CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 48: Application of Reciprocal Lattice in Crystal Geometry

Continuing from the previous lecture on the reciprocal lattice, we now examine the geometry of the reciprocal lattice in greater detail and explore how this concept can facilitate geometrical calculations for the real space lattice.

Consider the reciprocal lattice vectors $\overline{a}^*$, $\overline{b}^*$, and $\overline{c}^*$. Let α^* denote the angle between $\overline{b}^*$ and $\overline{c}^*$, β^* the angle between $\overline{c}^*$ and $\overline{a}^*$, and γ^* the angle between $\overline{a}^*$ and $\overline{b}^*$. This is analogous to the real space lattice, where the vectors $\overline{a}$, $\overline{b}$, and $\overline{c}$ form angles α, β, and γ, respectively.

To determine γ^*, consider the dot product $\overline{a}^* \cdot \overline{b}^*$. Expressing the reciprocal vectors in terms of the real lattice vectors, we have:

$$\overline{a}^* = \frac{\overline{b}\times\overline{c}}{V}, \quad \overline{b}^* = \frac{\overline{c}\times\overline{a}}{V},$$

where V is the volume of the unit cell. The dot product can also be expressed as:

$$\overline{a}^* \cdot \overline{b}^* = |\overline{a}^*|\,|\overline{b}^*| cos\gamma^*.$$

The magnitudes of the reciprocal vectors are:

$$|\overline{a}^*| = \frac{|\overline{b}\times\overline{c}|}{V} = \frac{bc sin\alpha}{V}, \quad |\overline{b}^*| = \frac{|\overline{c}\times\overline{a}|}{V} = \frac{ca sin\beta}{V}.$$

The numerator of the dot product is:

$$(\overline{b} \times \overline{c})\cdot(\overline{c} \times \overline{a}) = (\overline{b} \cdot \overline{c})(\overline{c} \cdot \overline{a}) - (\overline{c} \cdot \overline{c})(\overline{b} \cdot \overline{a}) = bc cos\alpha \cdot ac cos\beta - c^2 \cdot ab cos\gamma.$$

Substituting these results into the expression for $cos\gamma^*$ yields:

$$\cos\gamma^{*} = \frac{\cos\alpha\cos\beta-\cos\gamma}{\sin\alpha\sin\beta}.$$

Similarly, one obtains:

$$\cos\beta^{*} = \frac{\cos\gamma\cos\alpha-\cos\beta}{\sin\gamma\sin\alpha}, \quad \cos\alpha^{*} = \frac{\cos\beta\cos\gamma-\cos\alpha}{\sin\beta\sin\gamma}.$$

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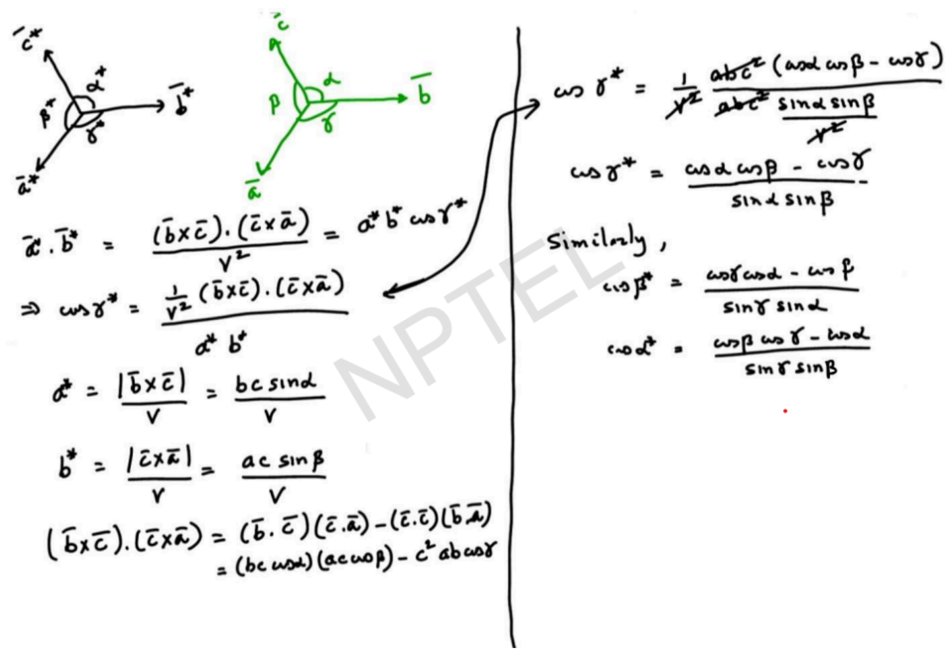

These relationships define the angles α^{*}, β^{*}, and γ^{*} of the reciprocal lattice in terms of the real lattice angles α, β, and γ.

Next, we consider the geometry of the real space lattice using the reciprocal lattice. Denote the reciprocal lattice vector corresponding to a set of planes $(h\ k\ l)$ as:

$$\overline{r^{*}_{hkl}} = h\overline{a^{*}} + k\overline{b^{*}} + l\overline{c^{*}}.$$

This vector is perpendicular to the $(h\ k\ l)$ plane, and its magnitude is the reciprocal of the interplanar spacing d_{hkl}:

$$|\overline{r^{*}_{hkl}}| = \frac{1}{d_{hkl}}.$$

The magnitude of any vector v is defined by:

$$|\overline{v}| = \sqrt{\overline{v} \cdot \overline{v}}.$$

Applying this to $\overline{r^*_{hkl}}$, we have:

For a general crystal system, one must first determine the reciprocal vectors $\overline{a^*}$, $\overline{b^*}$, and $\overline{c^*}$, compute the dot products, and then obtain $|\overline{r^*_{hkl}}|$ to find the interplanar spacing $d_{hkl} = 1/|\overline{r^*_{hkl}}|$.

In the case of an orthorhombic lattice, where all axes are mutually perpendicular ($\alpha^* = \beta^* = \gamma^* = 90^\circ$), the cross terms vanish because $cos 90^\circ = 0$. Consequently, the magnitude of the reciprocal lattice vector simplifies to:

$$|\overline{r^*_{hkl}}|^2 = h^2|\overline{a^*}|^2 + k^2|\overline{b^*}|^2 + l^2|\overline{c^*}|^2.$$

This provides a straightforward expression for the interplanar spacing of $(h\ k\ l)$ planes in an orthorhombic lattice.

For an orthogonal axis system, the reciprocal lattice vectors $\overline{a^*}$, $\overline{b^*}$, and $\overline{c^*}$ can be determined from the definitions:

$$\overline{a^*} = \frac{\overline{b}\times\overline{c}}{V}, \quad \overline{b^*} = \frac{\overline{c}\times\overline{a}}{V}, \quad \overline{c^*} = \frac{\overline{a}\times\overline{b}}{V},$$

where V is the volume of the unit cell. In an orthogonal system, the angle between any two real lattice vectors is 90°, and the volume is simply $V = abc$. Since $sin 90^\circ = 1$, it follows that the magnitudes of the reciprocal vectors are:

$$|\overline{a^*}| = \frac{1}{a}, \quad |\overline{b^*}| = \frac{1}{b}, \quad |\overline{c^*}| = \frac{1}{c}.$$

Therefore, for an orthorhombic lattice, the square of the reciprocal lattice vector corresponding to the $(h\ k\ l)$ plane is:

$$|r^*|^2 = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} = \frac{1}{d^2_{hkl}},$$

which reproduces the familiar relationship for the interplanar spacing d_{hkl} in an orthorhombic crystal system.

This formalism also provides a straightforward derivation of the Zone Weiss Law. For any plane $(h\ k\ l)$, let the reciprocal lattice vector be

$$\overline{r^*_{hkl}} = h\overline{a^*} + k\overline{b^*} + l\overline{c^*}.$$

If a direction $[u\ v\ w]$ lies within the plane $(h\ k\ l)$, then $\overline{r^*_{hkl}}$ is perpendicular to it:

$$\overline{r^*_{hkl}} \cdot \overline{u} = 0, \quad where \quad \overline{u} = u\overline{a} + v\overline{b} + w\overline{c}.$$

Expanding the dot product yields:

$$hu\,\overline{a^*} \cdot \overline{a} + kv\,\overline{b^*} \cdot \overline{b} + lw\,\overline{c^*} \cdot \overline{c} = 0,$$

and since $\overline{a^*} \cdot \overline{a} = \overline{b^*} \cdot \overline{b} = \overline{c^*} \cdot \overline{c} = 1$, we obtain the Zone Weiss Law:

$$hu + kv + lw = 0.$$

This demonstrates the utility of the reciprocal lattice in simplifying crystallographic problems.

Another application is the determination of angles between two planes. Consider planes $(h_1\ k_1\ l_1)$ and $(h_2\ k_2\ l_2)$ in the lattice. Let their normals in reciprocal space be

$$\overline{r^*_1} = h_1\overline{a^*} + k_1\overline{b^*} + l_1\overline{c^*}, \quad \overline{r^*_2} = h_2\overline{a^*} + k_2\overline{b^*} + l_2\overline{c^*}.$$

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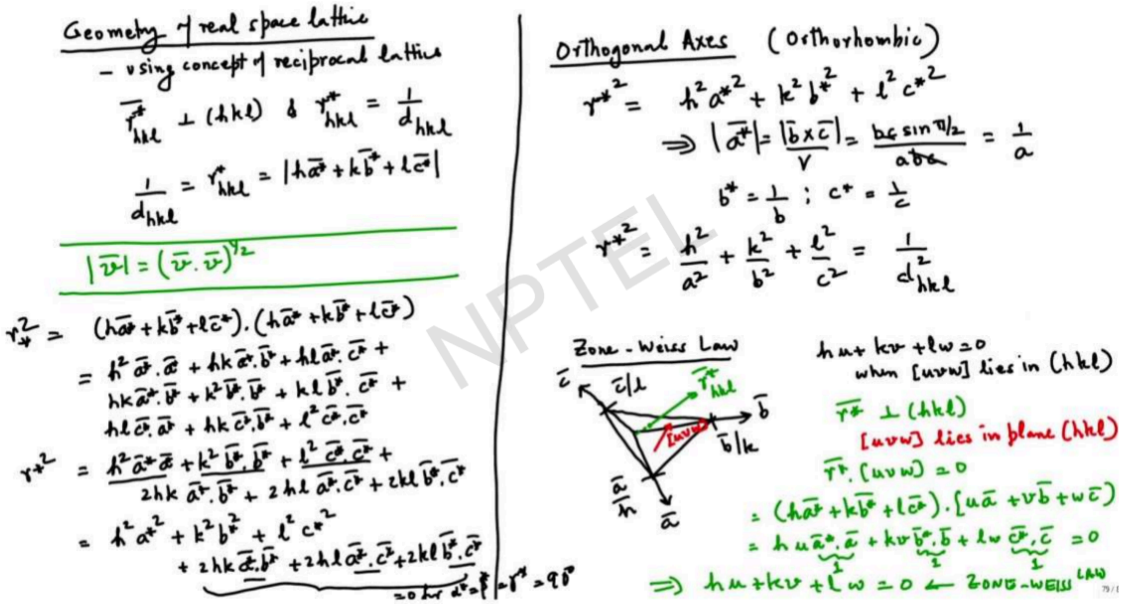

The angle θ between the planes is the angle between their normals:

$$cos\theta = \frac{\overline{r_1^*}\cdot\overline{r_2^*}}{|\overline{r_1^*}|\,|\overline{r_2^*}|}.$$

For an orthorhombic lattice, where all axes are mutually perpendicular, the reciprocal vectors satisfy $\overline{a^*}\cdot\overline{b^*} = \overline{a^*}\cdot\overline{c^*} = \overline{b^*}\cdot\overline{c^*} = 0$, and their magnitudes are $|\overline{a^*}| = 1/a$, $|\overline{b^*}| = 1/b$, $|\overline{c^*}| = 1/c$. Thus, the dot product simplifies to:

$$\overline{r_1^*}\cdot\overline{r_2^*} = \frac{h_1h_2}{a^2} + \frac{k_1k_2}{b^2} + \frac{l_1l_2}{c^2},$$

and the magnitudes are:

$$|\overline{r_1^*}| = \sqrt{\frac{h_1^2}{a^2} + \frac{k_1^2}{b^2} + \frac{l_1^2}{c^2}}, \quad |\overline{r_2^*}| = \sqrt{\frac{h_2^2}{a^2} + \frac{k_2^2}{b^2} + \frac{l_2^2}{c^2}}.$$

Hence, the angle between the planes in an orthorhombic lattice is:

$$cos\theta = \frac{\frac{h_1h_2}{a^2}+\frac{k_1k_2}{b^2}+\frac{l_1l_2}{c^2}}{\sqrt{\frac{h_1^2}{a^2}+\frac{k_1^2}{b^2}+\frac{l_1^2}{c^2}}\sqrt{\frac{h_2^2}{a^2}+\frac{k_2^2}{b^2}+\frac{l_2^2}{c^2}}}.$$

For a cubic lattice, where $a = b = c$, this expression simplifies further to:

$$cos\theta = \frac{h_1h_2+k_1k_2+l_1l_2}{\sqrt{h_1^2+k_1^2+l_1^2}\sqrt{h_2^2+k_2^2+l_2^2}}.$$

Thus, using reciprocal lattice vectors, the angles between any two planes in a lattice can be easily determined. This concludes the discussion of angles between planes using reciprocal lattice concepts.

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Angles (θ) between $(h_1k_1l_1)$ and $(h_2k_2l_2)$

$$\overline{r_1^*} = h_1\overline{a^*} + k_1\overline{b^*} + l_1\overline{c^*}$$

$$\overline{r_2^*} = h_2\overline{a^*} + k_2\overline{b^*} + l_2\overline{c^*}$$

Find angle (θ) between $\overline{r_1^*}$ and $\overline{r_2^*}$

$$\overline{r_1^*}\cdot\overline{r_2^*} = r_1^* r_2^* \cos\theta$$

$$\cos\theta = \frac{\overline{r_1^*}\cdot\overline{r_2^*}}{r_1^* r_2^*}$$

Orthorhombic

$$a^* = \frac{1}{a};\ b^* = \frac{1}{b},\ c^* = \frac{1}{c}$$

$$\overline{a^*}\cdot\overline{b^*} = \overline{a^*}\cdot\overline{c^*} = \overline{b^*}\cdot\overline{c^*} = \ldots = 0$$

$$\overline{a^*}\cdot\overline{a^*} = \frac{1}{a^2};\ \overline{b^*}\cdot\overline{b^*} = \frac{1}{b^2};\ \overline{c^*}\cdot\overline{c^*} = \frac{1}{c^2}$$

$$\cos\theta = \frac{\frac{h_1h_2}{a^2}+\frac{k_1k_2}{b^2}+\frac{l_1l_2}{c^2}}{\left(\frac{h_1^2}{a^2}+\frac{k_1^2}{b^2}+\frac{l_1^2}{c^2}\right)^{1/2}\left(\frac{h_2^2}{a^2}+\frac{k_2^2}{b^2}+\frac{l_2^2}{c^2}\right)}$$

Cubic

$$a = b = c$$

$$\cos\theta = \frac{h_1h_2+k_1k_2+l_1l_2}{(h_1^2+k_1^2+l_1^2)^{1/2}(h_2^2+k_2^2+l_2^2)^{1/2}}.$$