interior of the crystals ; tha is, in connection with the fixation of the positions of the atoms on the crystal lattice, the measurement c distances between atoms and the associated internal symmetry. Such a study is possible because of th fact that the intensities of diffracted beams and their directions are related to the atomic arrangement i crystals. Thus, measurements of their intensities and directions would provide the desired informatic about crystals. It is in this sense a very important chapter. Moreover, it is so because the X-ray diffractic represents a wave propagation in a periodic structure— a problem of central importance in solid sta physics. The concepts developed in this chapter can, therefore, be carried over to other forms of wa (*e.g.* electromagnetic waves, elastic waves, electron waves) propagation in crystalline (that is, periodi solids. The principle of diffraction will now be discussed.

To start with, consider the influence of the X-rays on an atom. When the atom is exposed to monochromatic beam of X-rays, the electric field vector of the radiation forces its electrons to carry out harmonic vibrations of a frequency equal to that of the incident beam and thus to undergo acceleration. These accelerated charges in turn re-emit the radiation at the frequency of their vibration, that is, at the incident wave frequency. The emitted wave have a spherical wavefront centered about the atom, so the energy goes off in all directions. Now, since in a crystal we are concerned with a group of atoms arranged in a regular pattern, let us next consider a row of identical atoms upon which there falls a plane X-ray wave normally, according to fig. 1. Each atom of the row emits radiation in the manner explained

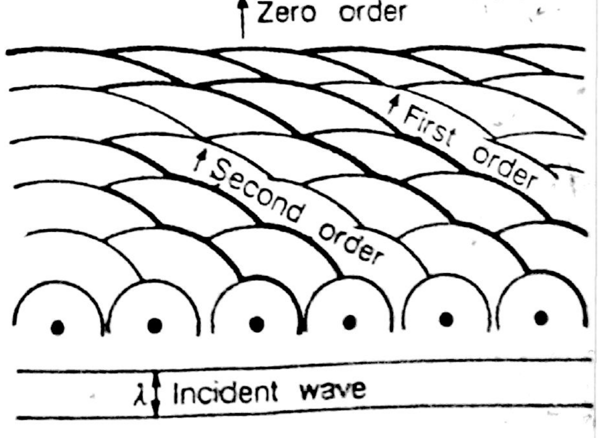

Fig. 1. Reinforcement of scattered waves producing diffracted beams of different orde

above. Assuming the incident wave crests to be parallel to the row of atoms, the envelope of the wavelets emitted by individual atoms forms new wave crests and we see that besides a beam propagated in the same direction as the incident beam, there are beams in few other (specific) directions also. Thus, although the individual atoms scatter (re-emit) radiation in all directions, there are only a few directions in which these wavelets reinforce each other to produce plane waves. These waves are said to be produced by diffraction and are designated as zero order, first order, second order, etc., diffracted beams.

The problem of a row of atoms was considered only for simplicity. Actual crystals, however, are not hypothetical linear array of fig. 1 ; they have three-dimensional character. The principle consequence of the additional two dimensions is that additional geometrical conditions must be satisfied before a given incident wave can be diffracted, making the geometry of diffraction more restrictive. There are two ways of calculating the conditions of diffraction in actual crystals : that due to Bragg and that due to Von Laue. Both are informative and will be discussed.

The Bragg Treatment

W. L. Bragg investigated the conditions for *X*-ray diffraction by means of a model which gives the correct mathematical results in a very simple way. He found that the directions of diffracted beams can be accounted for by making the assumption that the *X*-rays are specularly (*i.e.* mirror-like) reflected from parallel atomic planes in the crystal and the multiple reflections interfere constructively in those directions. It is common practice, therefore, to interchange the words diffraction and reflection of *X*-rays.

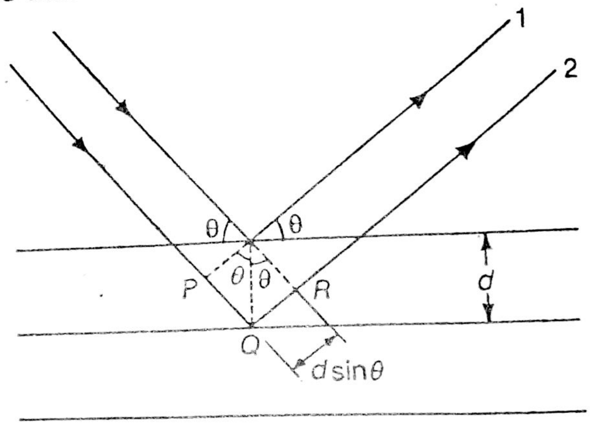

Fig. 2. Geometry for the derivation of the Bragg equation $2d \sin \theta = n\lambda$; here d is the spacing of parallel atomic planes and $2n\pi$ is the difference in phase between reflections from successive planes.

Suppose the horizontal lines in fig. 2 represent parallel planes of atoms which partly reflect incident *X*-radiation, the distance between successive planes being d. Assuming the truth of Snell's law (*i.e.* incident beam, reflected beam, and normal are in one plane for mirror reflection ; and angle of incidence equals angle of reflection) the path difference for rays 1 and 2 reflected from adjacent planes is the length PQR, which is equal to $2d \sin \theta$. Now, the rays reflected from adjacent planes will be in phase and their amplitudes will reinforce to produce a strong reflection only if this path difference is equal to an integral number n of wavelength λ. Thus, the Bragg condition for diffraction is

$$2d \sin \theta = n\lambda . \qquad \text{...(1)}$$

This is known as Bragg law, n being the order of diffraction. It is now obvious that there are only certain directions θ in which the reflections of a given wavelength λ from all parallel planes add up in phase to give a strong reflected (diffracted) beam; the first few directions correspond to $n = 1, 2, 3, \ldots$ *etc.* We also conclude accordingly that a beam of monochromatic *X*-rays incident on a crystal with an arbitrary angle θ is in general not reflected. Also, because $\sin \theta \leq 1$, wavelengths $\lambda \leq 2d$ are essential if the Bragg reflection is to occur. Since $d \approx 10^{-8}$ cm., this condition is equivalent to $\lambda \lesssim 10^{-8}$ cm. It is for this reason that *X*-rays are most useful for crystal analysis. Just by the way of illustration, long wavelength visible light, having λ in the range of 4×10^{-5} cm. is not Bragg reflected. Instead, the well-known effects of optical refraction and reflection are observed with it.