Crystal Structure

Diffraction by atoms

To consider diffraction of X-ray by crystal which is a three-dimensional grating let us consider at first diffraction of light from one dimensional optical grating. If X-ray beam is directed to a row of equally spaced atoms, then each atom scatter the X-ray in all directions. The figure represents only one dimensional representation of scattering. The scattered waves reinforce in certain directions to produce zero, first, second order or higher order diffracted beam. 1st order diffraction pattern means adjacent wave fronts which are superimposing have one wave length difference from one another, i.e, 1st wave crest from an atom superimposes with the 2nd crest from the adjacent atom which in turn again superimposes with the 3rd crest from its adjacent atoms and so on. The direction of the 1st order.

diffracted beam is indicated by the arrow perpendicular to the wave front and is nearest to the direction of the incident X-ray. Similarly 2nd order diffraction pattern means adjacent waves which are superimposing with one another have two wavelength difference. This diffracted beam makes a greater angle with the direction of the incident X-ray. Thus, the higher is the order of diffraction the direction of the diffracted beam deviates more the direction of the from the incident X-ray beam (Fig. 23).

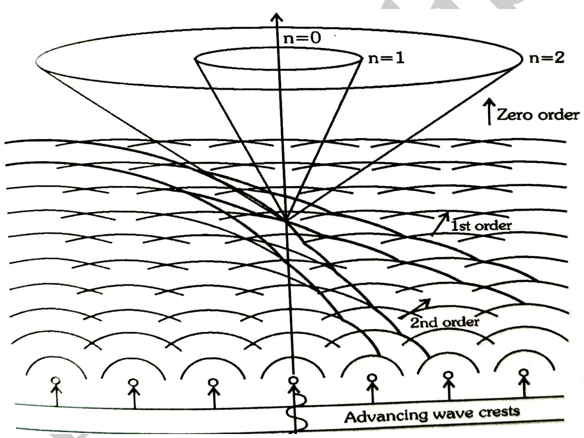

Fig. 23:Reinforcement of scattered waves producing defracted beams in the different orders. The upper rings for diffracted beams are produced when diffraction occurs from two dimension arrangement of points

If we consider diffraction by rows of atoms present in two dimension, and place a photographic plate behind the atoms, then the 1^{st} order diffraction beam forms a ring on the photographic plate surrounding the central brightest spot for the main X-ray beam. The ring for the 1" order diffraction is closest to the central bright spot. The ring for 2^{nd} order diffraction has higher radius and it increases with the order of diffraction.

Bragg's Law

A crystal contains infinite number of parallel planes of atoms. Atoms of each plane scatter incident X-ray and the zero order. 1st order, 2nd order diffracted beams are produced as described above. The diffracted beams from any set of parallel planes reinforces in such a manner that incident and scattered rays for a particular order of diffraction make equal angles with the atomic planes. It is then possible to regard the plane of beams as a reflector that is reflecting a portion of X-ray following law of reflection. The scattered bean then can be considered as the reflected beam. To understand this let us consider a set of parallel hkl planes of atoms of which two are represented by aa' and bb' (fig 24). Supporting the monochromatic X-ray beam is directed at the planes in the direction L_1M_1 making angle θ with the plane. The line L_1L_2 perpendicular to L_1M_1 represents one of the crests of the advancing monochromatic X-ray beam i.e. throughout the line L_1L_2 rays are in the same phase. When the reaches each of the atoms of the parallel planes, the atom generates a scattered ray, the crests of all the scattered rays from M_1 move along M_1N_1 and the crest of all the scattered rays the atoms, such as M, M_1, M_2 etc. fall on the line NN_1N_2. Since the L_1L_2 and NN_1N_2 both represent crests of the incident and reflected beam respectively, along these two lines, rays are at the same phase. So the path traversed by the rays $L_1M_1N_1$ when the crest of the incident ray strikes atom at M_1 and $L_2M_2N_2$ when the crest of the incident ray strikes atom at M_2 are obviously an integral multiple of wavelength λ. Let us draw perpendicular M_1P and M_1Q from M to the lines and M_2N_2 and M_2N_2 respectively. Therefore, at the points M_1 and P the rays will have the same phase and similarly at the points M_1 and Q the rays will also be in the same phase. Henes the path traversed by the ray along PM_2Q must be an integral multiple of wavelength otherwise destructive interference will occur between the rays scattered from M_1

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and M_2. So to have constructive interference i.e to have the reflected beam the distance ($PM_2 + M_2Q$) must be an integral multiple of wavelength. Let us connect $M_1$and M_2 by the line M_1M_2. The line M_1M_2 is the distance between two adjacent hkl planes.

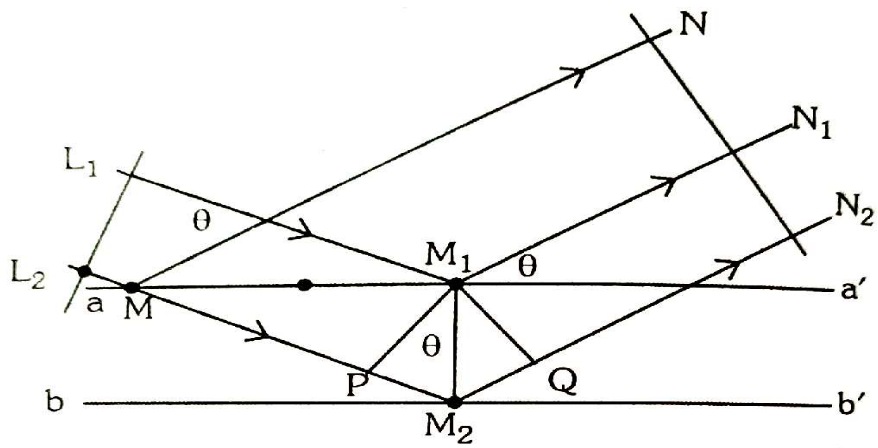

Fig 24: Constructive interference occurs when path difference is integral multiple of wave length

Now, $PM_2 = M_1M_2 \, Sin\theta$ and $M_2Q = M_1M_2 \, Sin\theta$

therefore $PM_2 + M_2Q = 2M_1M_2 Sin\theta = 2d_{hkl} \, Sin\theta$.

For constructive interference, $2d_{hkl}Sin\theta = n\lambda$ Where n = 1, 2, 3 etc and is called order of reflection.

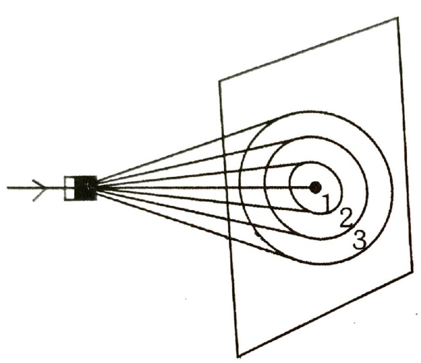

Fig.25: Diffracted beams produce circular rings on photographic place

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This is the famous Bragg's equation.

First order reflection means rays from successive planes when reinforce they differ by one waveleng i.e. x^{th} crest from one plane, $(x + 1)^{th}$ crest from the adjacent plane, $(x + 2)^{th}$ crest from the next adjacent plane will coincide and will form the scattered beam. Or, in other words 1st order diffracted beams from the parallel planes constitute 1 order reflected beam.

For a given set of planes, 1st, 2^{nd} order reflections occur when the incident X-ray strikes the planes at certain definite angle. Therefore when θ is changed, strong reflections flash out each time when the equation $2d\sin\theta = n\lambda$ holds with n = 1, 2, 3… At other intermediate values of θ, the path difference between the two adjacent rays is not an integral multiple of λ and the consequence is the destructive interference lowering the intensity of reflected beam. Moreover intensity of reflected beam from any set of parallel planes decreases with the increase in the value of n, the order of reflection. This is due to the fact that in 1^{st} order reflection the diffracted beam forms a narrow cone surrounding the path of the incident beam and the beam strikes the flat photographic plate forming ring of lowest radius. The radius of the ring increases with the order of reflection. Since number of photons is same in all of the cases the 1^{st} order reflection becomes brightest, i.e. intensity is maximum. (Fig. 25)

Certain consequences of Bragg's Law are

1. Maximum value of sinθ= 1 So, the maximum limit of θ is 90° Under this condition for n = 1

$d_{hkl} = \lambda/2$

Therefore for a given monochromatic radiation there is a lower limit of spacing of the planes to produce diffraction spectra or for a given crystal the maximum wavelength of X-ray used is $2d_{hkl}$

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2. For different reflections from the same planes of a crystal with a monochromatic X-ray (ie. d and λ are constant)

We have, Sinθ=n X constant.

That is sines of the angles of reflection of maximum intensities bear a simple ratio. For cubic face of NaCl, the angles of reflection for strong beams are 5.9°, 11.85° and 18.15°. So, $n_1 : n_2 : n_3$ = Sin 5.9° : Sin 11.85°: sin 18.15°

3. If d_{hkl} be the separation between hkl planes, then the separation between dnh, nk, nl plane is,

$$d_{nh,nk,nl} = \frac{1}{\sqrt{\frac{n^2h^2}{a^2} + \frac{n^2k^2}{b^2} + \frac{n^2l^2}{c^2}}}$$

$$= \frac{1}{n} \cdot \frac{1}{\sqrt{\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}}$$

$$= \frac{d_{hkl}}{n}$$

∴ from the relation, $2\, d_{hkl} \sin\theta = n\lambda$

or, $2\, \frac{d_{hkl}}{n} \sin\theta = 1 \cdot \lambda$

i.e . nth order reflection from hkl plane means first order reflection from (nh,nk.nl) plane.