Ans. Laue's equations. Laue's diffraction equations give the conditions under which X-rays scattered from different atoms of a crystal combine to form a diffracted beam. For this purpose we study the X-ray diffraction pattern produced by identical scattering centres located at the *lattice points* of a three dimensional crystal lattice. Let P_1 and P_2 be two such lattice points separated by a vector $\vec{r}$. Suppose a parallel beam of X-rays is incident on P_1P_2 along the direction of unit vector $\hat{i}$. The scattered beam is also parallel and let it be in any arbitrary direction given by unit vector $\hat{s}$. Draw P_1A perpendicular to the incident wave direction and P_2B perpendicular to the scattered wave direction, then P_1A is incident and P_2B the scattered wave front. The path difference between the two scattered waves – one scattered from P_2, and the other scattered from P_1 is given by

$$P_2A - P_1B = \vec{r}\cdot\hat{i} - \vec{r}\cdot\hat{s} = \vec{r}\cdot(\hat{i} - \hat{s}) = \vec{r}\cdot\vec{S}$$

where $\vec{S} = (\hat{i} - \hat{s})$ is a vector in the direction of the normal to the reflecting plane.

If θ is the angle that the incident beam makes with the reflecting plane, then the angle that the scattered (reflected) beam makes with the reflecting plane is also equal to θ and the angle between the unit vectors $\hat{i}$ and $\hat{s} = 2\theta$ as shown in Fig. 2.4.

$$\therefore \quad |\vec{S}| = 2\sin\theta \qquad [\because \hat{i} \text{ and } \hat{s} \text{ are unit vectors}]$$

The phase difference between the waves scattered at the lattice points P_1 and P_2 is given by

$$\phi = \frac{2\pi}{\lambda}(\vec{r}\cdot\vec{S})$$

The intensity of the diffracted beam is a *maximum* in the direction in which ϕ is an integral multiple of 2π.

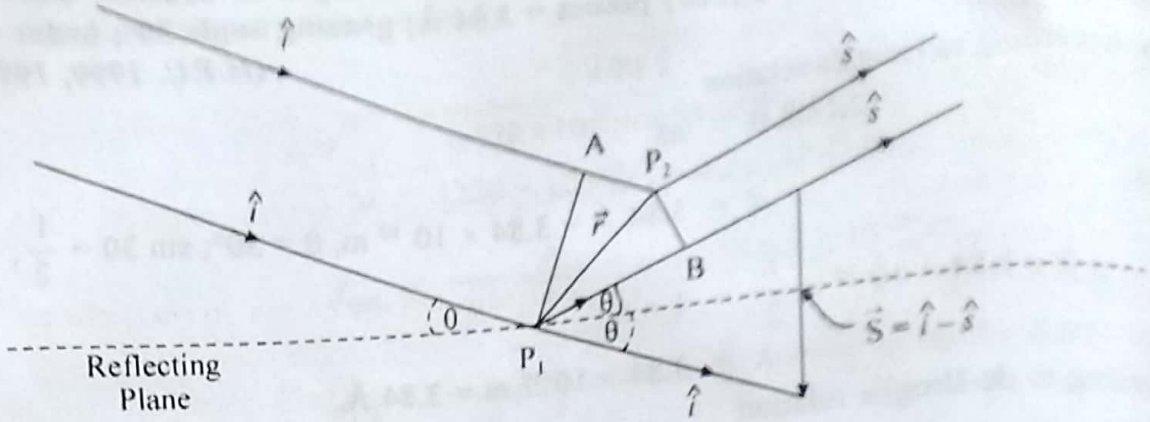

Fig. 2.4

If $\vec{a}$, $\vec{b}$ and $\vec{c}$ are the primitive lattice vectors of the point P_2 with respect to the point P_1 then

$$\vec{r} = \vec{a} + \vec{b} + \vec{c}$$

and the above condition can be put in the form of three separate conditions *i.e.*,

$$\phi_a = \frac{2\pi}{\lambda}(\vec{a}\cdot\vec{S}) = 2\pi h$$

$$\phi_b = \frac{2\pi}{\lambda}(\vec{b}\cdot\vec{S}) = 2\pi k$$

and $$\phi_c = \frac{2\pi}{\lambda}(\vec{c}\cdot\vec{S}) = 2\pi l$$

where h, k, l are integers and ϕ_a, ϕ_b and ϕ_c are phase differences between the waves scattered from the two ends of the primitive lattice vectors $\vec{a}$, $\vec{b}$ and $\vec{c}$ respectively.

If α, β, γ are the angles between the normal to the reflecting plane and $\vec{a}$, $\vec{b}$ and $\vec{c}$ respectively, then

$$\vec{a}\cdot\vec{S} = |\vec{a}||\vec{S}|\cos\alpha = 2a\sin\theta\cos\alpha$$

$$\vec{b}\cdot\vec{S} = |\vec{b}||\vec{S}|\cos\beta = 2b\sin\theta\cos\beta$$

$$\vec{c}\cdot\vec{S} = |\vec{c}||\vec{S}|\cos\gamma = 2c\sin\theta\cos\gamma$$

From (*i*), (*ii*) and (*iii*), we have

$$\vec{a}\cdot\vec{S} = h\lambda, \quad \vec{b}\cdot\vec{S} = k\lambda \quad \text{and} \quad \vec{c}\cdot\vec{S} = l\lambda$$

$$\therefore \quad 2a\sin\theta\cos\alpha = h\lambda$$

$$2b\sin\theta\cos\beta = k\lambda$$

$$2c\sin\theta\cos\gamma = l\lambda$$

These are the Laue's equations for X-ray diffraction.

EC-(5)

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