# CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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## Lecture 43: Scattering of X-Rays: The Laue Equations - II

In the last lecture, we started looking at scattering from a crystal of finite size. In this analysis, we assumed a finite crystal with $N_1$ atoms along the $a$ axis, $N_2$ atoms along the $b$ axis, and $N_3$ atoms along the $c$ axis. The way we visualize this scattering is as follows. Let us consider a lattice point at the origin, marked as point $A$, and another lattice point at point $B$. The location of lattice point $B$ with respect to $A$ is given by the vector $\overline{r}$, as shown in the figure.

From this construction, one determines the path difference when the X-rays reach a point $Q$. If the path difference is an integral multiple of the wavelength, then constructive interference occurs. Based on this idea, we proceeded further and determined the resultant wave at point $Q$, which is obtained by summing over all $\overline{r}$ vectors. The vector $\overline{r}$ itself is a lattice translation vector given by

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

where the scattering centers are located only at the corners of a primitive unit cell.

By expanding this summation, the resultant wave at point $Q$ was written in the form of three separate summations. As we saw towards the end of the last lecture, each of these summations is a geometric series, summed over $N_1$ terms, $N_2$ terms, and $N_3$ terms, respectively. Using the formula for the summation of a geometric series, we obtained the summation results for the first, second, and third terms.

Note that the parameters $\psi_1$, $\psi_2$, and $\psi_3$ are defined as

$$\psi_1 = \frac{\pi}{\lambda}\overline{S} \cdot \overline{a}, \quad \psi_2 = \frac{\pi}{\lambda}\overline{S} \cdot \overline{b}, \quad \psi_3 = \frac{\pi}{\lambda}\overline{S} \cdot \overline{c},$$

where $S$ is the scattering vector and $a$, $b$, and $c$ are the unit cell translation vectors.

Proceeding further, we write down the resultant amplitude at point $Q$ by multiplying all three summations. The resultant wave at point $Q$ can be written as

$$Y = \frac{\Phi_0}{R} e^{i\omega t} \left( \frac{1 - e^{i2N_1\psi_1}}{1 - e^{i2\psi_1}} \right) \left( \frac{1 - e^{i2N_2\psi_2}}{1 - e^{i2\psi_2}} \right) \left( \frac{1 - e^{i2N_3\psi_3}}{1 - e^{i2\psi_3}} \right)$$

Now, we want to determine the resulting intensity. The intensity $I$ is given by the product of the amplitude and its complex conjugate,

$$I = YY^*$$

To proceed, let us briefly consider the complex conjugate of the terms appearing in the summation. Each numerator and denominator term is of the form $1 - e^{i2x}$. The complex conjugate of this expression is $1 - e^{-i2x}$. If we multiply a term by its complex conjugate, we obtain

$$(1 - e^{i2x})(1 - e^{-i2x}).$$

Expanding this expression gives

$$2 - e^{i2x} - e^{-i2x}.$$

Using the trigonometric identities

$$e^{i2x} = cos2x + isin2x, \quad e^{-i2x} = cos2x - isin2x,$$

we find that

$$(1 - e^{i2x})(1 - e^{-i2x}) = 2(1 - cos2x) = 4sin^2x.$$

Now, let us calculate the resulting intensity explicitly. Writing the full complex conjugate, we have

$$Y^* = \frac{\Phi_0}{R} e^{-i\omega t} \left( \frac{1 - e^{-i2N_1\psi_1}}{1 - e^{-i2\psi_1}} \right) \left( \frac{1 - e^{-i2N_2\psi_2}}{1 - e^{-i2\psi_2}} \right) \left( \frac{1 - e^{-i2N_3\psi_3}}{1 - e^{-i2\psi_3}} \right)$$

Multiplying $Y$ and $Y^*$, the exponential terms $e^{i\omega t}$ and $e^{-i\omega t}$ cancel out. The resulting intensity becomes

$$I = \frac{\phi_0^2}{R^2}\frac{sin^2(N_1\psi_1)}{sin^2\psi_1}\frac{sin^2(N_2\psi_2)}{sin^2\psi_2}\frac{sin^2(N_3\psi_3)}{sin^2\psi_3}.$$

We now investigate these individual functions of the form

$$\frac{sin^2(N\psi)}{sin^2\psi}.$$

To understand where maxima occur, let us examine the behavior of a general function

$$\frac{sin^2(Nx)}{sin^2x}$$

as $x$ approaches an integral multiple of π. Direct substitution gives an indeterminate form $0/0$, so we apply L'Hôpital's rule. Differentiating the numerator and denominator, and applying the limit twice, we find that

$$\lim_{x\rightarrow h\pi}\frac{sin^2(nx)}{sin^2x} = \lim_{x\rightarrow h\pi}\frac{2nsin(nx)\text{cos}cos\,(nx)}{2\,sinx\,cosx}$$

$$= \lim_{x\rightarrow h\pi}\frac{nsin(nx)}{sin2x}$$

$$= \lim_{x\rightarrow h\pi}\frac{2n^2cos2nx}{2cos2x} = n^2,$$

where $h$ is an integer

Plots of this function show that for large $N$, the function is nearly zero everywhere except at specific values such as $0$, π, 2π, and so on, where sharp peaks appear. As $N$ decreases, the peaks broaden and subsidiary maxima appear. This implies that smaller crystal sizes produce broader diffraction peaks, while larger crystals with more scattering centers produce sharper peaks.

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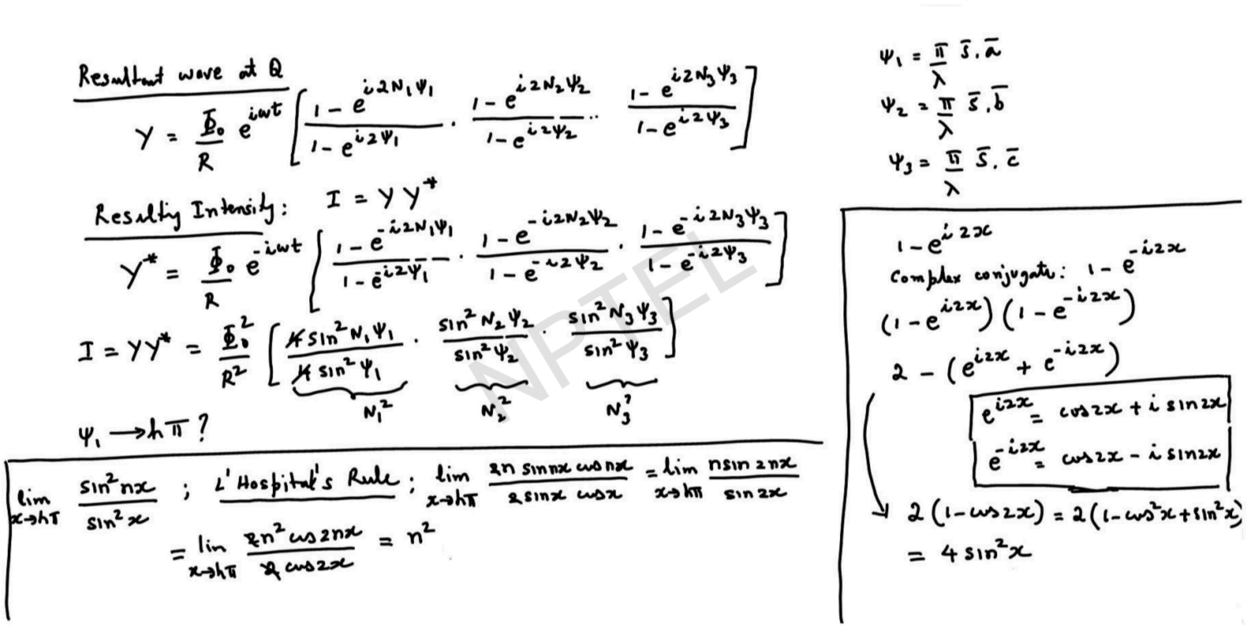


Therefore, the intensity reaches a maximum when

$$\psi_1 = h\pi, \quad \psi_2 = k\pi, \quad \psi_3 = l\pi,$$

where $h$, $k$, and $l$ are integers. All three conditions must be satisfied simultaneously; otherwise, the intensity goes to zero.

Substituting the definitions of $\psi_1$, $\psi_2$, and $\psi_3$, we obtain

$$\overline{S} \cdot \overline{a} = h\lambda, \quad \overline{S} \cdot \overline{b} = k\lambda, \quad \overline{S} \cdot \overline{c} = l\lambda.$$

These are known as the Laue conditions.

At these maxima, the intensity becomes

$$I_{max} = \frac{\phi_0^2}{R^2} N_1^2 N_2^2 N_3^2.$$

Now, let us give a geometric interpretation of the Laue conditions. The scattering vector $S$ is defined as the difference between the scattered beam unit vector and the incident beam unit vector. Geometrically, it is perpendicular to an imaginary reflecting plane. The incident beam makes an angle θ with this plane, and the scattered beam makes the same angle θ. Since both unit vectors have unit magnitude, the magnitude of the scattering vector is

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

Let us now express the Laue conditions in crystal coordinates. Let the scattering vector $\overline{S}$ make angles α, β, and γ with the $a$, $b$, and $c$ axes, respectively. Then,

$$\overline{S} \cdot \overline{a} = 2asin\theta cos\alpha,$$

$$\overline{S} \cdot \overline{b} = 2bsin\theta cos\beta,$$

$$\overline{S} \cdot \overline{c} = 2csin\theta cos\gamma$$

Now, consider an imaginary plane in crystal space with Miller indices $(hkl)$. This plane intersects the $a$, $b$, and $c$ axes at $a/h$, $b/k$, and $c/l$, respectively. The interplanar spacing $d$ for this plane can be written as

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

Substituting this expression into the Laue conditions gives

$$2dsin\theta = \lambda,$$

which is the well-known Bragg equation.

If the plane $(hkl)$ has a common factor $n$, the reflection condition can be interpreted either as an $n^{th}$-order reflection from the plane $(h/n\, k/n\, l/n)$ or as a first-order reflection from the plane $(hkl)$. Thus, we see that the Laue diffraction conditions and the Bragg diffraction condition are equivalent and converge to the same result.

With this, I conclude this lecture.

Thank you.

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