CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

Prof. Sandeep Sangal

IIT Kanpur

Lecture 47: The Reciprocal Lattice

In this lecture, I introduce an important concept known as the reciprocal lattice. We examine how the reciprocal lattice is related to the real lattice and discuss its applications in crystallography and X-ray diffraction. We therefore begin our discussion with the reciprocal lattice.

We start with what is referred to as the real-space lattice. A real-space lattice is defined by the vectors $\bar{a}$, $\bar{b}$, and $\bar{c}$, which are the unit-cell vectors that we have been using so far. Corresponding to this real lattice, we define another lattice, called the reciprocal lattice, which is described by a different set of three vectors denoted as $\overline{a^*}$, $\overline{b^*}$, and $\overline{c^*}$.

Let us now examine the relationship between the vectors $\bar{a}$, $\bar{b}$, $\bar{c}$ and their corresponding reciprocal vectors $\overline{a^*}$, $\overline{b^*}$, and $\overline{c^*}$. This relationship can be expressed in terms of dot products. One set of relationships is given by taking the dot product of each reciprocal lattice vector with its corresponding real-space vector. Thus, $\overline{a^*} \cdot \bar{a}$, $\overline{b^*} \cdot \bar{b}$, and $\overline{c^*} \cdot \bar{c}$ are all equal to the same positive quantity. In crystallography, this quantity is conventionally chosen to be unity. Hence, we use the relations

$$\overline{a^*} \cdot \bar{a} = \overline{b^*} \cdot \bar{b} = \overline{c^*} \cdot \bar{c} = 1.$$

A second set of relationships involves dot products between reciprocal lattice vectors and non-corresponding real-space vectors. Specifically,

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

If we are given a set of vectors $\bar{a}$, $\bar{b}$, and $\bar{c}$ along with another set $\overline{a^*}$, $\overline{b^*}$, and $\overline{c^*}$, and if these two sets satisfy the above relationships, then the two lattices are related in a reciprocal manner. They are referred to as reciprocal lattices because of these mutually orthogonal and normalized properties.

Let us now examine how one can determine the reciprocal lattice vectors when a given set of real-space vectors $\overline{a}$, $\overline{b}$, and $\overline{c}$ is known. Consider the relationships stated above. From $\overline{a^*} \cdot \overline{b} = 0$ and $\overline{a^*} \cdot \overline{c} = 0$, it follows that the reciprocal lattice vector $\overline{a^*}$ is perpendicular to both $\overline{b}$ and $\overline{c}$. This implies that $\overline{a^*}$ is perpendicular to the bc plane of the real lattice. Similarly, the reciprocal lattice vector $\overline{b^*}$ is perpendicular to the ac plane, and the reciprocal lattice vector $\overline{c^*}$ is perpendicular to the ab plane of the real lattice.

Let us now explicitly determine the reciprocal lattice vector $\overline{a^*}$. Since $\overline{a^*}$ is perpendicular to the bc plane, it must be parallel to the vector $\overline{b} \times \overline{c}$. Therefore, a^* can be written as a scalar multiple of this cross product,

$$\overline{a^*} = \beta(\overline{b} \times \overline{c}),$$

where β is a scalar constant.

To determine β, we take the dot product of both sides with $\overline{a}$. This gives

$$\overline{a^*} \cdot \overline{a} = \beta \overline{a} \cdot (\overline{b} \times \overline{c}).$$

From the defining reciprocal-lattice condition, we already have $\overline{a^*} \cdot \overline{a} = 1$. Hence,

$$\beta \overline{a} \cdot (\overline{b} \times \overline{c}) = 1.$$

The quantity $\overline{a} \cdot (\overline{b} \times \overline{c})$ has a clear geometric interpretation. Consider the real-space unit cell defined by the vectors $\overline{a}$, $\overline{b}$, and $\overline{c}$. The magnitude of $\overline{b} \times \overline{c}$ is equal to $bc\sin\alpha$, where α is the angle between $\overline{b}$ and $\overline{c}$. This represents the area of the parallelogram formed by $\overline{b}$ and $\overline{c}$. Taking the dot product with $\overline{a}$ introduces the factor $\cos\theta$, where θ is the angle between $\bar{a}$ and $\bar{b} \times \bar{c}$. Multiplying this area by the component of a perpendicular to the bc plane gives the volume of the unit cell, denoted by V. Thus,

$$\bar{a} \cdot (\bar{b} \times \bar{c}) = V.$$

This immediately implies that

$$\beta = \frac{1}{V}.$$

Therefore, the reciprocal lattice vector $\overline{a^*}$ can be written as

$$\overline{a^*} = \frac{\bar{b}\times\bar{c}}{V} = \frac{\bar{b}\times\bar{c}}{\bar{a}\cdot(\bar{b}\times\bar{c})}.$$

In a similar manner, the remaining reciprocal lattice vectors can be obtained as

$$\overline{b^*} = \frac{\bar{c}\times\bar{a}}{V}, \qquad \overline{c^*} = \frac{\bar{a}\times\bar{b}}{V}.$$

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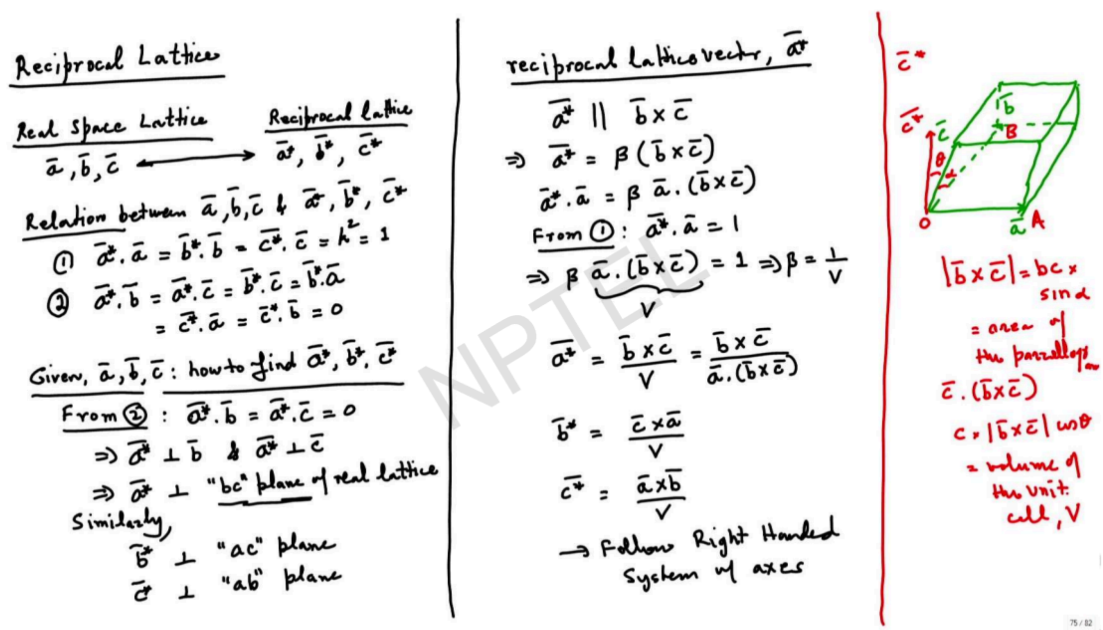

One important point to note here is that we must be very careful while writing cross products. For example, we cannot arbitrarily write $\bar{a} \times \bar{b}$ in place of $\bar{b} \times \bar{a}$. The order of the vectors in a cross product matters because we are following a right-handed coordinate system. If the order is reversed, the resulting vector will point in the opposite direction. Thus, $\overline{a} \times \overline{b}$ and $\overline{b} \times \overline{a}$ represent vectors of equal magnitude but opposite direction.

Let us now examine what happens if we take the reciprocal of the reciprocal lattice. Taking the reciprocal of the reciprocal lattice involves forming cross products of the reciprocal lattice vectors and dividing by the volume of the reciprocal unit cell. For example, the real-space lattice vector $\overline{a}$ can be obtained as

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

where V^* is the volume of the reciprocal unit cell. Similarly, the real-space lattice vector $\overline{b}$ is given by

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

and the real-space lattice vector $\overline{c}$ is given by

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

Thus, taking the reciprocal of the reciprocal lattice leads us back to the original real-space lattice.

We now examine how the volume of the reciprocal unit cell V^* is related to the volume V of the real-space unit cell. Consider the dot product between $\overline{c}$ and $\overline{c^*}$. From the defining properties of the reciprocal lattice, we already know that

$$\overline{c} \cdot \overline{c^*} = 1.$$

The reciprocal lattice vector $\overline{c^*}$ can be written as

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

and the real-space vector c can be expressed, in terms of reciprocal lattice vectors, as

$$\bar{c} = \frac{\bar{a}^* \times \bar{b}^*}{V^*}.$$

Taking the dot product gives

$$\bar{c} \cdot \bar{c}^* = \frac{(\bar{a} \times \bar{b}) \cdot (\bar{a}^* \times \bar{b}^*)}{VV^*}.$$

Expanding the numerator using vector identities, this expression can be written as

$$\frac{(\bar{a}^* \cdot \bar{a})(\bar{b} \cdot \bar{b}^*) - (\bar{b} \cdot \bar{a}^*)(\bar{a} \cdot \bar{b}^*)}{VV^*}.$$

From the reciprocal lattice relations, $\bar{a}^* \cdot \bar{a} = 1$ and $\bar{b} \cdot \bar{b}^* = 1$, while the mixed dot products $\bar{b} \cdot \bar{a}^*$ and $\bar{a} \cdot \bar{b}^*$ are zero. Hence, the numerator reduces to unity, and we obtain

$$\bar{c} \cdot \bar{c}^* = \frac{1}{VV^*}.$$

Since this dot product is also equal to 1, it follows that

$$V^* = \frac{1}{V}.$$

Thus, the volume of the reciprocal unit cell is the reciprocal of the volume of the real-space unit cell.

We now consider a more general reciprocal lattice vector. Just as in real space we can define a lattice vector $\bar{r}$, in reciprocal space we can also define a reciprocal lattice vector, which we denote by $\bar{r}^*$. Because the reciprocal lattice also possesses translational symmetry, a general reciprocal lattice vector can be written as

$$\bar{r}^* = h\bar{a}^* + k\bar{b}^* + l\bar{c}^*,$$

where h, k, and l are integers.

We now wish to establish the relationship between the reciprocal lattice vector $\bar{r}^*$ and the real-space lattice planes indexed by (hkl). Consider the real-space axes defined by a, b, and c, and let the plane (hkl) intersect the a, b, and c axes at points A, B, and C, respectively. In terms of Miller indices, the intercepts are given by $\overline{OA} = a/h$, $\overline{OB} = b/k$, and $\overline{OC} = c/l$.

Let us now examine the relationship between $\overline{r}^*$ and the plane (hkl). Consider the vector $\overline{AB}$ lying in the plane. This vector can be written as

$$\overline{AB} = \overline{OB} - \overline{OA} = \frac{\overline{b}}{k} - \frac{\overline{a}}{h}.$$

Taking the dot product of $\overline{r}^*$ with AB gives

$$\overline{r}^* \cdot \overline{AB} = \left(h\overline{a}^* + k\overline{b}^* + l\overline{c}^*\right) \cdot \left(\frac{\overline{b}}{k} - \frac{\overline{a}}{h}\right).$$

Expanding this expression term by term, we observe that all mixed dot products vanish because $\overline{a}^* \cdot \overline{b} = 0$, $\overline{b}^* \cdot \overline{a} = 0$, and similarly for the remaining mixed terms. The only surviving terms are

$$-\overline{a}^* \cdot \overline{a} + \overline{b}^* \cdot \overline{b},$$

which evaluates to $-1 + 1 = 0$. Hence,

$$\overline{r}^* \cdot \overline{AB} = 0.$$

By similar arguments, it can be shown that $\overline{r}^*$ is also perpendicular to the vectors $\overline{BC}$ and $\overline{AC}$. Therefore, the reciprocal lattice vector

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

is perpendicular to the real-space plane (hkl).

We now determine the magnitude of $\overline{r}^*$. Let n be a unit vector normal to the plane (hkl). The dot product of n with the vector $\overline{OA}$ gives the interplanar spacing d_{hkl}. Since $\overline{r}^*$ is

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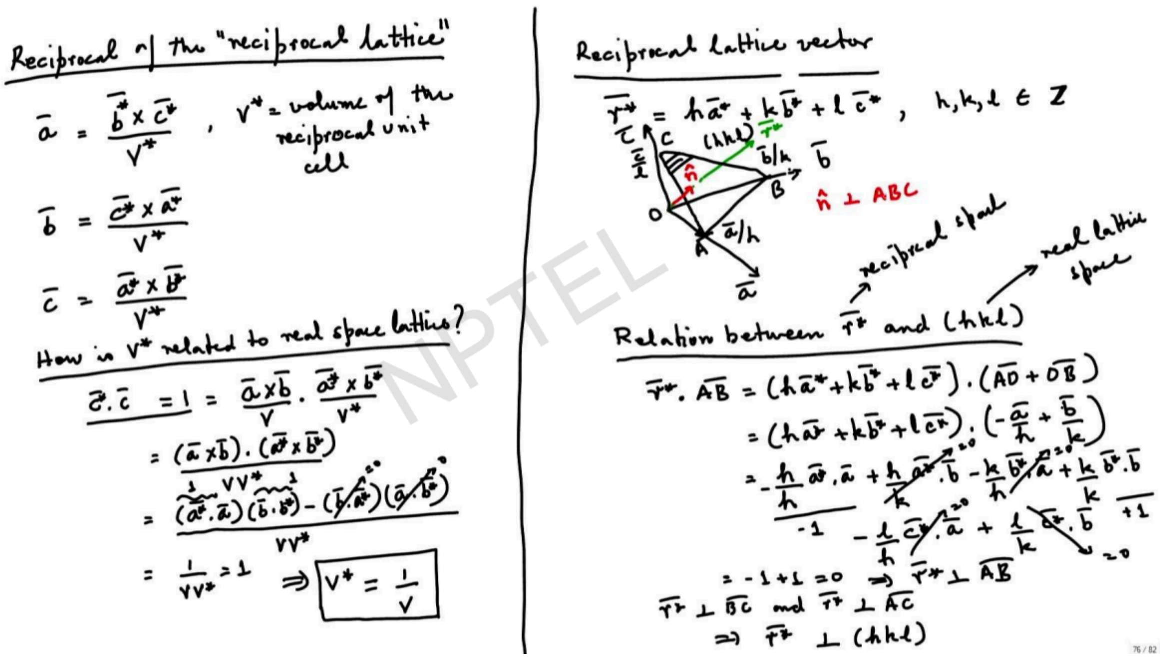

normal to the plane, the unit vector n can be written as

$$\hat{n} = \frac{\overline{r}^*}{|\overline{r}^*|}.$$

Thus,

$$d_{hkl} = \hat{n} \cdot \overline{OA} = \frac{\overline{r}^*}{|\overline{r}^*|} \cdot \frac{\overline{a}}{h}.$$

Substituting $r^* = h\overline{a}^* + k\overline{b}^* + l\overline{c}^*$, the only nonzero contribution arises from the term involving $\overline{a}^* \cdot \overline{a} = 1$. Hence,

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

Therefore, the magnitude of the reciprocal lattice vector r^* is simply the reciprocal of the interplanar spacing of the plane to which it is perpendicular. We will continue this discussion in the next lecture.

Thank you.

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Magnitude of $\overline{r^*}$?

$$d = \hat{n} \cdot \overline{OA}$$

d = interplanar spacing of (hkl)

$$\hat{n} = \frac{\overline{r^*}}{|\overline{r^*}|} = \frac{\overline{r^*}}{r^*}$$

$$d = \frac{\overline{r^*} \cdot \overline{OA}}{r^*} = \frac{(h\bar{a}^* + k\bar{b}^* + l\bar{c}^*) \cdot \bar{a}/h}{r^*}$$

$$= \frac{(h/h)\,\bar{a}^* \cdot \bar{a}}{r^*} = \frac{1}{r^*} \quad (\bar{a}^* \cdot \bar{a} = 1)$$

$$\therefore r^* = \frac{1}{d}$$