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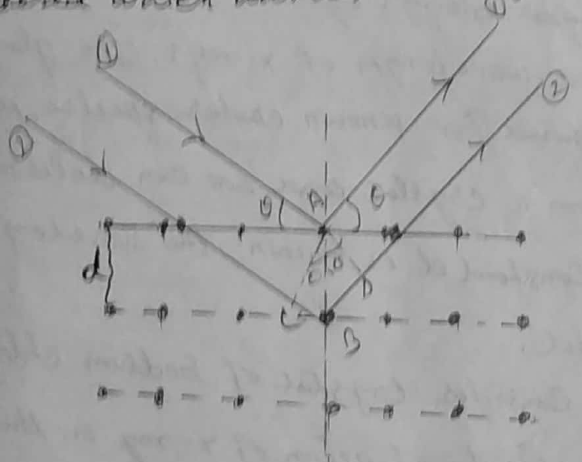
Bragg's law

According to W. L. Bragg, when a monochromatic beam of x-rays falls on the atoms in a crystal, it is scattered by that atoms which are placed in a parallel planes. If the path difference between two reflected rays from two different planes is an integral multiple of wavelength, the intensity of the reflected beam at a given angle will be maximum.

Let us consider the distance between the centre of atoms (or ions) be d. Let θ be the angle made by x-rays of wave length λ with the planes. Each atom becomes scattering centre. Bragg suggested that only those rays will be considered which was deflected by an angle θ.



Let us assume two rays scattered from atom A and B, clearly ray (2) traverses more distance in composition to ray (1). The path difference between two rays (1) and (2) be $CB + BD = n\lambda$

$$\Rightarrow 2CB = n\lambda$$

$$\Rightarrow 2d\sin\theta = n\lambda \quad \rightarrow (1) \quad \left(\because \sin\theta = \frac{CB}{d} \quad \therefore CB = d\sin\theta\right)$$

eqn (1) is called Bragg's equation. θ is known as glancing angle and n is the order of diffraction. If the distance between the atoms d be known, the wavelength λ of x-rays of maximum intensity can be calculated.

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Significance :- The interpretation of Bragg's law gives that the diffraction intensities can be stronger only at certain values of θ for specific values of λ and d. Therefore a knowledge of experimentally observed diffraction angles and wavelength of X-rays can provided the information about the inter planar spacing of the crystal. Thus the space, shape, ~~shape~~ and orientation of the unit cell can be determined from ~~diffraction~~ experiment using monochromatic X-rays.
~~This will be clear from the example of~~

Measurement of X-ray's wave length by using Bragg's law.

With the help of ~~equat~~ Bragg's equation $2d\sin\theta = n\lambda$ we can measure the wave length of X-rays. The glancing angle θ is measured for known order spectra produced by reflection from a crystal and we can determine λ/d. If lattice constant d is known, the wave length λ can be determined.

Let us consider crystal of sodium chloride (NaCl). From the study of action of X-ray on this crystal we found that this crystal is cubic and sodium and chloride ions are arranged alternately at the corners of the elementary cube. Every elementary cube has eight ions at its corners, four of sodium and four of chlorine. Every elementary cube is surrounded on all sides by other similar cubes. Hence each ion of NaCl is shared between two cubes and each elementary cube contains half a molecule of NaCl. Hence

$$\text{Mass of elementary cube} = \frac{M}{2N_0}$$

Where M = Molecular weight of Sodium chloride

$$= 23 + 35.5 = 58.5$$

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N_0 = Avogadro's number
$= 6.06 \times 10^{23}$

$\therefore$ mass of elementary cube $= \dfrac{58.5}{2 \times 6.06 \times 10^{23}}$

Because each side of elementary cube is d, hence the volume of elementary cube $= d^3 = \dfrac{\text{mass}}{\text{Density}}$

$$\text{or } d^3 = \frac{58.5}{2 \times 6.06 \times 10^{23} \times 2.17}$$

Where density of sodium chloride $= 2.17 \dfrac{gm}{c.c.}$

$$\text{or } d = \left[\frac{58.5}{2 \times 6.06 \times 10^{23} \times 2.17}\right]^{1/3}$$

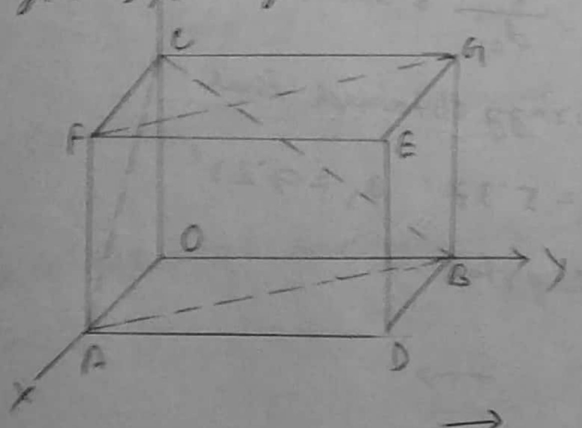
$$\therefore \quad d = 2.82 \times 10^{-8} \text{ cm.}$$

The value of θ for first order spectrum of X-rays from platinum target found by Bragg was 11.4° Hence

$$\lambda = 2 \times 2.82 \times 10^{-8} \times \sin 11.4^\circ \quad \left(\begin{matrix}\text{For first order} \\ n = 1\end{matrix}\right.$$
$$= 1.10 \times 10^{-8} \text{ cm.}$$
$$= 1.10 \times 10^{-10} \text{ m}$$
$$= 1.10 \text{ Å} \qquad (10^{-10} \text{ m} = 1 \text{ Å})$$

DETERMINATION OF CRYSTAL STRUCTURE

In order to determine the crystal structure the lattice constant 'd' is determined by using different planes of crystal as a reflecting surface for some known wave length of X-rays. The structure of crystal is analyzed.



1. Plane ADEF and its parallel plane.

According to Miller indices, this plane is called (100) plane and the distance between two such parallel planes be d_{100}.

2. Plane ABGF and its parallel plane.

This plane is called (110) plane and the distance between two such parallel planes be d_{110}.

3. Plane ABC and its parallel plane.

This plane is called (111) plane and the distance between two such parallel planes be d_{111}.

It can be shown that for simple cubic type crystal

$$\frac{1}{d_{100}} : \frac{1}{d_{110}} : \frac{1}{d_{111}} = 1 : \sqrt{2} : \sqrt{3}$$

For body centred cubic type crystal

$$\frac{1}{d_{100}} : \frac{1}{d_{110}} : \frac{1}{d_{111}} = 1 : \frac{1}{\sqrt{2}} : \sqrt{3}$$

For face centred cubic type crystal

$$\frac{1}{d_{100}} : \frac{1}{d_{110}} : \frac{1}{d_{111}} = 1 : \sqrt{2} : \frac{\sqrt{3}}{2}$$

If there is maximum intensity for glancing angles θ_1, θ_2 and θ_3 for 1st order of set of planes (100), (110), and (111) of crystal, then from Bragg's equation

$$2d_{100} \sin\theta_1 = \lambda$$

$$2d_{110} \sin\theta_2 = \lambda$$

$$2d_{111} \sin\theta_3 = \lambda$$

and $\frac{1}{d_{100}} : \frac{1}{d_{110}} : \frac{1}{d_{111}} = \sin\theta_1 : \sin\theta_2 : \sin\theta_3$

For KCl crystal Bragg obtained that

$\theta_1 = 5^\circ 23'$ $\theta_2 = 5^\circ 37'$ $\theta_3 = 9^\circ 23'$

Hence for KCl crystal.

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$\frac{1}{d_{100}} : \frac{1}{d_{110}} : \frac{1}{d_{111}} = \sin 5^\circ 23' : \sin 5^\circ 37' : \sin 9^\circ 23'$

$= 0.0938 : 0.1326 : 0.1630$

$\therefore \frac{1}{d_{100}} : \frac{1}{d_{110}} : \frac{1}{d_{111}} = 1 : \sqrt{2} : \sqrt{3}$

This ratio is for simple cubic type crystal and hence we conclude that structure of KCl is simple cubic type.