Bragg's Law:

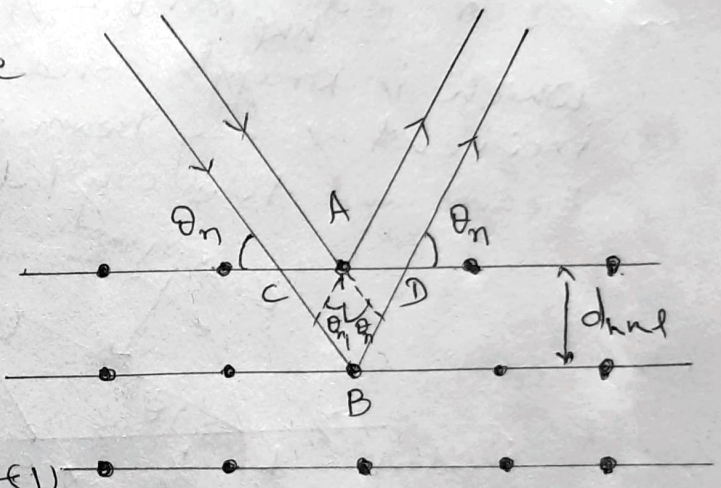
W.L. Bragg presented a simple explanation of the observed angles of the diffracted x-ray beams from a crystal. For this he considered a series of parallel rows of planes in which the atoms are arranged. A parallel beam of x-rays are incident in a direction making a glancing angle θ with planes. Each atom of the planes acts as a centre of disturbance and reflects the x-rays. The diffracted (here reflected) beams from different layers interfere and give rise to maxima and minima according as the conditions of maxima and minima are satisfied.

The path difference between diffracted beams shown in the figure is given by

$$\Delta = 2CB$$

$$\Delta = CB + BD = 2AB\sin\theta_n$$

$$= 2(d_{hkl})\sin\theta_n$$



For maxima, we have

$$2d_{hkl}\sin\theta_n = n\lambda \quad \text{---(1)}$$

Where n is an integer 1, 2, 3 ----

Equation (1) is known as Bragg's law.

Here d_{hkl} is the spacing of the (hkl) planes.

Bragg's condition in terms of the reciprocal lattice.

The Bragg's condition can be expressed as

$$\sin\theta = \frac{\lambda}{2d_{hkl}} \quad \text{---(2)}$$

in which the order of reflection is included. This can also be written as

$$\sin\theta = \frac{1/d_{hkl}}{2\lambda} \quad \text{---(3)}$$

A geometrical interpretation of equation (3) is given in figure-1. SO is a vector whose length is $1/\lambda$. This vector is taken along the direction of the incident x-ray beam and ends at the origin of the reciprocal lattice. Now a sphere of radius

$1/\lambda$ is drawn with S as centre. If this sphere passes through a reciprocal point P in the reciprocal lattice, then OP is a reciprocal lattice vector. The vector is ⊥ler to a lattice plane (hkl) and the length of this vector is $1/d_{hkl}$. But from figure

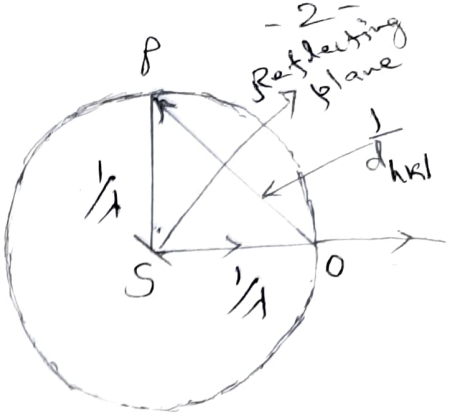


Fig. 1

$$OP = 2\sin\theta/\lambda$$

Thus, $$\frac{1}{d_{hkl}} = 2\sin\theta/\lambda$$

or $$2d_{hkl}\sin\theta = \lambda$$

Which is Bragg's condition. The direction of the incident x-ray beam the direction of the diffracted beam and the crystal plane are shown in the fig. 2.

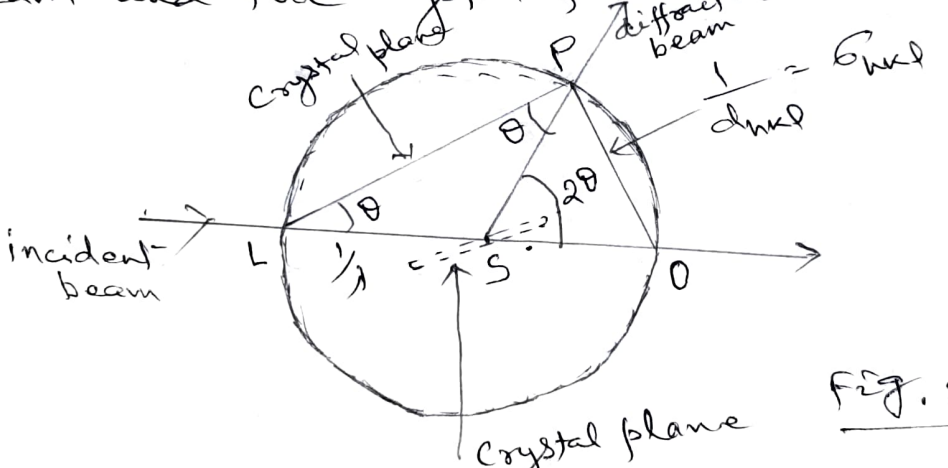


Fig. 2

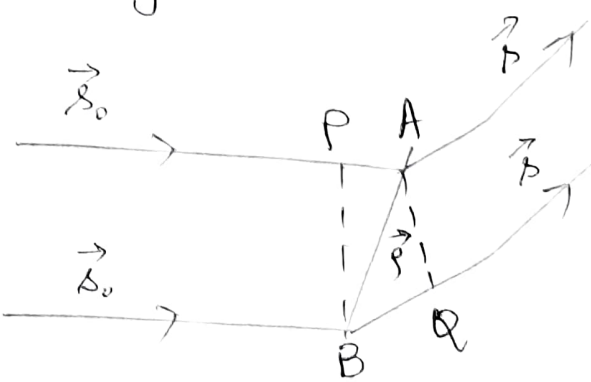
Von Laue treatment of X-ray diffraction

Let us consider the radiation scattered by two identical scattering centres A and B separated by a distance $\vec{r}$ as shown in fig. - 1. Here the incident radiation is assumed to be parallel and the scattered beam is detected at a long distance away. Let $\vec{S_0}$ and $\vec{S}$ be the unit vectors along the incident and scattered beams respectively.

The path difference between the two diffracted beams is given by

$$A - BP - AQ = \vec{S_0}\cdot\vec{r} - \vec{S}\cdot\vec{r}$$

$$= (\vec{S_0} - \vec{S})\cdot\vec{r}$$



The vector $\vec{s}_0 - \vec{s}$ represents the direction normal to the plane that reflects the incident radiation to scattered radiation as shown in fig.-2. The reflecting plane can be regarded as a Bragg's reflecting plane.

If 2θ be the angle between $\vec{s}$ and $\vec{s}_0$, then

$$|\vec{s}_0 - \vec{s}| = 2\sin\theta$$

Thus, the phase diff.

$$\phi = \frac{2\pi}{\lambda} \cdot \Delta$$

$$= \frac{2\pi}{\lambda} (\vec{s}_0 - \vec{s}) \cdot \vec{\rho} \quad \text{——— (1)}$$

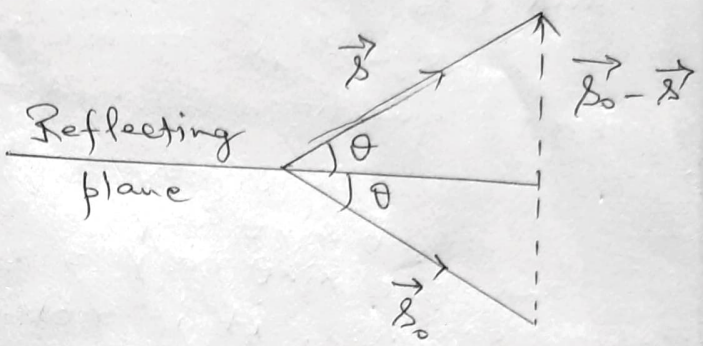


Fig.2

For maxima, the phase diff. must be an integral multiple of 2π. This condition can be satisfied in the case of nearest-neighbour atoms if the radiation scattered by them are in phase.

We know that the nearest neighbour atoms are separated by primitive translation vector $\vec{a}$, $\vec{b}$ and $\vec{c}$. Hence replacing $\vec{\rho}$ by $\vec{a}$, $\vec{b}$ or $\vec{c}$ in equation (1), we get the following conditions for maxima,

$$\frac{2\pi}{\lambda}(\vec{s}_0 - \vec{s}) \cdot \vec{a} = 2\pi h'$$

$$\frac{2\pi}{\lambda}(\vec{s}_0 - \vec{s}) \cdot \vec{b} = 2\pi k' \quad (2)$$

$$\frac{2\pi}{\lambda}(\vec{s}_0 - \vec{s}) \cdot \vec{c} = 2\pi l'$$

Here h', k' and l' may any three integers. Writing $h' = nh$, $k' = nk$ and $l' = nl$, where h, k, l are integers and n is a common factor (integer) in h', k' and l'. Thus we have from (2)

$$(\vec{s}_0 - \vec{s}) \cdot \vec{a} = nh\lambda$$
$$(\vec{s}_0 - \vec{s}) \cdot \vec{b} = nk\lambda \quad \text{——— (3)}$$
$$(\vec{s}_0 - \vec{s}) \cdot \vec{c} = nl\lambda$$

These conditions are known Laue's equations.

Bragg's law from Laue's equations

Let α, β and γ be the angles between $(\vec{S_0}-\vec{S})$ and the a-, b-, and c-axes of the crystal respectively.

$$\therefore (\vec{S_0}-\vec{S})\cdot\vec{a} = 2\sin\theta \cdot a\cos\alpha = 2a\sin\theta\cos\alpha$$

and $(\vec{S_0}-\vec{S})\cdot\vec{b} = 2b\sin\theta\cos\beta$ (4)

$$(\vec{S_0}-\vec{S})\cdot\vec{c} = 2c\sin\theta\cos\gamma$$

From equations (3) and (4), we have

$$2a\sin\theta\cos\alpha = n h\lambda$$
$$2b\sin\theta\cos\beta = n k\lambda \quad \text{— (5)}$$
$$\text{and} \quad 2c\sin\theta\cos\gamma = n l\lambda$$

From eqns. (5), it is noted that the direction cosines of the vector $(\vec{S_0}-\vec{S})$ are proportional to h/a, k/b and l/c. We also know that the direction cosines of the normal to (hkl) planes are proportional to h/a, k/b and l/c. Thus, it is concluded that the scattering normal $(\vec{S_0}-\vec{S})$ is identical to the normal to (hkl) planes. Hence (hkl) planes may be regarded as the reflecting planes in the sense of Bragg's treatment.

If d_{hkl} be the spacing between the adjacent planes of a family of (hkl) planes, then we have

$$d_{hkl} = \frac{a}{h}\cos\alpha = \frac{b}{k}\cos\beta = \frac{c}{l}\cos\gamma$$

then from any of the equation (5), we have

$$2d_{hkl}\sin\theta = n\lambda$$

which is Bragg's condition. Here n is the order of diffraction which is the greatest common factor of the integers h', k', l' of the Laue's equations (2). It is convention to refer an observed X-ray reflection by numbers h', k', l' inclosed in parenthesis. Thus the first order diffraction maxima by (111) planes is refered as (111) reflection. Similarly, the second order reflection maxima is referred as (222) reflection and so on.

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