CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 42: Scattering of X-Rays: The Laue Equations - I

So, let us consider a crystal of finite size where atoms are located only at the corners of the unit cell, and we will consider each atom to be a point scatterer. So, we are now going to look at the phenomenon of scattering from a crystal of finite size. Here, atoms are only at the corners of a unit cell, and atoms are considered as point scatterers.

Though the phenomenon of scattering of X-rays from atoms occurs as a result of electrons, and strictly speaking they are not point scatterers, for all practical purposes we can carry out the analysis by assuming that they are point scatterers. So, if there is a point scatterer, the incoming X-ray beam will get scattered in all directions in three-dimensional space.

Now, we are considering a crystal of finite size. Let us say that there are N_1 atoms along the a axis, N_2 atoms along the b axis, and N_3 atoms along the c axis. So, the total number of atoms is essentially $N_1 \times N_2 \times N_3$.

Now, let us consider just two-point scatterers. Let us label one point scatterer as A and another point scatterer as B, and remember that all of these point scatterers are at the corners of the unit cell. Now, the vector $\overline{AB}$, let me call it the vector $\overline{r}$. Now, we have an incoming X-ray beam of a specific wavelength, and the beam hits these two point scatterers.

Let us take a particular scattering direction and consider a point far away, say point Q, where we place the detector. Now, these two rays, call them ray 1 and ray 2, depending on the path difference, could result in constructive interference or destructive interference, and to find that out we need to calculate the path difference.

Let me call point A as the origin, and with respect to this origin we will do all the calculations. The distance of point Q from the crystal is let us say R, and this R is much, much greater than the magnitude of the small vector r, which essentially means that we can assume that point Q is almost equidistant from all the point scatterers. Because R is much larger than the size of the crystal, we can also assume that ray 1 and ray 2 are parallel when they meet at point Q.

Now, what is the path difference? Let us call the path difference between ray 1 and ray 2 as δ. In order to find this, let us do a small construction. We drop a perpendicular from point B onto ray 1, and another perpendicular from point A onto ray 2, and let us label these points as C and D. So, the path difference δ is nothing but $AC - BD$.

$$\delta = AC - BD$$

Now, let me write down the equation for the incoming radiation. We will consider this as a plane wave and write it in complex form. Let us consider ray 1 and write down the wave at point Q, and let me call this y_1. This corresponds to ray 1 at point Q.

$$y_1 = \frac{\phi_0}{R} e^{i\omega t}$$

Now, ray 2 would have travelled a different distance compared to ray 1, and hence I can write the wave due to ray 2 by adding a phase difference. This phase difference is given by $\frac{2\pi}{\lambda}$ times the path difference. So, δ is the path difference, and $\frac{2\pi}{\lambda}\delta$ is the phase difference.

When the path difference is an integral multiple of λ, the phase difference is an integral multiple of 2π, and the two waves are in phase. When the path difference is $\lambda/2$, for example, the waves are completely out of phase.

$$y_2 = \frac{\phi_0}{R} e^{i(\omega t + \frac{2\pi}{\lambda}\delta)}$$

Now, we have to find δ. To do this, let us add a few more details to the diagram. Let us say the incoming radiation direction is defined by a unit vector $\hat{s}_0$, and the scattered beam direction is defined by another unit vector $\hat{s}$. These represent the incident beam direction and the scattered beam direction, respectively.

Now, let us write down the path difference. We already stated that $\delta = AC - BD$. The segment AC can be written as the projection of the vector $\bar{r}$ onto the scattered beam direction. Hence,

$$AC = \bar{r} \cdot \hat{s}$$

Similarly,

$$BD = \bar{r} \cdot \hat{s}_0$$

Therefore, the path difference can be written as

$$\delta = \bar{r} \cdot (\hat{s} - \hat{s}_0)$$

Now, let us define a new vector,

$$S = \hat{s} - \hat{s}_0,$$

which we call the scattering vector. Hence, the path difference becomes

$$\delta = \bar{r} \cdot \bar{S}$$

Before proceeding further, let us spend some time understanding the scattering vector $\bar{S}$. Geometrically, if $\hat{s}_0$ is the incident beam direction and $\hat{s}$ is the scattered beam direction, then the scattering vector $\bar{S}$ is simply the vector difference of these two unit vectors. If we bisect the angle between $\hat{s}_0$ and $\hat{s}$ using an imaginary plane, then the scattering vector $\bar{S}$ is perpendicular to this imaginary plane.

From this construction, we can see that the incoming radiation makes an angle θ with this imaginary plane, and the scattered radiation also makes the same angle θ. This makes it appear as if reflection is taking place from this imaginary plane, although physically no reflection occurs.

From this geometry, since $\hat{s}_0$ and $\hat{s}$ are unit vectors, the magnitude of the scattering vector is

$$|\bar{S}| = 2sin\theta.$$

We will take note of this result and return to it later.

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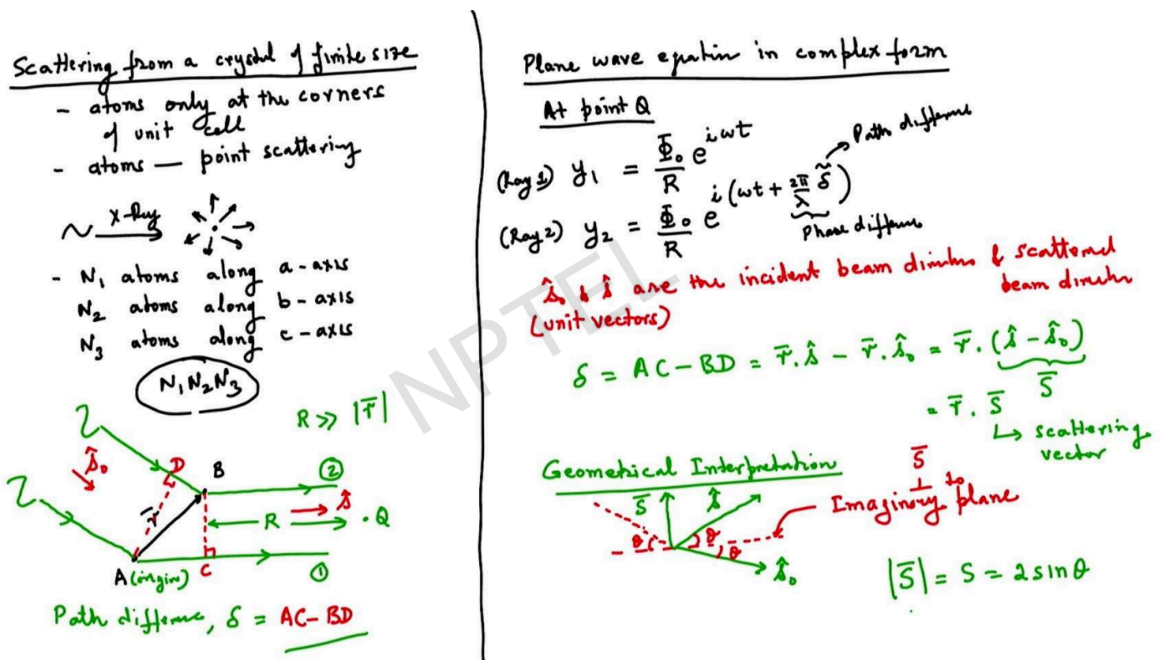

Now, we want to find the resultant wave at point Q by adding all the scattered waves coming from all the scattering centers in the crystal. The total number of scattering centers is $N_1N_2N_3$. We take point A as the origin, and all scattering centers are defined with respect to this origin by different vectors $\bar{r}$.

The resultant wave at point Q can be obtained by summing the contribution from all scattering centers. Thus, the resultant wave can be written as a summation over all $\bar{r}$ vectors:

$$Y = \frac{\phi_0}{R} \sum_{\bar{r}} e^{i(\omega t + \frac{2\pi}{\lambda} \bar{r} \cdot \bar{S})}$$

Here, ϕ_0 / R and $e^{i\omega t}$ can be taken outside the summation, giving

$$Y = \frac{\phi_0}{R} e^{i\omega t} \sum_{\bar{r}} e^{i(\frac{2\pi}{\lambda} \bar{r} \cdot \bar{S})}$$

Now, what is the vector $\bar{r}$? Since scattering centers are only at the corners of the unit cell, $\bar{r}$ is a lattice translation vector. Hence,

$$\bar{r} = u\bar{a} + v\bar{b} + w\bar{c},$$

where $\bar{a}$, $\bar{b}$, and $\bar{c}$ are the unit cell vectors. The integer u varies from 0 to $N_1 - 1$, v varies from 0 to $N_2 - 1$, and w varies from 0 to $N_3 - 1$.

Therefore, the summation can be written as three separate summations:

$$Y = \frac{\phi_0}{R} e^{i\omega t} \sum_{u=0}^{N_1 - 1} e^{i\frac{2\pi}{\lambda} u\bar{S} \cdot \bar{a}} \sum_{v=0}^{N_2 - 1} e^{i\frac{2\pi}{\lambda} v\bar{S} \cdot \bar{b}} \sum_{w=0}^{N_3 - 1} e^{i\frac{2\pi}{\lambda} w\bar{S} \cdot \bar{c}}$$

Let us examine the first summation. Expanding it,

$$1 + e^{i\frac{2\pi}{\lambda} \bar{S} \cdot \bar{a}} + e^{i\frac{2\pi}{\lambda} \bar{S} \cdot \bar{a} \cdot 2} + \cdots + e^{i\frac{2\pi}{\lambda} \bar{S} \cdot \bar{a}(N_1 - 1)}$$

This is a geometric series. For a geometric series with first term $t_0 = 1$ and common ratio $f = e^{i\frac{2\pi}{\lambda} \bar{S} \cdot \bar{a}}$, For geometric series of n terms,

$$t_0 + t_0 f + t_0 f^2 + \ldots + t_0 f^n = \frac{t_0(1 - f^n)}{1 - f}$$

So, the summation of N_1 terms is,

$$\frac{1-f^{N_1}}{1-f}.$$

Let us define

$$\psi_1 = \frac{\pi}{\lambda}\overline{S}\cdot\overline{a}.$$

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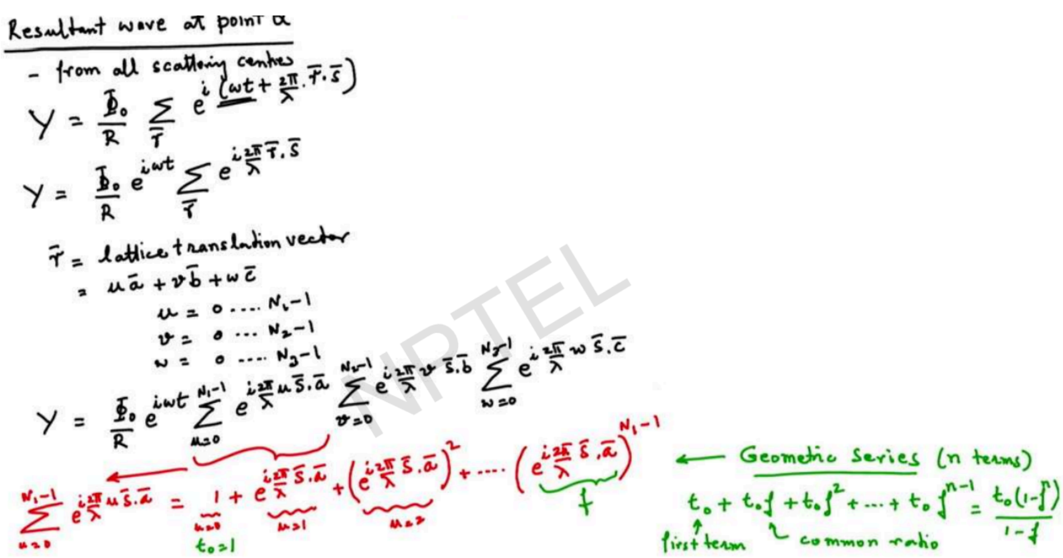

Then the summation can be written as

$$\sum_{u=0}^{N_1-1} e^{i\frac{2\pi}{\lambda}u\overline{S}\cdot\overline{a}} = \frac{1-e^{i2N_1\psi_1}}{1-e^{i2\psi_1}}.$$

Similarly, defining

$$\psi_2 = \frac{\pi}{\lambda}\overline{S}\cdot\overline{b}, \quad \psi_3 = \frac{\pi}{\lambda}\overline{S}\cdot\overline{c},$$

the other two summations can be written as

$$\sum_{v=0}^{N_2-1} e^{i\frac{2\pi}{\lambda}v\bar{S}\cdot\bar{b}} = \frac{1-e^{i2N_2\psi_2}}{1-e^{i2\psi_2}},$$

$$\sum_{v=0}^{N_2-1} e^{i\frac{2\pi}{\lambda}v\bar{S}\cdot\bar{c}} = \frac{1-e^{i2N_3\psi_3}}{1-e^{i2\psi_3}}.$$

Thus, we have derived an expression for the resultant wave at point Q by summing the contributions from all scattering centers in the finite crystal. In the next lecture, we will determine the intensity of this wave at point Q.

Thank you.

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