The Reciprocal Lattice

Two types of lattice are of a great importance:

1. Reciprocal lattice
2. Direct lattice (which is the Bravais lattice that determines a given reciprocal lattice).

What is a reciprocal lattice?

A reciprocal lattice is regarded as a geometrical abstraction. It is essentially identical to a "wave vector" k-space.

Definition:

Since we know that $\vec{R}$ may construct a set of points of a Bravais lattice, thus a reciprocal lattice can be defined as:

- The collection of all wave vectors that yield plane waves with a period of the Bravais lattice.[Note: any $\vec{R}$ vector is a possible period of the Bravais lattice]
- A collection of vectors $\vec{G}$ satisfying $e^{i\vec{G}\bullet\vec{R}}=1$ or $\vec{G}\bullet\vec{R}=2\pi n$, where n is an integer and is defined as: $k_1n_1+k_2n_2+k_3n_3$. Here $\vec{G}$, is a reciprocal lattice vector which can be defined as: $\vec{G}=k_1\vec{b}_1+k_2\vec{b}_2+k_3\vec{b}_3$, where k_1, k_2 and k_3 are integers. [Note: In some text books you may find that $\vec{G}=\vec{K}$].
- The reciprocal lattice vector $\vec{G}$ which generates the reciprocal lattice is constructed from the linear combination of the primitive vectors $\vec{b}_1,\vec{b}_2$, and $\vec{b}_3$, where $\vec{b}_1=2\pi\frac{\vec{a}_2\times\vec{a}_3}{V_{cell}}$ and $\vec{b}_2$ and $\vec{b}_3$ can be obtained from cyclic permutation of 1 2 3.

Notes:

1. Since $\vec{G}\bullet\vec{R}=2\pi n$, this implies that $\vec{b}_i\bullet\vec{a}_j=2\pi\delta_{ij}$, where $\delta_{ij}=1$ if $i=j$ and $\delta_{ij}=0$ if $i\neq j$.
2. The two lattices (reciprocal and direct) are related by the above definitions in 1.
3. Rotating a crystal means rotating both the direct and reciprocal lattices.

4. The direct crystal lattice has the dimension of $[L]$ while the reciprocal lattice has the dimension of $[L^{-1}]$.

Why do we need a reciprocal lattice?

Reciprocal lattice provides a simple geometrical basis for understanding:

a) All things of "wave nature" (like behavior of electron and lattice vibrations in crystals.
b) The geometry of x-ray and electron diffraction patterns.

Reciprocal lattice to simple cubic (sc) lattice:

The simple cubic primitive lattice, which has the primitive vectors $\vec{a}_1 = a\hat{x}$, $\vec{a}_2 = a\hat{y}$ and $\vec{a}_3 = a\hat{z}$, has a volume of cell equal to $V_{cell} = a^3$.

The corresponding primitive vectors in the reciprocal lattice can be obtained as:

$$\vec{b}_1 = 2\pi \frac{a^2(\hat{y}\times\hat{z})}{a^3} \quad \Rightarrow \quad \vec{b}_1 = (\frac{2\pi}{a})\hat{x},$$

$$\vec{b}_2 = 2\pi \frac{a^2(\hat{z}\times\hat{x})}{a^3} \quad \Rightarrow \quad \vec{b}_2 = (\frac{2\pi}{a})\hat{y} \text{ and}$$

$$\vec{b}_3 = 2\pi \frac{a^2(\hat{x}\times\hat{y})}{a^3} \quad \Rightarrow \quad \vec{b}_3 = (\frac{2\pi}{a})\hat{z} .$$

The corresponding volume in reciprocal lattice is $(\frac{2\pi}{a})^3 = \frac{(2\pi)^3}{V_{cell}}$.

It must be noted that the reciprocal lattice of a sc is also a sc but with lattice constant of $(\frac{2\pi}{a})$.

Reciprocal lattice to bcc lattice:

When a set of primitive vectors for the bcc lattice are given by $\vec{a}_1 = a\hat{x}$, $\vec{a}_2 = a\hat{y}$ and $\vec{a}_3 = \frac{a}{2}(\hat{x}+\hat{y}+\hat{z})$, as shown in figure 11, where a is the side of the conventional cell, the primitive lattice vectors of the reciprocal lattice are found as:

$$\vec{b}_1 = 2\pi \frac{[\frac{a^2}{2}(\hat{y})\times(\hat{x}+\hat{y}+\hat{z})]}{\frac{a^3}{2}} \qquad \Rightarrow \quad \vec{b}_1 = (\frac{2\pi}{a})(\hat{x}-\hat{z}),$$

$$\vec{b}_2 = 2\pi \frac{[\frac{a^2}{2}(\hat{x}+\hat{y}+\hat{z})\times(\hat{x})]}{\frac{a^3}{2}} \qquad \Rightarrow \quad \vec{b}_2 = (\frac{2\pi}{a})(\hat{y}-\hat{z}),$$

$$\vec{b}_3 = 2\pi \frac{[a^2(\hat{x}\times\hat{y})]}{\frac{a^3}{2}} \qquad \Rightarrow \quad \vec{b}_3 = (\frac{2\pi}{a})(2\hat{z}).$$

You can easily show that the volume of primitive reciprocal lattice is $2(\frac{2\pi}{a})^3$. This can be compared to the volume of primitive direct lattice $V_{cell} = \frac{a^3}{2}$.

Notes:

a) The *bcc* primitive lattice vectors in the reciprocal lattice are just the primitive vectors of an fcc lattice.

b) The general reciprocal lattice vector $\vec{G} = k_1\vec{b}_1 + k_2\vec{b}_2 + k_3\vec{b}_3$ has a special expression for *bcc* primitive reciprocal lattice as: $\vec{G} = \frac{2\pi}{a}[(k_2+k_3)\hat{x} + (k_1+k_3)\hat{y} + (k_1+k_2)\hat{z}]$.

Reciprocal lattice to *fcc* lattice:

We know that the primitive vectors of *fcc* primitive lattice may be defined by: $\vec{a}_1 = \frac{a}{2}(\hat{y}+\hat{z})$, $\vec{a}_2 = \frac{a}{2}(\hat{x}+\hat{z})$ and $\vec{a}_3 = \frac{a}{2}(\hat{y}+\hat{x})$, [see figure 10]. Thus the primitive vectors in the reciprocal lattice are:

$$\vec{b}_1 = (\frac{2\pi}{a})(-\hat{x}+\hat{y}+\hat{z}),\ \vec{b}_2 = (\frac{2\pi}{a})(\hat{x}-\hat{y}+\hat{z}) \text{ and } \vec{b}_3 = (\frac{2\pi}{a})(\hat{x}+\hat{y}-\hat{z}).$$

It must be noted that these latter vectors are the primitive lattice vectors of a *bcc* lattice.

The volume of the primitive cell of the reciprocal lattice is $4(\frac{2\pi}{a})^3$. [Try to find $\vec{G}$ for the *fcc* primitive reciprocal lattice, for example, when $k_1=1$, $k_2=-2$ and $k_3=3$].

Reciprocal lattice to simple hexagonal lattice:

Recalling the primitive vectors of a simple hexagonal $\vec{a}_1 = a\hat{x}$, $\vec{a}_2 = \frac{a}{2}(\hat{x}+\sqrt{3}\hat{y})$ and $\vec{a}_3 = c\hat{z}$, as shown in figure 15.

The corresponding primitive vectors can simply be determined by using: $\vec{b}_1 = 2\pi\frac{\vec{a}_2\times\vec{a}_3}{V_{cell}}$, $\vec{b}_2 = 2\pi\frac{\vec{a}_3\times\vec{a}_1}{V_{cell}}$ and $\vec{b}_3 = 2\pi\frac{\vec{a}_1\times\vec{a}_2}{V_{cell}}$.

The volume of primitive cell for the direct lattice is $V_{cell} = \frac{\sqrt{3}}{2}a^2c$.

$$\vec{b}_1 = 2\pi\frac{\frac{a}{2}(\hat{x}+\sqrt{3}\hat{y})\times c\hat{z}}{\frac{\sqrt{3}}{2}a^2c} \quad \Rightarrow \quad \vec{b}_1 = (\frac{2\pi}{a})(\hat{x}-\frac{1}{\sqrt{3}}\hat{y}),$$

$$\vec{b}_2 = 2\pi\frac{c\hat{z}\times a\hat{x}}{\frac{\sqrt{3}}{2}a^2c} \quad \Rightarrow \quad \vec{b}_2 = (\frac{2\pi}{a})(\frac{2}{\sqrt{3}}\hat{y}) \text{ and}$$

$$\vec{b}_3 = 2\pi\frac{a\hat{x}\times\frac{a}{2}(\hat{x}+\sqrt{3}\hat{y})}{\frac{\sqrt{3}}{2}a^2c} \quad \Rightarrow \quad \vec{b}_3 = (\frac{2\pi}{c})\hat{z}.$$

Using a common origin for both reciprocal and direct lattices, we can build up the primitive reciprocal lattice by determining the magnitudes of $\vec{b}_1 = (\frac{2\pi}{a})(\hat{x}-\frac{1}{\sqrt{3}}\hat{y})$ and $\vec{b}_2 = (\frac{2\pi}{a})(\frac{2}{\sqrt{3}}\hat{y})$ and the angle between them. This will give you a clue how the base of the new reciprocal lattice looks like. Thus both vectors have the magnitude of $|\vec{b}_1| = |\vec{b}_2| = (\frac{4\pi}{\sqrt{3}a})$. Obviously the magnitude of the third vector is $|\vec{b}_3| = (\frac{2\pi}{c})$. These can be compared to the magnitudes of the primitive vectors, $|\vec{a}_1| = a$, $|\vec{a}_2| = a$ and $|\vec{a}_3| = c$, respectively, as shown in figures 27 and 28). The angle between the two vectors $\vec{b}_1$ and $\vec{b}_2$ can be directly obtained as $\theta = \cos^{-1}(\frac{\vec{b}_1 \bullet \vec{b}_2}{|\vec{b}_1||\vec{b}_2|}) = 120^\circ$.

Now what is left is to determine the angle between the vectors $\vec{a}_1$ and $\vec{b}_1$ which is obtained by applying the relation $\vec{b}_i \bullet \vec{a}_j = 2\pi\delta_{ij}$ and it is ($\pi/6$). This implies the necessity to rotate the plane of the two reciprocal vectors $\vec{b}_1$ and $\vec{b}_2$ by $\pi/6$. (See figure 27).

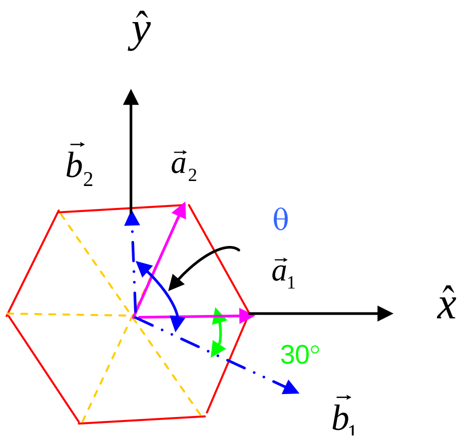

Figure 27: The primitive vectors of base of simple hexagonal conventional cell in direct space lattice as compared to their corresponding vectors in reciprocal space lattice.

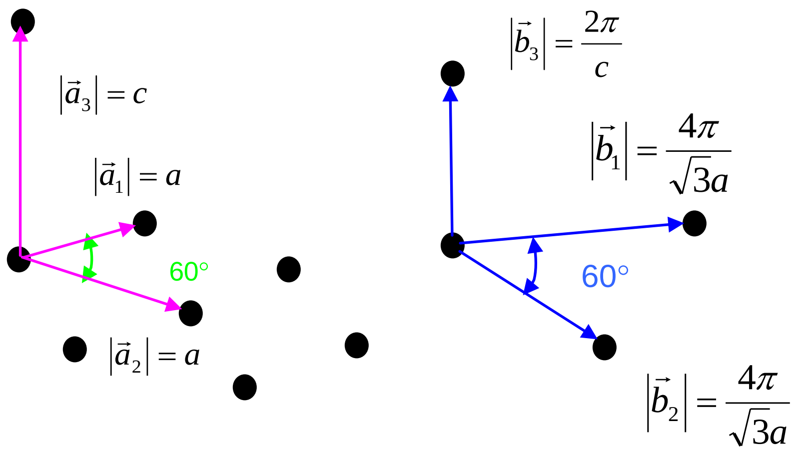

Figure 28: The three primitive vectors of simple hexagonal conventional cell in direct space lattice as compared to their corresponding vectors in reciprocal space lattice.

Conclusion:

This shows that the reciprocal lattice to a simple hexagonal lattice with lattice constant a and c is also another simple hexagonal lattice, with lattice constants $\frac{4\pi}{\sqrt{3}a}$ and $\frac{2\pi}{c}$, but rotated through $\pi/6$ about the c-axis with respect to the direct lattice (in a clockwise direction). [See problem 5.2.a in Solid State Physics by N. Ashcroft & N. Mermin].