6 Reciprocal lattice. Miller indices.

The structure of crystals can be studied using EM waves (X-rays) with wavelengths comparable with the lattice constants of a crystal. Let’s consider a plane wave \( e^{i(\omega t + kr)} \) with wave vector \( \mathbf{k} \) in any direction that travels through a Bravais lattice with lattice constant \( \mathbf{R} \). We can select a set of those \( \mathbf{K} \) vectors that yield plane waves with the periodicity of the lattice, i.e. for which

\[
e^{\mathbf{K} \cdot (\mathbf{r} + \mathbf{R})} = e^{\mathbf{K} \cdot \mathbf{r}} \quad \forall \mathbf{r}
\]

from which

\[
e^{\mathbf{K} \cdot \mathbf{R}} = 1 \quad \forall \mathbf{K}
\]

6.1 The reciprocal lattice.

The possible values of \( \mathbf{K} \) can be considered as points of a „\( k \)-space” with axes \( k_x, k_y, k_z \), where they determine another Bravais lattice, the so called reciprocal lattice of the given Bravais lattice. The original Bravais lattice is called the direct lattice. That the set of \( \mathbf{K} \) vectors is itself a Bravais lattice can be seen from (6.2) because the letters \( \mathbf{K} \) and \( \mathbf{R} \) may be interchanged in the formula. This also proves that the reciprocal lattice of the reciprocal lattice is the direct lattice.

There exists an algebraic formula between the \( \mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3 \) primitive reciprocal lattice vectors and the three primitive direct lattice vectors \( \mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3 \)

\[
\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \\
\mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \\
\mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}
\]

(6.3)

Easy to see that these vectors satisfy (6.2):

\[
\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi \delta_{ij}
\]

(6.4)

The fact the space of the reciprocal vectors is the same as space of the wave vectors is very important both for crystallography as well as for the theory of conductivity.

Example: With (6.3) we can easily prove that the reciprocal lattice of an fcc lattice is a bcc lattice:

Start with the following selection of primitive fcc lattice vectors:
Then the 3 primitive vectors are

\[ \mathbf{a}_1 = \frac{a}{2} (\mathbf{i} + \mathbf{k}) \]
\[ \mathbf{a}_2 = \frac{a}{2} (\mathbf{i} + \mathbf{j}) \]
\[ \mathbf{a}_3 = \frac{a}{2} (\mathbf{j} + \mathbf{k}) \] (6.5)

Determine first the denominator in (6.3), which is the volume of the primitive cell:

\[ \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) = \frac{a}{2} (\mathbf{i} + \mathbf{k}) \cdot \left( \frac{a}{2} (\mathbf{i} + \mathbf{j}) \times \frac{a}{2} (\mathbf{j} + \mathbf{k}) \right) \]
\[ = \frac{a^3}{8} (\mathbf{i} + \mathbf{k}) \cdot (\mathbf{i} \times (\mathbf{j} + \mathbf{k})) \]
\[ = \frac{a^3}{8} (\mathbf{i} \cdot (\mathbf{i} \times (\mathbf{j} + \mathbf{k}))) \]
\[ = \frac{a^3}{8} (\mathbf{i} \cdot (\mathbf{j} \times \mathbf{k}) + \mathbf{k} \cdot (\mathbf{i} \times \mathbf{j})) \]
\[ \] here we used that \( \mathbf{i}, \mathbf{j} \) and \( \mathbf{k} \) are perpendicular to each other.

Furthermore

\[ \mathbf{i} \times \mathbf{j} = \mathbf{k}, \mathbf{j} \times \mathbf{k} = \mathbf{i} \quad \text{and} \quad \mathbf{k} \times \mathbf{i} = \mathbf{j} \]

Therefore

\[ \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) = \frac{a^3}{4} \] (6.6)

Now work with the numerators using the same formulas for \( \mathbf{i}, \mathbf{j} \) and \( \mathbf{k} \):

\[ \mathbf{a}_2 \times \mathbf{a}_3 = \frac{a^2}{4} (\mathbf{k} - \mathbf{j} + \mathbf{i}) \mathbf{a}_3 \times \mathbf{a}_1 = \frac{a^2}{4} (\mathbf{i} - \mathbf{k} + \mathbf{j}) \mathbf{a}_1 \times \mathbf{a}_2 = \frac{a^2}{4} (\mathbf{j} - \mathbf{i} + \mathbf{k}) \]

Which gives us the reciprocal base vectors:

\[ \mathbf{b}_1 = \frac{2\pi}{a} \frac{a^2}{4} (\mathbf{k} - \mathbf{j} + \mathbf{i}) \]
\[ \mathbf{b}_2 = \frac{2\pi}{a} (\mathbf{i} - \mathbf{k} + \mathbf{j}) \] (6.6)
\[ \mathbf{b}_3 = \frac{2\pi}{a} (\mathbf{j} - \mathbf{i} + \mathbf{k}) \]

Compare (6.6) with vectors on Fig. 14 to see that we, in fact got the primitive vectors of a bcc lattice. The only difference is that the length is now \( \frac{2\pi}{a} \). This means that the volume of the primitive cell in a reciprocal lattice is \( \frac{(2\pi)^3}{V} \) where \( V \) is the volume of the primitive cell of the original lattice.
Because the reciprocal lattice of a reciprocal lattice is the original (direct) lattice, we also proved that the reciprocal lattice of a bcc lattice is an fcc lattice.

**Brillouin zone**

The Wigner-Seitz cell of a reciprocal lattice is called the first Brillouin zone.

### 6.2 Miller indices

*Lattice planes* are those imaginary planes in the crystal which contain at least 3 non co-linear points. All such planes contain an infinite number of lattice points. 

*Miller indices* form a notation system in crystallography for planes and directions in crystal (Bravais) lattices.

Notation: Let $\mathbf{e}_1$, $\mathbf{e}_2$, and $\mathbf{e}_3$ stand for the unit vectors in the direction of the $k_x$, $k_y$, and $k_z$ axes of the reciprocal lattice and let $h, k, l$ be integers. Then the following notations are used:

- **(hkl)** - miller index of a family of parallel lattice planes perpendicular to the direction given by the reciprocal vector $h\mathbf{e}_1 + k\mathbf{e}_2 + l\mathbf{e}_3$ (the coordinates of the wave vector of a wave with the same periodicity as the selected lattice planes). By convention, negative integers are written with a bar above the number, as in $-3$ unless they are larger than 9, but such indices are rare. The integers are usually written in lowest terms, i.e. their greatest common divisor should be 1. Miller index (100) represents a plane orthogonal to direction $\mathbf{e}_1$; index (010) represents a plane orthogonal to direction $\mathbf{e}_2$, and index 001 represents a plane orthogonal to $\mathbf{e}_3$.

- **\{hkl\}** - denotes all planes which are equivalent in the crystal. E.g. in simple cubic crystals planes (100),(010),(001) are equivalent and \{100\} means all and any of these

- **[hkl]** - denotes a direction in the direct lattice
- **\{hkl\}** - denotes all equivalent directions in the direct lattice

There are two ways to calculate the Miller indices for a given crystal:

- via a point in the reciprocal lattice
- as the inverse intercepts along the lattice vectors in the direct lattice

Select three lattice vectors $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)$ that define the unit cell. These determine the 3 primitive lattice vectors $(\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3)$ in the reciprocal lattice.

**Method 1**

The 3 integers $h, k, l$ determine a direction in the reciprocal lattice:

$$ \mathbf{g}_{hkl} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3 $$

which is the direction the plane wave with the same periodicity as the lattice planes that lie perpendicular to this direction travels. $\mathbf{g}_{hkl}$ is a vector of k-space. The
requirement of lowest terms means that it is the shortest reciprocal lattice vector in the given direction. The planes of indices (hkl) are perpendicular to this vector, and their distance is the length of \( g_{hkl} \).

Method 2

The planes of constant phase of a plane wave traveling in the direction given by \( g_{hkl} \) intersects the three \((a_1, a_2, a_3)\) direct lattice vectors at the three points \((a_1/h, a_2/k, a_3/l)\) or some multiple thereof.

**Derivation**

The equation of the lattice planes is:

\[
K \cdot r = A = \text{const}
\]

where \( r \) is any vector to a point in the plane. Let’s take a plane that intersects the primitive cell and denote the coordinates of the intersections of this plane with the three primitive vectors by \( x_1, x_2 \) and \( x_3 \). From the equation above:

\[
K \cdot x_1 \cdot a_1 = K \cdot x_2 \cdot a_2 = K \cdot x_3 \cdot a_3 = A
\]

But \( K \cdot a_1 = 2\pi h \), \( K \cdot a_2 = 2\pi k \) and \( K \cdot a_3 = 2\pi l \), therefore

\[
x_1 = \frac{A}{2\pi h}, x_2 = \frac{A}{2\pi k}, x_3 = \frac{A}{2\pi l}
\]

That is, the Miller indices are proportional to the inverses of the intercepts of the plane, in the basis of the lattice vectors.

If one of the indices is zero, it means that the planes do not intersect that axis (the intercept is “at infinity”).

It is clear from the above that the distance \( d_{hkl} \) between adjacent lattice planes are given by

\[
d_{hkl} = \frac{2\pi}{|g_{hkl}|}
\]

(6.7)
Example: Determine the Miller indices for the plane on the figure!

Solution:
The intersections with the three axes are at $4a_1$, $3a_2$ and $2a_3$. Then the inverse intercepts in lattice vector units are:

$$\frac{1}{4}, \frac{1}{3}, \frac{1}{2}$$

To get integer numbers we have to calculate the lowest common denominator of this fraction, which is 12. Multiplying each fraction with 12 gives the three Miller indices: $(346)$

Example: Draw all 9 lattice planes and determine the Miller indices in a simple cubic Bravais lattice.

Solution:

(Where is the origin of the 3 lattice vectors in the cubes?)