Chapter 2 Reciprocal Lattice

An important concept for analyzing periodic structures

Reasons for introducing reciprocal lattice

• Theory of crystal diffraction of x-rays, neutrons, and electrons.
  Where are the diffraction maximum? What is the intensity?

• Abstract study of functions with the periodicity of a Bravais lattice
  Fourier transformation. Reciprocal lattice is closely related to Fourier transformation

• Consideration of how momentum conservation will be modified in periodic potential

Basic knowledge: \( e^{i\vec{k} \cdot \vec{r}} \) is a plane wave

\[
e^{i\vec{k} \cdot \vec{r}} = \cos(\vec{k} \cdot \vec{r}) + i \sin(\vec{k} \cdot \vec{r})
\]

a periodic function

Wave vector \( \vec{k} = \frac{2\pi}{\lambda} \hat{n} \)
One dimensional reciprocal lattice

\( f(x) \) One dimensional periodic function

\[
f(x + a) = f(x)
\]

Expand \( f(x) \) into Fourier series

\[
f(x) = f_0 + \sum_{n>0} \left[ c_n \cos\left(\frac{2\pi nx}{a}\right) + s_n \sin\left(\frac{2\pi nx}{a}\right) \right]
\]

\[
= f_0 + \sum_{n>0} \left[ c_n \frac{e^{i\frac{2\pi nx}{a}} + e^{-i\frac{2\pi nx}{a}}}{2} + s_n \frac{e^{i\frac{2\pi nx}{a}} - e^{-i\frac{2\pi nx}{a}}}{2i} \right]
\]

\[
= f_0 + \sum_{n>0} \left[ \left( \frac{c_n}{2} + \frac{s_n}{2i} \right) e^{i\frac{2\pi nx}{a}} + \left( \frac{c_n}{2} - \frac{s_n}{2i} \right) e^{-i\frac{2\pi nx}{a}} \right]
\]

Redefine coefficients

We have

\[
f(x) = \sum_n a_n e^{i\frac{2\pi nx}{a}} = \sum_n a_n e^{iGx}
\]

\[
\text{Constraint that ensures } f(x) \text{ is a real function}
\]

\[
a_n = a_{-n}^*
\]

\( f(x) \) is expanded into a series of plane waves, with a set of wave vectors \( G \)'s.

Each plane wave \( e^{iGx} \) preserve the periodicity of \( f(x) \).

The set of discrete points \( G = \frac{2\pi n}{a} \) is one dimensional reciprocal lattice
• Reciprocal lattice points of a Bravais lattice indicate the allowed terms in the Fourier series of a function with the same periodicity as the Bravais lattice.

• Reciprocal lattice depends on the Bravais lattice, but does not depend on the particular form of \( f(x) \), as long as \( f(x) \) has the periodicity of the Bravais lattice.

• But reciprocal lattice does not indicate the magnitude of each Fourier term \( a_n \), which depends on the exact form of \( f(x) \).

\[
a_n = \frac{1}{a} \int_0^a dx \ f(x) e^{- \frac{2\pi i nx}{a}} = \frac{1}{a} \int_0^a dx \ f(x) e^{-iGx}
\]

Expand to three dimensional case:

Three dimensional periodic function \( f(\vec{r}) \) that satisfies \( f(\vec{r}) = f(\vec{r} + \vec{R}) \)

Fourier expansion:

\[
f(\vec{r}) = \sum_{\vec{G}} a_{\vec{G}} e^{i\vec{G} \cdot \vec{r}} \quad a_{\vec{G}} = \frac{1}{V \text{cell}} \int dV \ f(\vec{r}) e^{-i\vec{G} \cdot \vec{r}}
\]
General definition of reciprocal lattice

Bravais lattice \( \vec{R} \)

a plane wave \( e^{i\vec{G} \cdot \vec{r}} \)

The set of all wave vectors \( \vec{G} \) that yield plane waves \( e^{i\vec{G} \cdot \vec{r}} \) with the periodicity of a given Bravais lattice \( \vec{R} \) is known as its reciprocal lattice.

Analytically, the definition is expressed as 
\[
e^{i\vec{G} \cdot (\vec{r} + \vec{R})} = e^{i\vec{G} \cdot \vec{r}}
\]

The set of \( \vec{G} \) satisfying 
\[
e^{i\vec{G} \cdot \vec{R}} = 1
\]
for all \( \vec{R} \) in a Bravais lattice

- A reciprocal lattice is defined with reference to a particular Bravais lattice
- A set of vectors \( \vec{G} \) satisfying \( e^{i\vec{G} \cdot \vec{R}} = 1 \) is called a reciprocal lattice only if the set of \( \vec{R} \) is a Bravais lattice
- Reciprocal lattice is a Bravais lattice (proven in the following)
Construction of a reciprocal lattice
and Proof that $\vec{G}$ is a Bravais lattice

$\vec{a}_1 \quad \vec{a}_2 \quad \vec{a}_3$ are primitive vectors of a Bravais lattice

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

The reciprocal lattice can be generated by the primitive vectors

$\vec{b}_1 \quad \vec{b}_2 \quad \vec{b}_3$

$\vec{b}_i = 2\pi \frac{\vec{a}_i \times \vec{a}_j}{\vec{a}_i \cdot (\vec{a}_2 \times \vec{a}_3)}$

$V = \vec{a}_i \cdot (\vec{a}_2 \times \vec{a}_3)$

volume of primitive cell

Apparently $\vec{b}_i \cdot \vec{a}_j = 2\pi \delta_{ij}$

An arbitrary vector in reciprocal space can be written as a linear combination of

$\vec{g} = g_1 \vec{b}_1 + g_2 \vec{b}_2 + g_3 \vec{b}_3$

To qualify for a reciprocal lattice, $e^{i\vec{g} \cdot \vec{R}} = 1$ for all $\vec{R}$

$g_i$ has to be integers

Reciprocal lattice vector $\vec{G} = v_1 \vec{b}_1 + v_2 \vec{b}_2 + v_3 \vec{b}_3$

$\vec{b}_i$ is an integer

Apparently, it is also a Bravais lattice with $\vec{b}_i$ as its primitive vectors
The reciprocal of the reciprocal lattice

The reciprocal lattice is a Bravais lattice, one can construct its reciprocal lattice, which turns out to be nothing but the original direct lattice.

\[ \vec{R} \quad \text{Direct lattice} \]
\[ \vec{G} \quad \text{Reciprocal lattice} \]

\[ e^{i\vec{G} \cdot \vec{R}} = 1 \quad \text{for all } \vec{R} \]

Or, every \( \vec{R} \) satisfies \( e^{i\vec{R} \cdot \vec{G}} \) for all \( \vec{G} \)

Look for the reciprocal of the reciprocal lattice: \( \vec{K} \) which satisfies \( e^{i\vec{K} \cdot \vec{G}} = 1 \)

The set of vectors \( \vec{R} \) is a subset of the set of vectors \( \vec{K} \)

\[ \vec{R} \subseteq \vec{K} \]

For any vector that does not belong to the direct lattice \( \vec{R} \):

\[ \vec{r} = x_1 \vec{a}_1 + x_2 \vec{a}_2 + x_3 \vec{a}_3 \quad \text{At least one } x_i \text{ is non-integer} \]

For \( \vec{G} = \vec{b}_i \) we have

\[ e^{i\vec{r} \cdot \vec{G}} = e^{i\vec{r} \cdot \vec{b}_i} = e^{ix_i \vec{a}_i \cdot \vec{b}_i} = e^{i2\pi x_i} \neq 1 \]

So \( r \) does not belong to \( \vec{K} \)

So the set of vectors \( \vec{R} \) is identical to the set of vectors \( \vec{K} \)
Examples of reciprocal lattice

Simple cubic Bravais lattice

\[ \vec{a}_1 = a\hat{x} \quad \vec{a}_2 = a\hat{y} \quad \vec{a}_3 = a\hat{z} \]

Reciprocal lattice

\[ \vec{b}_1 = \frac{2\pi}{a} \hat{x} \quad \vec{b}_2 = \frac{2\pi}{a} \hat{y} \quad \vec{b}_3 = \frac{2\pi}{a} \hat{z} \]

Also a simple cubic lattice

Cubic unit cell with an edge of \( \frac{2\pi}{a} \)

Face centered cubic

\[ \vec{a}_1 = \frac{a}{2} (\hat{y} + \hat{z}) \quad \vec{a}_2 = \frac{a}{2} (\hat{z} + \hat{x}) \quad \vec{a}_3 = \frac{a}{2} (\hat{x} + \hat{y}) \]

\[ V = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = \frac{1}{4}a^3 \]

Primitive vectors of Reciprocal lattice

\[ \vec{b}_1 = \frac{2\pi}{a} (-\hat{x} + \hat{y} + \hat{z}) \quad \vec{b}_2 = \frac{2\pi}{a} (\hat{x} - \hat{y} + \hat{z}) \quad \vec{b}_3 = \frac{2\pi}{a} (\hat{x} + \hat{y} - \hat{z}) \]

They are the primitive vectors of a body centered cubic lattice

Size of the cubic cell: \( \left( \frac{4\pi}{a} \right)^3 \)
Body centered cubic

Primitive vectors

\[
\bar{a}_1 = \frac{a}{2} (-\hat{x} + \hat{y} + \hat{z}) \quad \bar{a}_2 = \frac{a}{2} (\hat{x} - \hat{y} + \hat{z}) \quad \bar{a}_3 = \frac{a}{2} (\hat{x} + \hat{y} - \hat{z})
\]

Primitive vectors for reciprocal lattice

\[
\bar{b}_1 = \frac{2\pi}{a} (\hat{y} + \hat{z}) \quad \bar{b}_2 = \frac{2\pi}{a} (\hat{x} + \hat{z}) \quad \bar{b}_3 = \frac{2\pi}{a} (\hat{x} + \hat{y})
\]

They are the primitive vectors of a fcc lattice

Fcc and bcc are reciprocal to each other

Brillouin Zones

The Wigner Seitz primitive cell of the reciprocal lattice is known as the first Brillouin zone.
The first Brillouin zone is enclosed by perpendicular bisectors between the central lattice point and its 12 nearest neighbors.

It is a regular 12 faced solid.
First Brillouin zone of fcc structure

Primitive vectors of fcc structure

Brillouin zones of fcc structure

The reciprocal lattice is bcc lattice
Lattice planes and reciprocal lattice vectors

Lattice planes: any plane that contains at least three noncollinear Bravais lattice points

Due to translational symmetry, any lattice plane will contain infinitely many lattice points, which form a two dimensional Bravais lattice.

Family of lattice planes:
A set of parallel, equally spaced lattice planes which together contains all the points of the three dimensional Bravais lattice.

Theorem:
For any family of lattice planes separated by a distance $d$, there are reciprocal lattice vectors perpendicular to the planes, the shortest of which have a length of $\frac{2\pi}{d}$. Conversely, for any reciprocal lattice vector $\vec{G}$, there is a family of lattice planes normal to $\vec{G}$ and separated by a distance $d$, where $\frac{2\pi}{d}$ is the length of the shortest reciprocal lattice vector parallel to $\vec{G}$.

The theorem is a direct consequence of
(1) The definition of reciprocal lattice $\quad e^{i\vec{G} \cdot \vec{R}} = 1$
(2) the fact that a plane wave has the same value at all points lying in a family of planes that are perpendicular to its wave vector and separated by an integral number of wavelength.
Proof of the first part of the theorem:

Given a family of lattice planes with a separation of $d$, let $\hat{n}$ be a unit vector normal to the planes. Let’s make up a wave vector:

$$\vec{K} = \frac{2\pi}{d} \hat{n}$$

We need to prove that $\vec{K}$ is a reciprocal lattice vector, and it is the shortest one in that direction.

To qualify for a reciprocal vector, $e^{i\vec{K} \cdot \vec{R}} = 1$ has to be satisfied for all $\vec{R}$ of the Bravais lattice.

We know this condition is satisfied for the origin of the Bravais lattice $\vec{r} = 0$ because $e^{i\vec{K} \cdot \vec{0}} = 1$.

Then $e^{i\vec{K} \cdot \vec{r}} = 1$ must be true for all the lattice points $\vec{r}$ in the lattice plane that contains the origin $\vec{r} = 0$.

Because $\vec{K}$ is perpendicular to that plane, and $\vec{K} \cdot \vec{r}$ should be a constant in the plane

$e^{i\vec{K} \cdot \vec{r}}$ is a periodic function with a wavelength $\lambda = \frac{2\pi}{|\vec{K}|} = d$ in the direction of its wave vector.

The wavelength $\lambda = d$ happens to be the separation of the planes.

Therefore for all the lattice points $\vec{R}$ in the family of planes, $e^{i\vec{K} \cdot \vec{R}} = 1$ is satisfied.

So $\vec{K}$ is a reciprocal vector, and we can write it as $\vec{G} = \frac{2\pi}{d} \hat{n}$. 


If there is another vector \( \vec{G}' \) shorter than \( \vec{G} \),

\[ |\vec{G}'| < |\vec{G}| \]

The wavelength of \( \vec{G}' \) is

\[ \lambda' = \frac{2\pi}{|\vec{G}'|} > d \]

It is impossible for \( e^{i\vec{G}' \cdot \vec{r}} = 1 \) to have the same value on two planes with a distance shorter than the wavelength. So \( \vec{G}' \) can not be a reciprocal vector.

**Proof of the converse of the theorem**

Given a reciprocal lattice vector, let \( \vec{G} \) be the shortest parallel reciprocal lattice vector.

Let's construct a set of real space planes (not necessarily lattice planes) on which \( e^{i\vec{G} \cdot \vec{r}} = 1 \).

Now we need to prove that this set of planes are lattice planes and contains all the Bravais lattice points.

These planes must contain \( \vec{r} = 0 \). They must be all perpendicular to \( \vec{G} \) and separated by a distance \( d = \lambda = \frac{2\pi}{|G|} \).

For all Bravais lattice vector \( \vec{R} \), \( e^{i\vec{G} \cdot \vec{R}} = 1 \) must be true for any reciprocal vector.

So the set of planes must contain all the Bravais lattice points.

Lastly, we need to prove that each of these planes contain lattice points instead of every nth of them.

Suppose only every nth of the planes contain lattice points. According to the first part of the theorem, the shortest reciprocal vector perpendicular to the planes will be, \( \frac{2\pi}{nd} = \frac{G}{n} \), which contradict with assumption that \( G \) is the shortest reciprocal vector in that direction.
Reciprocal lattice vectors and Miller indices of lattice planes

The miller indices of a lattice plane are the coordinates of the shortest reciprocal lattice vector normal to that plane, with respect to a specified set of primitive reciprocal lattice vectors. Thus a plane with Miller indices h, k, l, is normal to the reciprocal lattice vector \( \mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3 \)

Proof

Consider a plane with miller indices h, k, l. \( \mathbf{G} = h'\mathbf{b}_1 + k'\mathbf{b}_2 + l'\mathbf{b}_3 \) is the shortest reciprocal vector normal to that plane. Let’s prove that \( h' = h \quad k' = k \quad l' = l \)

For any point \( \mathbf{r} \) on plane, \( \mathbf{G} \cdot \mathbf{r} = A \)

So

\[
\begin{align*}
\mathbf{G} \cdot (x_1\mathbf{a}_1) &= A \\
\mathbf{G} \cdot (x_2\mathbf{a}_2) &= A \\
\mathbf{G} \cdot (x_3\mathbf{a}_3) &= A
\end{align*}
\]

Then it follows that

\[
h' : k' : l' = \frac{1}{x_1} : \frac{1}{x_2} : \frac{1}{x_3}
\]

Since \( \mathbf{G} \) is the shortest reciprocal vector perpendicular to the plane. There should be no common factors between \( h' \quad k' \quad l' \). These parameters satisfy the original definition of miller indices.

Therefore \( h' = h \quad k' = k \quad l' = l \)