Chapter #2:
X-Ray Diffraction and the Reciprocal Lattice

Lecture 3: Reciprocal Lattice – Formal Definition, Properties, and Diffraction Condition

1. Introduction

In the previous lectures, we derived Bragg's law and established the condition for constructive interference in X-ray diffraction. The set of points in reciprocal space that satisfy Bragg's condition form what is known as the reciprocal lattice.

Therefore, reciprocal space provides a simpler geometric interpretation of diffraction phenomena.

Why do we need the reciprocal lattice?

We need the reciprocal lattice because waves (like X-rays, electrons, neutrons) interact with crystals in wave-vector (momentum) space, not real space. The reciprocal lattice is the natural language for describing diffraction, Bragg conditions, and electronic structure.

2. Definition of Reciprocal Lattice Vectors

If the primitive vectors of the direct lattice are $\mathbf{a_1}$, $\mathbf{a_2}$, and $\mathbf{a_3}$, we define three new vectors $\mathbf{b_1}$, $\mathbf{b_2}$, and $\mathbf{b_3}$ such that:

1- $$e^{i\Delta\vec{k}.\vec{R}} = 1$$

2- $$a_i . b_j = 2\pi\delta_{ij}$$

where δ_{ij} is the Kronecker delta symbol:

$\delta_{ij} = 1$ if $i = j$

$\delta_{ij} = 0$ if $i \neq j$

$$a_1 . b_1 = 2\pi$$
$$a_1 . b_2 = 0$$

The vectors $\mathbf{b_1}$, $\mathbf{b_2}$, and $\mathbf{b_3}$ are called the reciprocal lattice primitive vectors.

3. Dimensional Analysis

The dimensions of direct lattice vectors are length (L), while the dimensions of reciprocal lattice vectors are inverse length (L^{-1}). Therefore, the wave vector **k** has the same physical dimension as a reciprocal lattice vector.

$$a_i \sim length$$

$$b_i \sim \frac{1}{length}$$

This confirms that reciprocal space is naturally associated with momentum space.

Remember that:

$$k = \frac{2\pi}{\lambda}$$

$$p = \hbar k$$

4. Explicit Form of Reciprocal Lattice Vectors

The reciprocal lattice vectors can be written as:

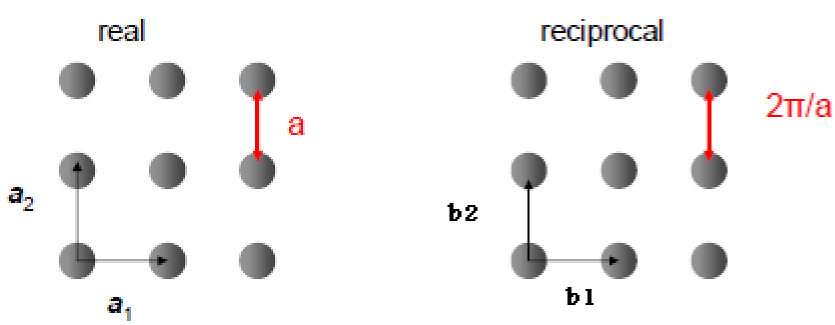
$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 x \vec{a}_3}{V} = 2\pi \frac{\vec{a}_2 x \vec{a}_3}{\vec{a}_1 . (\vec{a}_2 x \vec{a}_3)}$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 x \vec{a}_1}{V}$$

$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 x \vec{a}_2}{V}$$

where $V = \vec{a}_1 . (\vec{a}_2 x \vec{a}_3)$ is the volume of the primitive cell.

In crystallography, the factor 2π is sometimes omitted, while in solid-state physics it is typically retained.



5. Orthogonality Properties

Let's check the validation of equations (1) and (2).

$$\vec{a}_1.\vec{b}_1 = \vec{a}_1.2\pi \ \frac{\vec{a}_2 x\vec{a}_3}{\vec{a}_1.(\vec{a}_2 x\vec{a}_3)} = 2\pi \frac{\vec{a}_1.(\vec{a}_2 x\vec{a}_3)}{\vec{a}_1.(\vec{a}_2 x\vec{a}_3)} = 2\pi$$

$$\vec{a}_1.\vec{b}_2 = \vec{a}_1. \ 2\pi \ \frac{\vec{a}_3 x\vec{a}_1}{\vec{a}_1.(\vec{a}_2 x\vec{a}_3)} = 2\pi a^3 \frac{\hat{x}.(\hat{z} \ \mathrm{x} \ \hat{x})}{\vec{a}_1.(\vec{a}_2 x\vec{a}_3)} = 2\pi a^3 \frac{\hat{x}.\hat{y}}{\vec{a}_1.(\vec{a}_2 x\vec{a}_3)} = 0$$

- Each reciprocal vector is perpendicular to the plane formed by the other two direct lattice vectors. For example, b_1 is perpendicular to the plane formed by a_2 and a_3.
- If the direct lattice vectors $\vec{a}_1, \vec{a}_2, and\ \vec{a}_3$ are mutually orthogonal, then the reciprocal lattice vectors also form an orthogonal set. In this special case, each reciprocal vector $\vec{b}_i$ is parallel to the corresponding direct vector $\vec{a}_i$.
- However, in non-orthogonal lattices (i.e., Monoclinic, Triclinic), the reciprocal lattice vectors are not necessarily parallel to the direct lattice vectors.

6. General Reciprocal Lattice Vector

A general reciprocal lattice vector can be written as:

$$\vec{G} = m_1\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3$$

where m_1, m_2, m_3 are integers.

We can also check the validations of equations (1) and (2).

$$e^{i\vec{G}.\vec{R}} = e^{i(m_1\vec{b}_1+m_2\vec{b}_2+m_3\vec{b}_3).(n_1\vec{a}_1+n_2\vec{a}_2+n_3\vec{a}_3)}$$

$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

Since; $a_i.b_j = 2\pi\delta_{ij}$

Then, $$e^{i2\pi(m_1n_1+m_2n_2+m_3n_3)} = e^{i2\pi n} = 1$$

Where **n** is an integer.

7. Diffraction Condition in Reciprocal Space

Theory: the set of reciprocal lattice vectors G determines the possible X-ray diffractions.

From the diffraction condition derived in the previous lecture:

$$(\vec{k}^\backslash - \vec{k}).\vec{R} = \Delta\vec{k}.\vec{R} = 2\pi n$$

Therefore, we can say that the scattering vector $\Delta\vec{k}$ is equivalent to the reciprocal lattice vector $\vec{G}$.

($\Delta\vec{k} = \vec{G}$)

This means that diffraction occurs when the change in wave vector equals a reciprocal lattice vector. This condition is completely equivalent to Bragg's law.

Therefore, the set of reciprocal lattice vectors determines all possible X-ray reflections.

- This is the Laue condition for diffraction.

See some visualizations of the reciprocal lattices

http://www.msm.cam.ac.uk/doitpoms/tlplib/reciprocal_lattice/reciprocal_lattice.php

http://www.matter.org.uk/diffraction/geometry/lattice_vectors.htm

❑ Reciprocal Lattices to SC, FCC, and BCC

	Direct lattice	Reciprocal lattice	Volume
SC	$\begin{cases} \mathbf{a}_1 = a\mathbf{x} \\ \mathbf{a}_2 = a\mathbf{y} \\ \mathbf{a}_3 = a\mathbf{z} \end{cases}$	$\begin{cases} \mathbf{b}_1 = (2\pi/a)\mathbf{x} \\ \mathbf{b}_2 = (2\pi/a)\mathbf{y} \\ \mathbf{b}_3 = (2\pi/a)\mathbf{z} \end{cases}$	$(2\pi/a)^3$
FCC	$\begin{cases} \mathbf{a}_1 = \frac{1}{2}a(\mathbf{x}+\mathbf{y}) \\ \mathbf{a}_2 = \frac{1}{2}a(\mathbf{y}+\mathbf{z}) \\ \mathbf{a}_3 = \frac{1}{2}a(\mathbf{z}+\mathbf{x}) \end{cases}$	$\begin{cases} \mathbf{b}_1 = \frac{2\pi}{a}(-\mathbf{x}+\mathbf{y}-\mathbf{z}) \\ \mathbf{b}_2 = \frac{2\pi}{a}(\mathbf{x}-\mathbf{y}+\mathbf{z}) \\ \mathbf{b}_3 = \frac{2\pi}{a}(\mathbf{x}+\mathbf{y}-\mathbf{z}) \end{cases}$	$2(2\pi/a)^3$
BCC	$\begin{cases} \mathbf{a}_1 = \frac{1}{2}a(\mathbf{x}+\mathbf{y}-\mathbf{z}) \\ \mathbf{a}_2 = \frac{1}{2}a(-\mathbf{x}+\mathbf{y}+\mathbf{z}) \\ \mathbf{a}_3 = \frac{1}{2}a(\mathbf{x}-\mathbf{y}+\mathbf{z}) \end{cases}$	$\begin{cases} \mathbf{b}_1 = \frac{2\pi}{a}(\mathbf{y}+\mathbf{z}) \\ \mathbf{b}_2 = \frac{2\pi}{a}(\mathbf{x}+\mathbf{z}) \\ \mathbf{b}_3 = \frac{2\pi}{a}(\mathbf{x}+\mathbf{y}) \end{cases}$	$4(2\pi/a)^3$

8. Exercises

1. Show that the reciprocal of the reciprocal lattice of a simple cubic lattice is again simple cubic.

2. Determine the Bravais lattice of the reciprocal lattice of BCC.

3. Determine the Bravais lattice of the reciprocal lattice of FCC.