Lecture 10

A few important examples of reciprocal lattices

(i) Reciprocal lattice of 2D simple square Bravais lattice:

If the primitive vectors of the direct lattice are $\vec{a}_1$ and $\vec{a}_2$, the reciprocal lattice vectors are –

$$\vec{b}_1 = 2\pi \frac{\theta \vec{a}_2}{\vec{a}_1 \cdot \theta \vec{a}_2} \quad \text{and} \quad \vec{b}_2 = 2\pi \frac{\theta \vec{a}_1}{\vec{a}_2 \cdot \theta \vec{a}_1} \quad \text{with } \theta \text{ being}$$

a 90° rotation matrix given by $\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$.

In matrix notation, $\vec{a}_1 \equiv \begin{pmatrix} a \\ 0 \end{pmatrix}$ and $\vec{a}_2 = \begin{pmatrix} 0 \\ a \end{pmatrix}$.

$$\therefore \vec{b}_1 = 2\pi \frac{\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ a \end{pmatrix}}{\begin{pmatrix} a & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ a \end{pmatrix}} = 2\pi \frac{\begin{pmatrix} a \\ 0 \end{pmatrix}}{\begin{pmatrix} a & 0 \end{pmatrix}\begin{pmatrix} a \\ 0 \end{pmatrix}} = \frac{2\pi}{a^2}\begin{pmatrix} a \\ 0 \end{pmatrix}$$

Similarly, $\vec{b}_2 = \frac{2\pi}{a^2}\begin{pmatrix} 0 \\ a \end{pmatrix}$.

$$\therefore \vec{b}_1 = \frac{2\pi}{a}\begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \vec{b}_2 = \frac{2\pi}{a}\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\therefore \vec{b}_1 = \frac{2\pi}{a}\hat{a}_1 \quad \text{and} \quad \vec{b}_2 = \frac{2\pi}{a}\hat{a}_2$$

So, the primitive vectors of the reciprocal lattice are same in length and is given by $\frac{2\pi}{a}$. So the reciprocal of the 2D square lattice with lattice constant a is another square lattice with lattice constant $\frac{2\pi}{a}$.

(ii) Reciprocal lattice of simple cubic lattice:

$$\vec{a}_1 = a\hat{x},\quad \vec{a}_2 = a\hat{y},\quad \vec{a}_3 = a\hat{z}$$

Now, $$\vec{b}_1 = 2\pi \frac{\vec{a}_2\times\vec{a}_3}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)} = \frac{2\pi}{a^3}a^2\hat{x} = \frac{2\pi}{a}\hat{x}$$

Similarly, $\vec{b}_2 = \frac{2\pi}{a}\hat{y}$ and $\vec{b}_3 = \frac{2\pi}{a}\hat{z}$.

So, the reciprocal of a simple cubic lattice is again a simple cubic lattice with cubic primitive cell of side $\frac{2\pi}{a}$.

(iii) For a fcc lattice,

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

$$\vec{b}_1 = 2\pi\frac{\frac{a^2}{4}(\hat{y}+\hat{z}-\hat{x})}{2\cdot a^3/8} = \frac{4\pi}{a}\cdot\frac{1}{2}(\hat{y}+\hat{z}-\hat{x})$$ which you can verify.

Similarly, $\vec{b}_2 = \frac{4\pi}{a}\frac{1}{2}(\hat{z}+\hat{x}-\hat{y})$ and $\vec{b}_3 = \frac{4\pi}{a}\frac{1}{2}(\hat{x}+\hat{y}-\hat{z})$

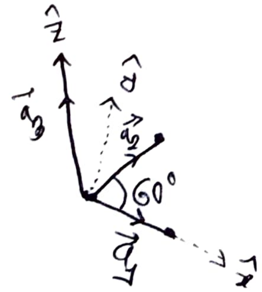
This is precisely the form of the bcc lattice primitive vectors, which has lattice constant of $\frac{4\pi}{a}$.

(iv) Reciprocal lattice of a bcc lattice: We can easily find the reciprocal lattice of the bcc lattice by the procedures we mentioned in earlier cases. However, we can do one better. The reciprocal of the reciprocal lattice is the direct lattice. Since, the reciprocal of the fcc is bcc, the reciprocal of bcc then must be fcc. Now, you get the fcc back if you start with bcc lattice with side length $\frac{4\pi}{a}$. However, for finding the reciprocal of bcc you will start with the direct lattice with side length a. Which you can verify that then, the reciprocal of bcc is just an fcc lattice with side ~~leng~~ length of $\frac{4\pi}{a}$.

(v) Reciprocal of a simple hexagonal lattice:

$$\vec{a}_1 = a\hat{x}, \quad \vec{a}_2 = a\cos 60^\circ\,\hat{x} + a\sin 60^\circ\,\hat{y}$$

$$= \frac{a}{2}\hat{x} + \frac{\sqrt{3}a}{2}\hat{y}$$



$$\vec{a}_3 = c\hat{z}$$

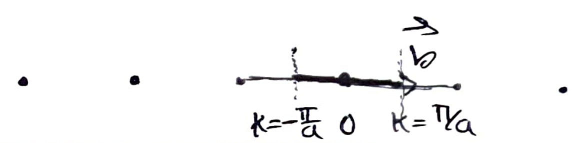
Starting from here, you should be able to prove that, the reciprocal to this lattice is again a hexagonal lattice with lattice constants $\frac{2\pi}{c}$ and $\frac{4\pi}{\sqrt{3}a}$, rotated through 30° about the c-axis with respect to the direct lattice.

First Brillouin Zone

In simplest term, the Wigner-Seitz primitive cell of the reciprocal lattice (in k-space) is called the first Brillouin zone. As the name suggests, there are higher Brillouin Zones. However, they are of immense importance for the analysis of the electronic energy-band structure of crystals. Here, in our study of diffraction, we will limit ourselves to the first Brillouin zone only.

Although the term "Wigner-Seitz cell" and "first Brillouin zone" refer to identical geometrical construction, in practice the latter term is applied only to the k-space cell. In particular, when reference is made to the first Brillouin zone of a particular r-space Bravais lattice (associated with a particular crystal structure), what is always meant is the Wigner-Seitz cell of the associated reciprocal lattice.

In 1D, the first Brillouin zone is just the following line segment, bounded by $k = \pm a$.



Reciprocal lattice

We have already talked about Wigner-Seitz cell for ~~&~~ two-dimensional lattices previously. The first Brillouin zone can then be easily found from the definition.

In 3D, the reciprocal of the square lattice is another square lattice in k-space. The boundaries of the first Brillouin zone for the square lattice are planes normal to the six lattice vectors $\pm\vec{b}_1$, $\pm\vec{b}_2$ and $\pm\vec{b}_3$ at their midpoints -

$$\pm\frac{1}{2}\vec{b}_1 = \pm\left(\frac{\pi}{a}\right)\hat{x}\,; \quad \pm\frac{1}{2}\vec{b}_2 = \pm(\pi/a)\hat{y}\,; \quad \pm\frac{1}{2}\vec{b}_3 = \pm(\pi/a)\hat{z}$$

These six planes bound a cube of edge $\frac{2\pi}{a}$ and of volume $\left(\frac{2\pi}{a}\right)^3$; this cube is the first Brillouin zone of the sc lattice.

The reciprocal of a bcc lattice is an fcc lattice. So, the first Brillouin zone of a bcc lattice is the Wigner-Seitz cell of an fcc lattice. The boundary of the first Brillouin zone are planes normal to the following twelve vectors:

$$\frac{2\pi}{a}(\pm\hat{y}\pm\hat{z})\,; \quad \frac{2\pi}{a}(\pm\hat{x}\pm\hat{z})\,; \quad \frac{2\pi}{a}(\pm\hat{x}\pm\hat{y})$$

which are vectors connecting the twelve nearest neighbours.

The zone is a regular twelve-faced solid, a rhombic dodecahedron.

Similarly the first Brillouin zone of an fcc lattice is the Wigner-Seitz primitive cell of BCC lattice. The boundary of the zone is mostly planes passing through the midpoint of the eight vectors –

$$\frac{2\pi}{a}\left(\pm\hat{x}\pm\hat{y}\pm\hat{z}\right)$$

which are the eight nearest neighbours. But the corners of the octahedron thus formed are cut by the planes that are the perpendicular bisectors of six other reciprocal lattice vectors:

$$\frac{2\pi}{a}\left(\pm 2\hat{x}\right) ; \frac{2\pi}{a}\left(\pm 2\hat{y}\right) ; \frac{2\pi}{a}\left(\pm 2\hat{z}\right)$$

The shape is a truncated octahedron.

Lattice planes from new perspective

Previously we discussed about the Miller indices and lattice planes, where we merily talked about a tenchnique to find Miller indices to lattice planes. We said that the reason behind taking the reciprocal of the intersections will be discussed in the reciprocal lattice section. As you know, the earth is round, and what goes around, comes around. Now is the time to talk about that in detail.

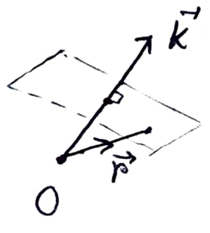
There is an intimate relation between vectors in the reciprocal lattice and planes of points in the direct lattice. This relation is of some importance in understanding the fundamental role the reciprocal lattice plays in the theory of diffraction, and will be applied soon.

Given a Bravais lattice, a "lattice plane" is defined to be any plane containing at least three non-colinear Bravais lattice points. Because of the translational symmetry of the Bravais lattice, any such plane will actually contain infinitely many lattice points, which will form a 2D Bravais lattice within the plane.

A family of lattice planes means a set of parallel, equally spaced lattice planes, which together contain all the points of the 3D Bravais lattice. Any lattice plane is a member of such a family. There are many such family of planes. The reciprocal lattice provides a very simple way to classify all possible families of lattice planes, which is embodied in the following 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 $\vec{K}$, there is a family of lattice planes normal to $\vec{K}$ and separated by a distance d, where $\frac{2\pi}{d}$ is the length of the shortest reciprocal lattice vectors parallel to $\vec{K}$.

To prove the first part of the theorem, let us first consider a plane that contains a set of points and let $\vec{K}$ be a vector perpendicular to the plane. Then,



$$\vec{K}.\vec{r} = \text{constant} = c$$

gives the equation of the plane where $\vec{r}$ is the position vector of any point in the plane. (The constant is found by $\vec{K}.\vec{r_0}$, where $\vec{r_0}$ is a known point on the plane). The minimum distance to the plane from the origin is given by d, which is found by,

$$\vec{K}.\vec{r} = c$$

$$\Rightarrow \vec{K}.d\hat{K} = c$$

$$\boxed{\therefore d = \frac{c}{|\vec{K}|}}$$

$\vec{d} \parallel \vec{K}$ since this is the perpendicular distance to the plane from the origin.

Now, consider a lattice plane that contains the origin point. So, $\vec{r} = \vec{0}$, and hence $e^{i\vec{K}.\vec{r}} = 1$ for any point $\vec{r}$ on the lattice plane. Now, we consider a family of planes, parallel to the one passing through the origin. They will be given by, the same condition $e^{i\vec{K}.\vec{r}} = 1$, or,

$$\vec{K}.\vec{r} = 2\pi m$$

For a particular plane, $\vec{K}.\vec{r} = 2\pi m$

For the next parallel plane, $\vec{K}.\vec{r} = 2\pi(m+1)$

The distance of the first plane from the origin $= \dfrac{2\pi m}{|\vec{K}|}$

Distance of the next plane from the origin $= \frac{2\pi(m+1)}{|\vec{K}|}$

$\therefore$ Distance between the planes, $d = \frac{2\pi(m+1)}{|\vec{K}|} - \frac{2\pi m}{|\vec{K}|}$

$$\boxed{\therefore d = \frac{2\pi}{|\vec{K}|}}$$

This means that, $\vec{K} = \frac{2\pi}{d}\hat{k}$. The fact that $\vec{K}$ is ~~the~~ a reciprocal lattice vector follows from the fact that, the plane wave $e^{i\vec{K}\cdot\vec{r}}$ is constant in planes perpendicular to $\vec{K}$ and has the same value separated by $\lambda = \frac{2\pi}{|\vec{K}|} = d$. Since the planes contain all the lattice points, $e^{i\vec{K}\cdot\vec{r}} = 1$ for all values of $\vec{r} = \vec{R}$. This suffices to show that $\vec{K}$ is indeed a reciprocal lattice vector. Conversely, if $\vec{K}$ is a reciprocal lattice vector, then the family of planes will contain all the lattice points.

The fact that $\vec{K}$ is the shortest reciprocal lattice vector is also evident now. If the wave vector is shorter than $\vec{K}$, the plane wave will have longer wavelength than $\frac{2\pi}{|\vec{K}|} = d$, and hence it will not have the same value on all the planes in the family of the planes.

This will break the construct and hence not possible.
So, $\vec{K} = \frac{2\pi}{d}\hat{x}$ is the smallest reciprocal lattice vector.

To prove the converse of the theorem, consider the shortest reciprocal lattice vector $\vec{K}$. Consider a set of real space planes on which $e^{i\vec{K}.\vec{r}} = 1$. Also consider, These planes (one of which contains $\vec{r}=\vec{0}$) are perpendicular to $\vec{K}$ and are separated by a distance $d = \frac{2\pi}{|\vec{K}|}$. Now, since the Bravais lattice vectors $\vec{R}$ all satisfies $e^{i\vec{K}.\vec{R}} = 1$, for any reciprocal lattice vector $\vec{K}$, the lattice points must lie within this planes. It means, the family of planes contain within it a family of lattice planes. Furthermore, the distance between the lattice planes is also d (rather than integer multiple of d). This is so, because, say, every n^{th} plane in the family of planes contain the Bravais lattice points, that is, a lattice plane. According to the first part of the theorem, the vector normal to the planes of length $\frac{2\pi}{(nd)}$, that is $\frac{\vec{K}}{n}$ will be the reciprocal lattice vectors. This would contradict our original assumption that no reciprocal lattice vector can be shorter than $\vec{K} = \frac{2\pi}{d}\hat{k}$. So, the spacing of the lattice planes will be d if the shortest reciprocal lattice vector is $\vec{K} = \frac{2\pi}{d}\hat{k}$.

Miller indices (again)

Quite generally, one describes the orientation of a plane by giving a vector normal to the plane. Since there are reciprocal lattice vectors that are normal to a family of lattice planes, it is natural to pick a reciprocal lattice vector to represent the normal. To make this choice unique, one uses the shortest such reciprocal lattice vector.

The Miller indices of a lattice plane are the coordinates of the shortest reciprocal lattice vector normal to that plane, with respect to a specific set of primitive reciprocal lattice vectors.

For example, the plane with Miller indices h, k, l is normal to the reciprocal lattice vector $h\vec{b_1} + k\vec{b_2} + l\vec{b_3}$.
So defined, Miller indices must be integers since $h, k, l \in \mathbb{Z}$. Since the normal to the plane is specified by the shortest perpendicular reciprocal lattice vector, h, k, l must have no common factor. Also, Miller indices depend on the choice of primitive vectors.

Now, consider a plane with Miller indices h, k, l; which is perpendicular to the reciprocal lattice vector $\vec{K} = h\vec{b_1} + k\vec{b_2} + l\vec{b_3}$. The lattice plane is contained in the continuous plane given by $\vec{K} \cdot \vec{r} = c$, where c is again a constant that satisfies $c = \vec{K} \cdot \vec{r_0}$. Say, the plane intersects at x_1, x_2, x_3 along the direct lattice primitive vectors $\vec{a_1}, \vec{a_2}, \vec{a_3}$.
So, we have points on the plane given by $x_1\vec{a_1}$, $x_2\vec{a_2}$ and $x_3\vec{a_3}$.

Now, $\vec{K} \cdot x_1\vec{a_1} = c \Rightarrow h\vec{b_1} \cdot x_1\vec{a_1} = c$ $\quad \Big| \quad \vec{b_1} \cdot \vec{a_2} = 0,\ \vec{b_1} \cdot \vec{a_3} = 0$

$$\therefore h = \frac{c}{2\pi x_1}$$

Similarly, $k = \frac{c}{2\pi x_2}$ and $l = \frac{c}{2\pi x_3}$.

Now you should see the connection and reason for taking the inverse of the intercepts and multiplying by common ~~numbers~~ factors to have the integer set.