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Reference Book:
Kittel, C., Introduction to Solid State Physics, 8^{th} ed., John Wiley & Sons Ltd, India (2005)

Reciprocal Lattice

The diffraction of x-rays occur from a set of parallel planes having different orientations and interplanar spacing. In certian situations involving the present of number of a set of parallel planes wirh diffrent orintations, it becomes difficulat to visualize all such plane sbecause of thier two dimentsional nature. The problem was simplifiled by P.P. Ewald by developing a new type of lattice known as reciprocal lattice.

A reciprocal lattice vector σ_{hkl} is defined as a vectro having magnitude equal to the reciprocal of the interplanar spacing d_{hkl} and direction coinciding with normal to (hkl) planes. Thus we have,

$$\sigma_{hkl} = \frac{1}{d_{hkl}}\hat{n} \tag{1}$$

where $\hat{n}$ is the unit vector normal to the (hkl) planes. In fact, a vector drawn from the origin to any point in the reciprocal lattice is a reciprocal lattice vector.

Like a direct lattice, a reciprocal lattice also has a unit cell whihc is of the form of a parallelopiped. The unit cell is formed by the shortest normals, along the three directions, i.e., along the normals to the planes (100), (010), and (001). These normals produce reciprocal lattice vectors designated as $\sigma_{100}, \sigma_{010}, \sigma_{001}$ which represent the *fundamental reciprocal lattice vectors*.

Let $\vec{a}, \vec{b}$, and $\vec{c}$ be the primitive translation vectors of the direct lattice as shown in figure. The base of the unit cell is formed by the vectors $\vec{b}$ and $\vec{c}$ and its height is equal to d_{100}. The volume of the cell is

$$V = (area) \times d_{100}$$
$$\Rightarrow \frac{1}{d_{100}} = \frac{area}{V} = \frac{|\vec{b}\times\vec{c}|}{V}$$

In vector form, it is written as

$$\frac{1}{d_{100}}\hat{n} = \frac{\vec{b}\times\vec{c}}{V} \tag{2}$$

where $\hat{n}$ is the unit vector normal to (100) planes.

From eq(1), we get,

$$\sigma_{100} = \frac{1}{d_{100}}\hat{n} \tag{3}$$

Denoting the fundamental reciprocal vectors $\sigma_{100}, \sigma_{010}$ and σ_{001} by a^*, b^*, and c^* respectively, eqs. (2) and (3) yield

$$a^* = \sigma_{100} = \frac{\vec{b}\times\vec{c}}{\vec{a}\cdot\vec{b}\times\vec{c}}; \quad b^* = \sigma_{010} = \frac{\vec{c}\times\vec{a}}{\vec{a}\cdot\vec{b}\times\vec{c}}; \quad c^* = \sigma_{001} = \frac{\vec{a}\times\vec{b}}{\vec{a}\cdot\vec{b}\times\vec{c}} \tag{4}$$

where $\vec{a}\cdot\vec{b}\times\vec{c}$ is the volume of the direct cell. Thus the reciprocal translation vectors bear a simple relationship to the crystal translation vectors as

$$a^* \text{ is normal to } \vec{b} \text{ and } \vec{c}; \quad b^* \text{ is normal to } \vec{c} \text{ and } \vec{a}; \quad c^* \text{ is normal to } \vec{a} \text{ and } \vec{b} \tag{5}$$

In vector notation, it means

$$\vec{a^*}\cdot\vec{b} = 0; \quad \vec{a^*}\cdot\vec{c} = 0; \quad \vec{b^*}\cdot\vec{c} = 0; \quad \vec{b^*}\cdot\vec{a} = 0; \quad \vec{c^*}\cdot\vec{a} = 0; \quad \vec{c^*}\cdot\vec{b} = 0. \tag{6}$$

Taking scalar product of $\vec{a^*}$, $\vec{b^*}$, and $\vec{c^*}$ with $\vec{a}$, $\vec{b}$, and $\vec{c}$ respectively and using eq (4) we find

$$\vec{a^*}\cdot\vec{a} = 1, \quad \vec{b^*}\cdot\vec{b} = 1, \quad \vec{c^*}\cdot\vec{c} = 1, \tag{7}$$

It appears from eqs (7) that $\vec{a^*}$, $\vec{b^*}$ and $\vec{c^*}$ are parallel to $\vec{a}$, $\vec{b}$ and $\vec{c}$ respectively. However, this is not always true. In non-cubic crystal systems, such as monoclinic crystal system, as shown in figure, $\vec{a^*}$ and a point in different directions, i.e. along OA' and OA respectively. THus all that is meant by eqs (7) is that the length of $\vec{a^*}$ is the reciprocal of $a\cos\theta$, where θ is the angle between $\vec{a^*}$ and $\vec{a}$.

In some cases, the primitive translation vectors $\vec{a}$, $\vec{b}$, and $\vec{c}$ of a direct lattice are related to the primitive translation vectors $\vec{a^*}$, $\vec{b^*}$ and $\vec{c^*}$ of the reciprocal lattice as

$$\vec{a^*}\cdot\vec{a} = \vec{b^*}\cdot\vec{b} = \vec{c^*}\cdot\vec{c} = 2\pi \tag{8}$$

These equations can be satisfied by choosing the reciprocal lattice vectors as

$$a^* = 2\pi\frac{\vec{b}\times\vec{c}}{\vec{a}\cdot\vec{b}\times\vec{c}}; \quad b^* = 2\pi\frac{\vec{c}\times\vec{a}}{\vec{a}\cdot\vec{b}\times\vec{c}}; \quad c^* = 2\pi\frac{\vec{a}\times\vec{b}}{\vec{a}\cdot\vec{b}\times\vec{c}} \tag{9}$$

It is now obvious that every crystal structure is associated with two important lattices - the direct lattice and reciprocal lattice. The two lattices are related to each other by eq (4). The fundamental translation vectors of the crystal lattice and reciprocal lattice have dimensions of $[L]$ and $[L^{-1}]$ respectively. This is why tha latter is called reciprocal lattice. Also, the volume of the unit cell of a reciprocal lattice is inversely proportional to the volume of the unit cell of its direct lattice.

A crystal lattice is a lattice in real or ordinary space, i.e., the space defined by the coordinates, whereas a reciprocal lattice is a lattice in the *reciprocal space*, *associated* ***k****-space* or *Fourier space*. A wave vector k is always drawn in k space. The points of the crystal lattice are given by

$$\vec{T} = m\vec{a} + n\vec{b} + p\vec{c} \tag{10}$$

where m, n, and p are integers. Similarly, the reciprocal lattice points or reciprocal lattice vectors may be defined as

$$\vec{G} = h\vec{a^*} + k\vec{b^*} + l\vec{c^*} \tag{11}$$

where h, k, and l are integers. Every point in Fourier space has a meaning, by the reciprocal lattice points are defined by eq (11) carry a spacial importance. In order to find the significance of G, we take the dot product of G and T:

$$\begin{aligned}\vec{G}\cdot\vec{T} &= \left(h\vec{a^*} + k\vec{b^*} + l\vec{c^*}\right)\cdot\left(m\vec{a} + n\vec{b} + p\vec{c}\right)\\ &= 2\pi\,(hm + kn + lp) = 2\pi(aninteger)\\ exp(i\vec{G}\cdot\vec{T}) &= 1\end{aligned}$$

Thus it is clear form eq (11) that h, k, and l define the coordinated of the points of reciprocal lattice space. In other words, it means that a point (hkl) in the reciprocal space corresponds to the set of parallel planes having the Miller indices (hkl). THe concept of reciprocal lattice is useful for redefining the Bragg's condition and introducing the concept of Brillouin zones.

Reciprocal Lattice to SC Lattice The primitive translation vectors of a simple cubic lattice may be written as

$$\vec{a} = a\hat{i}, \quad \vec{b} = a\hat{j}, \quad \vec{c} = a\hat{k}$$

$$\begin{aligned}\text{Volume of the simple cubic unit cell} &= \vec{a}\cdot\vec{b}\times\vec{c}\\ &= a^3\left(\hat{i}\cdot\hat{j}\times\hat{k}\right) = a^3\end{aligned}$$

Using eqs. (9), the reciprocal lattice vectors to the *sc* lattice are obtained as

$$\vec{a^*} = 2\pi\frac{\vec{b}\times\vec{c}}{\vec{a}\cdot\vec{b}\times\vec{c}} = 2\pi\frac{a\hat{j}\times a\hat{k}}{a^3} = \frac{2\pi}{a}\hat{i}; \qquad \vec{b^*} = \frac{2\pi}{a}\hat{j}; \quad \vec{c^*} = \frac{2\pi}{a}\hat{k} \tag{12}$$

The eq. (12) indicate that all the three reciprocal lattice vectors are equal in magnitude which means that the reciprocal lattice to *sc* lattice is also simple cubic but with lattice constant equal to $2\pi/a$.

Reciprocal Lattice to BCC Lattice The primitive translation vectors of a body-centered cubic lattice are,

$$\vec{a'} = \frac{a}{2}\left(\hat{i}+\hat{j}-\hat{k}\right); \quad \vec{b'} = \frac{a}{2}\left(-\hat{i}+\hat{j}+\hat{k}\right); \quad \vec{c'} = \frac{a}{2}\left(\hat{i}-\hat{j}+\hat{k}\right); \tag{13}$$

where a is the length of the cube edge and $\hat{i}$, $\hat{j}$ and $\hat{k}$ are the orthogonal unit vectors along the cube edges. The volume of the primitive cell is given by

$$\begin{aligned} V = \vec{a'}\cdot\vec{b'}\times\vec{c'} &= \frac{a}{2}\left(\hat{i}+\vec{j}-\vec{k}\right)\cdot\left[\frac{a^2}{4}\left(-\hat{i}+\hat{j}+\hat{k}\right)\times\left(\hat{i}-\hat{j}+\hat{k}\right)\right] \\ &= \frac{a}{2}\left(\hat{i}+\hat{j}-\hat{k}\right)\cdot\frac{a^2}{2}\left(\hat{i}+\hat{j}\right) \\ &= \frac{a^3}{2} \end{aligned}$$

Using eq. (9), the reciprocal lattice vectors are obtained as

$$\vec{a^*} = 2\pi\frac{\vec{b'}\times\vec{c'}}{\vec{a'}\cdot\vec{b'}\times\vec{c'}} = \frac{2\pi}{a}\left(\hat{i}+\hat{j}\right); \qquad \vec{b^*} = \frac{2\pi}{a}\left(\hat{j}+\hat{k}\right); \qquad \vec{c^*} = \frac{2\pi}{a}\left(\hat{k}+\hat{i}\right) \tag{14}$$

As will be seen later, these are the primitive transaltion vectors of *fcc* lattice. Thus the reciprocal lattice to a *bcc* lattice is *fcc* lattice.

Reciprocal Lattice to FCC Lattice The primitive translation vectors of an *fcc* lattice are,

$$\vec{a'} = \frac{a}{2}\left(\hat{i}+\hat{j}\right); \quad \vec{b'} = \frac{a}{2}\left(\hat{j}+\hat{k}\right); \quad \vec{c'} = \frac{a}{2}\left(\hat{k}+\hat{i}\right); \tag{15}$$

Volume of the primitive lattice is given by

$$\begin{aligned} V = \vec{a'}\cdot\vec{b'}\times\vec{c'} &= \frac{a}{2}\left(\hat{i}+\hat{j}\right)\cdot\left[\frac{a^2}{4}\left(\hat{j}+\hat{k}\right)\times\left(\hat{k}+\hat{i}\right)\right] \\ &= \frac{a}{2}\left(\hat{i}+\hat{j}\right)\cdot\frac{a^2}{4}\left(\hat{i}+\hat{j}-\hat{k}\right) \\ &= \frac{a^3}{4} \end{aligned}$$

Using eq (9), the primitive translation vectors of the reciprocal lattice are obtained as

$$\vec{a^*} = 2\pi\frac{\vec{b'}\times\vec{c'}}{\vec{a'}\cdot\vec{b'}\times\vec{c'}} = \frac{2\pi}{a}\left(\hat{i}+\hat{j}-\hat{k}\right); \qquad \vec{b^*} = \frac{2\pi}{a}\left(-\hat{i}+\hat{j}+\hat{k}\right); \qquad \vec{c^*} = \frac{2\pi}{a}\left(\hat{i}-\hat{j}+\hat{k}\right) \tag{16}$$

Comparing eq (16) with eq (13), we find that these are the primitive translation vectors of a *bcc* lattice having length of the cube edge as $2\pi/a$. Thus the reciprocal lattice to an *fcc* lattice is a *bcc* lattice.

Properties of Reciprocal Lattice

1. Each point in a reciprocal lattice corresponds to particular set of parallel planes of the direct lattice.
2. The distance of a reciprocal lattice point from a arbitrarily fixed origin is inversely proportional to the interplanar spacing of te corresponding parallel planes of the direct lattice.

3. The volume of a unit cell of the reciprocal lattice is inverrsely proportional to the volume of the corresponding unit cell of the direct lattice.
4. The unit cell of the reciprocal lattice need to be parallelopiped. It is customary to deal with Wigner-Seitz cell of the reciprocal lattice which constitutes the Brillioun zone.
5. The direct lattice is the reciprocal lattice to its own reciprocal lattice. Simple cubic lattice is self-reciprocal whereas *bcc* and *fcc* lattices are reciprocal to each other.

Bragg's Law in Reciprocal Lattice

The Bragg's diffraction condition obtained earlier by considering reflection from parallel lattice planes can be used to express geometrical relationship between the vectros in the reciprocal lattice. Consider a reciprocal lattice as shown in Figure. Starting from the point A (not necessarily a reciprocal lattice point), draw a vector $\vec{AO}$ of length $1/\lambda$ in the direction of the incident x-ray beam which terminates at the origin O of the reciprocal lattice. Taking A as the center, draw a sphere of radius AO which may intersect some point B of the reciprocal lattice.

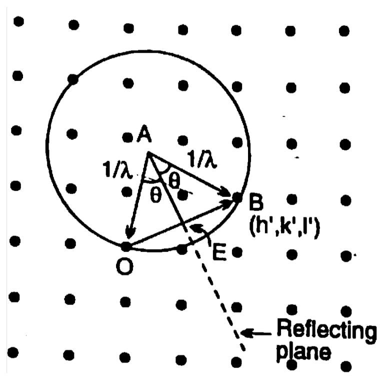


Figure 1: Ewald construction in the reciprocal lattice.

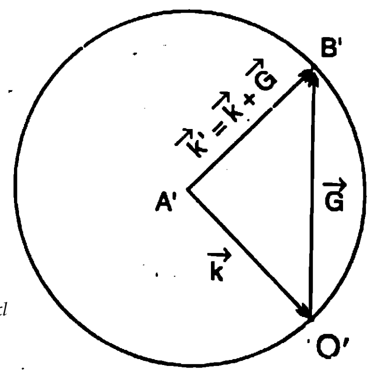
Let the coordinates of the point B be $(h'k'l')$ which may have a highest common factor n, i.e., the coordinates are of the type (nh, nk, nl), where h, k, and l do not have a common factor other than unity. Apparently, vector $\vec{OB}$ is the reciprocal vector. It must, therefore, be normal to the plane $(h'k'l')$ or (hkl) and should have length equal to $1/d_{h'k'l'}$ or n/d_{hkl}. Thus,

$$\left|\vec{OB}\right| = \frac{n}{d_{hkl}} \tag{17}$$

It follows from the geometry of figure (1) that one such plane is the plane AE. If $\angle EAO = \theta$ is the angle between the incident ray and the normal, then from ΔAOB, we have

$$OB = 2\,OE = 2\,OA\sin\theta = (2\sin\theta)/\lambda \tag{18}$$

From euations (17) and (18), we get



$$(2\sin\theta)/\lambda = n/d_{hkl}$$

$$\Rightarrow 2d_{hkl}\sin\theta = n\lambda$$

Figure 2: Magnified Ewald construction relating reciprocal lattice vector to the wave vectors of the incident and reflected radiation.

which is the Bragg's law, n being the order of reflection. Thus we notice that if the coordinates of a reciprocal point, (nh, nk, nl), contain a common factor n, then it represents n^{th} order reflection from the plane (hkl). It is also evident from the above geometrical construction that the Bragg's condition will be satisfied for a given wavelength λ provided the surface of radius $1/\lambda$ deawn about the point A intersects a point of the reciprocal lattice. Such a construction is called *Ewald construction*.

The Bragg's law itself takes a different form in the reciprocal lattice. To obtain the modified form of the Bragg's law, we redraw the vectors $\vec{AO}$, $\vec{OB}$ and $\vec{AB}$ such that each is magnified by a constant factor of 2π. Let the new vectors be $\vec{A'O'}$, $\vec{O'B'}$, and $\vec{A'B'}$ respectively as shown in Figure(2). Since

$$\vec{A'O'} = 2\pi(\vec{AO}) = 2\pi/\lambda$$

we can represent the wave vector $\vec{k}$ by the vector $\vec{A'O'}$. The vector $\vec{O'B'}$ is the reciprocal vector and is written as $\vec{G}$. Thus according to vector algebra, $\vec{A'B'}$ must be equal to $(\vec{k} + \vec{G})$. For diffraction to occur, the point B' must be on the sphere, i.e.,

$$\left|\vec{A'B'}\right| = \left|\vec{A'O'}\right|$$

$$\Rightarrow \left(\vec{k} + \vec{G}\right)^2 = k^2$$

$$\Rightarrow k^2 + 2\vec{k}\cdot\vec{G} + G^2 = k^2$$

$$\Rightarrow 2\vec{k}\cdot\vec{G} + G^2 = 0 \tag{19}$$

This is the vector form of Bragg's law and is used in the construction of the Brilliouin zones.

The vectors $\vec{A'B'}$ represents the direction of reflected or scattered beam. Denoting it by $\vec{k'}$, we get

$$\vec{k'} = \vec{k} + \vec{G}$$

which gives

$$k'^2 = k^2 \tag{20}$$

and

$$\vec{k'} - \vec{k} = \Delta\vec{k} = \vec{G} \tag{21}$$

This indicates that the scattering doesnot change the magnitude of wave vector $\vec{k}$; only its direction is changed. Also, the scattered wave differs from the incident wave by a reciprocal lattice vector $\vec{G}$.