CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 50: Reciprocal Lattice and Diffraction

In this lecture, we are going to now take up the ideas that we developed on the reciprocal lattice in the previous three lectures and develop the relationship between diffraction and reciprocal lattice.

So, in this Laue we had set up these Laue conditions in the following way that I have some scattering point A and another scattering point B. There is an incident X-ray beam falling on these scattering points and there is a scattered beam reflected in a certain direction.

So, the incident beam is given by the unit vector $\hat{s}_0$, and the scattered beam direction is given by the unit vector $\hat{s}$. Now, this can be considered to be a reflection along a certain (hkl) plane.

We also defined a scattering vector $\overline{S}$ which is perpendicular to this reflecting plane (hkl) . The incident beam makes an angle θ with the reflecting plane and it gets reflected from the plane, with the reflection angle also being θ.

The scattering vector itself from the above diagram simply becomes the difference of the two unit vectors:

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

As we see, the scattering vector $\overline{S}$ is perpendicular to the plane (hkl). The magnitude of the scattering vector from the above figure turns out to be $2sin\theta$.

From there, we got the Laue conditions:

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

where $\overline{a}$, $\overline{b}$, and $\overline{c}$ are the unit cell vectors of the real lattice.

Now, since the vector $\overline{S}$ is perpendicular to the plane (hkl) and the reciprocal lattice vector $\overline{r^*_{hkl}}$ is also perpendicular to the plane (hkl), the two vectors $\overline{S}$ and $\overline{r^*_{hkl}}$ are parallel.

This implies that I can write the scattering vector $\overline{S}$ as some scalar quantity β times the reciprocal lattice vector:

$$\overline{S} = \beta(h\overline{a^*} + k\overline{b^*} + l\overline{c^*})$$

Now, from the Laue conditions, I can write $\overline{S} \cdot \overline{a}$ as:

$$\overline{S} \cdot \overline{a} = \beta(h\overline{a^*} + k\overline{b^*} + l\overline{c^*}) \cdot a$$

Taking the dot product:

$$\beta(h\overline{a^*} \cdot \overline{a} + k\overline{b^*} \cdot \overline{a} + l\overline{c^*} \cdot \overline{a})$$

From the definition of the reciprocal lattice:

$$\overline{b^*} \cdot \overline{a} = 0, \quad \overline{c^*} \cdot \overline{a} = 0, \quad \overline{a^*} \cdot \overline{a} = 1$$

Hence, this reduces to βh. From the Laue condition $\overline{S} \cdot \overline{a} = h\lambda$, we obtain:

$$\beta h = h\lambda$$

which implies:

$$\beta = \lambda$$

Therefore, the scattering vector can be written as:

$$\overline{S} = \lambda(h\overline{a^*} + k\overline{b^*} + l\overline{c^*})$$

Dividing both sides by λ:

$$\frac{\bar{S}}{\lambda} = h\bar{a^*} + k\bar{b^*} + l\bar{c^*}$$

which is nothing but the reciprocal lattice vector $\bar{r^*}_{hkl}$.

This is another formulation of the diffraction condition. Whenever Bragg's law or the Laue conditions are satisfied, the vector $\bar{S}/\lambda$ must be a reciprocal lattice vector.

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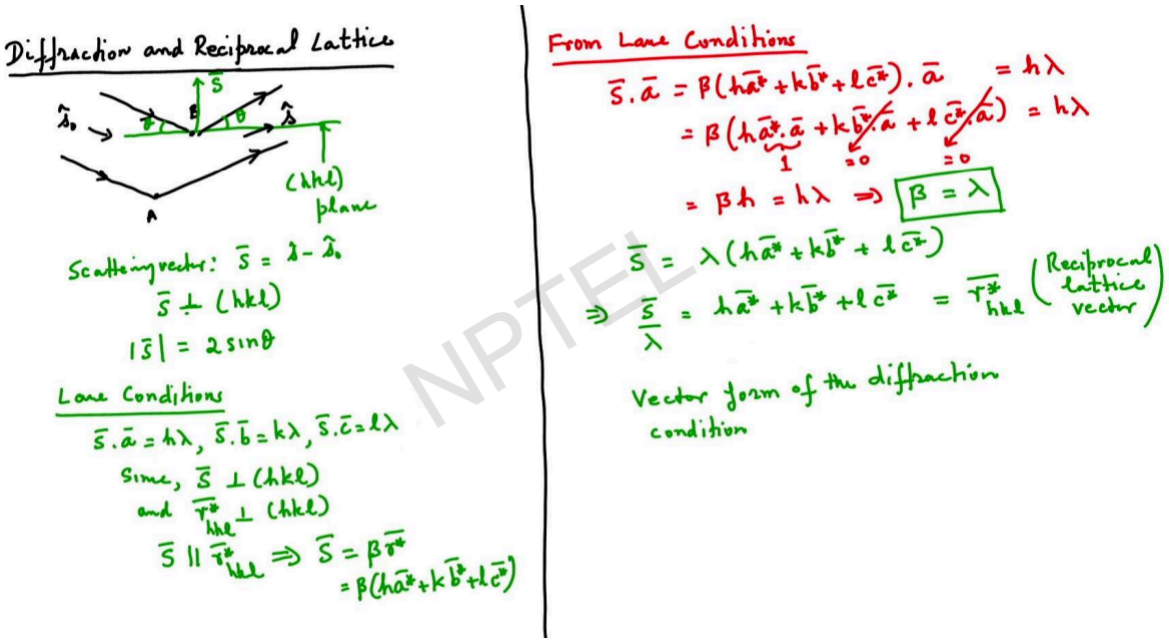

Now, this form of the diffraction condition can be set in a frame of reference called the Ewald construction.

The scattering vector is:

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

Dividing by the wavelength:

$$\frac{\bar{S}}{\lambda} = \frac{\hat{s}}{\lambda} - \frac{\hat{s}_0}{\lambda}$$

where $\hat{s}$ and $\hat{s}_0$ are unit vectors.

We now construct a sphere of radius $1/\lambda$. Let the center of the sphere be C, and let $\hat{s}_0/\lambda$ represent the incident beam direction. We mark this point as O, so CO represents the incident beam.

Let us now consider a scattered beam at some point P, represented by $\bar{S}/\lambda$, so CP represents the scattered beam. Clearly:

$$\overline{OP} = \frac{\bar{S}}{\lambda}$$

We take the point O as the origin of the reciprocal lattice. For diffraction to occur, the vector OP must be a reciprocal lattice vector. This implies that the point P must also be a reciprocal lattice point.

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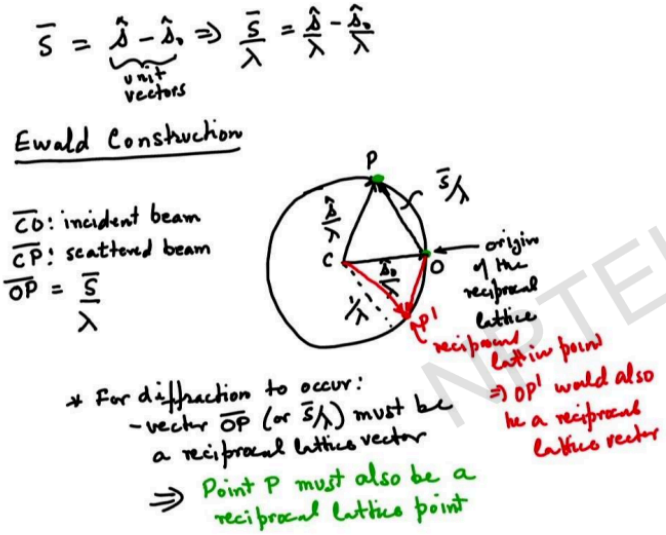

If another reciprocal lattice point P' lies elsewhere, then OP' would also be a reciprocal

lattice vector, giving rise to another scattered beam. This is the essence of the Ewald construction.

Now, we very briefly discuss experimental techniques used in X-ray diffraction. We begin with Bragg's law:

$$\lambda = 2dsin\theta$$

Suppose a crystal is placed randomly and irradiated with X-rays of wavelength λ, for example Cu K_{α} radiation with $\lambda = 1.54$ Å. In such a random orientation, the probability of satisfying Bragg's condition is very small.

Therefore, experimental techniques must be designed to obtain several diffractions from several (hkl) planes.

In the Bragg equation, there are three parameters: λ, θ, and d. For a given crystal, d is fixed. The parameters that can be varied are λ or θ, but not both simultaneously.

If both λ and θ are varied, the resulting diffraction pattern would be impossible to analyze.

Thus, either λ is varied while θ is fixed, or λ is fixed and θ is varied.

The locations of diffracted beams are recorded to obtain a diffraction pattern, which is then analyzed. Earlier methods used photographic films and chart recorders, while modern techniques use computers.

Experimental method	Parameter varied	Sample type	Major application
Laue method	λ	Single crystal	Crystal orientation
Rotating crystal method	θ	Single crystal	Crystal structure determination

Experimental method	Parameter varied	Sample type	Major application
X-ray diffractometer	θ	Powder / polycrystal	Phase identification and lattice parameter determination

Three general experimental methods are commonly used:For variable λ, white radiation is used, which provides a range of wavelengths. A single crystal is kept in a fixed position, and for a given (hkl) plane, the appropriate wavelength satisfying Bragg's law is selected automatically, producing diffraction.

With this, I conclude the lecture. In the next lecture, we will briefly analyze the Laue method and rotating crystal method using the reciprocal lattice, and then discuss the X-ray diffractometer in greater detail, including solving problems related to diffraction pattern analysis.

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