CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

Prof. Sandeep Sangal

IIT Kanpur

Lecture 49: Reciprocal Lattice Examples

In the last two lectures, we discussed the reciprocal lattice and its application to computations in crystallography. In this lecture, we examine how the reciprocal lattice and diffraction are related. Before proceeding, we will consider several examples in which a real lattice and its corresponding reciprocal lattice are drawn together to illustrate the relationship between real space and reciprocal space.

Let us begin with a primitive orthorhombic lattice. In real space, lattice points exist only at the corners. We consider a projection of the reciprocal lattice along the c axis, where the $\overline{a}$ and $\overline{b}$ vectors lie in the plane and the $\overline{c}$ vector is perpendicular to it. For clarity, we assign the following arbitrary values: $a = 2$ Å, $b = 4$ Å, and $c = 8$ Å.

Correspondingly, the reciprocal lattice is defined by vectors $\overline{a^*}$, $\overline{b^*}$, and $\overline{c^*}$. Since the lattice is orthorhombic, all three axes are mutually perpendicular, implying $\alpha = \beta = \gamma = 90^\circ$. Consequently, in reciprocal space, $\alpha^* = \beta^* = \gamma^* = 90^\circ$.

The magnitudes of the reciprocal lattice vectors are given by:

$$a^* = \frac{1}{a} = 0.5\ \text{Å}^{-1}, \quad b^* = \frac{1}{b} = 0.25\ \text{Å}^{-1}, \quad c^* = \frac{1}{c} = 0.125\ \text{Å}^{-1}.$$

Since we are considering the projection along $\overline{c}$, $\overline{c^*}$ is perpendicular to the figure. Although the shape of the reciprocal lattice mirrors that of the real lattice, the dimensions differ. Note that the units are inverse angstroms (Å^{-1}).

Consider a set of planes in the real lattice with Miller indices (110). In reciprocal space, these planes are represented by the reciprocal lattice point corresponding to the vector $\overline{r^*_{110}}$, given by

$$\overline{r^*_{110}} = 1 \cdot \overline{a^*} + 1 \cdot \overline{b^*} + 0 \cdot \overline{c^*}.$$

The vector $\overline{r^*_{110}}$ is perpendicular to the (110) plane, and its magnitude is the reciprocal of the interplanar spacing d_{110}:

$$|\overline{r^*_{110}}| = \frac{1}{d_{110}}.$$

Thus, each point in the reciprocal lattice represents a set of (hkl) planes in real space.

For a primitive cubic lattice with lattice parameters $a = b = c = 2$ Å, lattice points exist at the corners. Considering the reciprocal lattice, the magnitudes of $\overline{a^*}$, $\overline{b^*}$, and $\overline{c^*}$ are all equal:

$$a^* = b^* = c^* = \frac{1}{a} = 0.5\ \text{Å}^{-1},$$

with angles $\alpha^* = \beta^* = \gamma^* = 90^\circ$. A plane with Miller indices (110) in real space is represented by the reciprocal lattice vector $\overline{r^*_{110}}$, which is perpendicular to the

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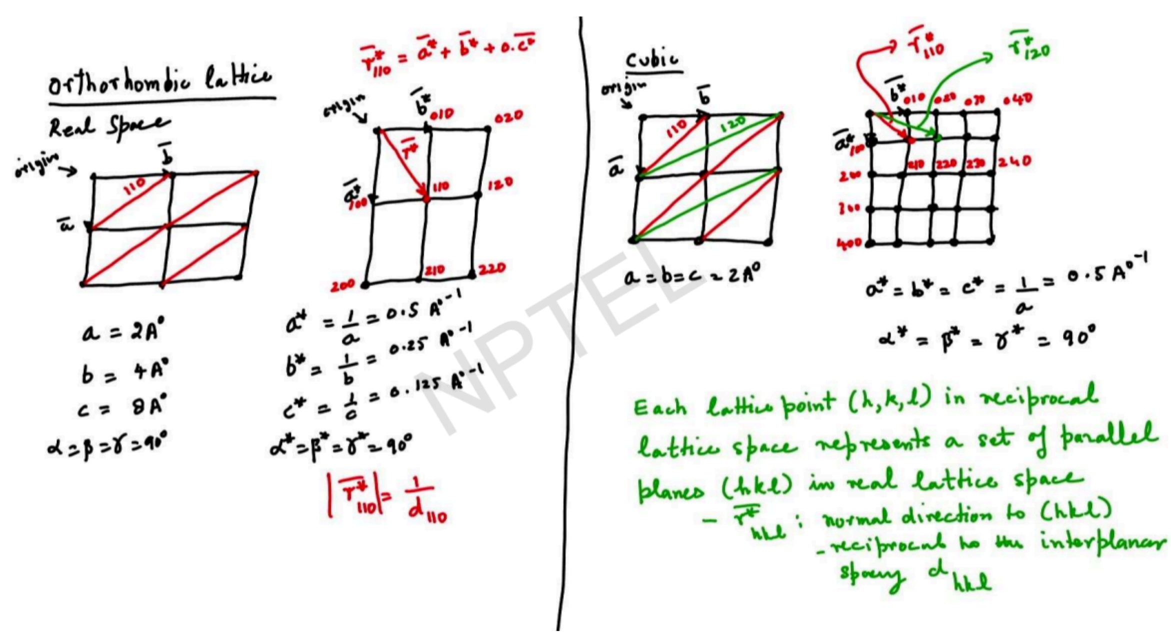

corresponding set of planes. Other planes, such as (120), are represented similarly by $\overline{r^*}_{120}$, with each vector perpendicular to the respective plane. In general, a reciprocal lattice point (hkl) represents a set of parallel (hkl) planes in real space, and the corresponding reciprocal lattice vector $\overline{r^*}_{hkl}$ encodes the normal direction to these planes. Its magnitude is the reciprocal of the interplanar spacing d_{hkl}.

Next, consider a primitive hexagonal lattice, where lattice points exist at all corners. Let $\overline{a}$ and $\overline{b}$ lie in the plane, $\overline{c}$ is perpendicular to the plane, and the angle between $\overline{a}$ and $\overline{b}$ is γ. Assume $a = b = 2$ Å, $c = 4$ Å, $\alpha = \beta = 90^\circ$, and $\gamma = 120^\circ$.

The reciprocal lattice vectors are defined as follows:

- $\overline{a^*}$ is perpendicular to $\overline{b}$ and $\overline{c}$,
- $\overline{b^*}$ is perpendicular to $\overline{a}$ and $\overline{c}$,
- $\overline{c^*}$ is perpendicular to $\overline{a}$ and $\overline{b}$.

If the real lattice vector b is horizontal, the corresponding $\overline{a^*}$ vector is vertical. The angle γ^* between $\overline{a^*}$ and $\overline{b^*}$ can be calculated using the relation:

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

Substituting $\alpha = \beta = 90^\circ$ and $\gamma = 120^\circ$, we obtain:

$$cos\gamma^* = - cos120^\circ = 0.5 \quad \Rightarrow \quad \gamma^* = 60^\circ.$$

The magnitudes of the reciprocal lattice vectors can also be calculated from first principles:

$$|\overline{a}^*| = |\overline{b}^*| = \frac{1}{\sqrt{3}}, \quad |\overline{c}^*| = \frac{1}{d_{001}} = \frac{1}{4\ \text{Å}} = 0.25\ \text{Å}^{-1}.$$

Thus, the reciprocal lattice provides a compact representation of the geometry of the real lattice. In the next lecture, we will relate these concepts to diffraction and examine how the reciprocal lattice framework can be applied to interpret diffraction patterns.

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