3.3 Reciprocal lattice

$$a^*.a = 2\pi \quad , \quad a^*.b = 0 \quad , a^*.c = 0$$

$$b^*.b = 2\pi \quad , \quad b^*.a = 0 \quad , b^*.c = 0 \qquad (14)$$

$$c^*.c = 2\pi \quad , \quad c^*.a = 0 \quad , c^*.b = 0$$

From equations (14) we see that the vector a^* is normal to the plan ($b \times c$) , b^* is normal to the plan ($c \times a$) , and the vector c^* is normal to the plan ($a \times b$).

In order to obtain reciprocal lattice vectors in term of real lattice vectors, one can multiply first group in eq.(14) by $(b \times c / b \times c)$, the second group by $(c \times a / c \times a)$, and the third group by $(a \times b / a \times b)$

$$a^* = 2\pi \frac{b \times c}{a.(b \times c)} = 2\pi \frac{b \times c}{V} \qquad (15)$$

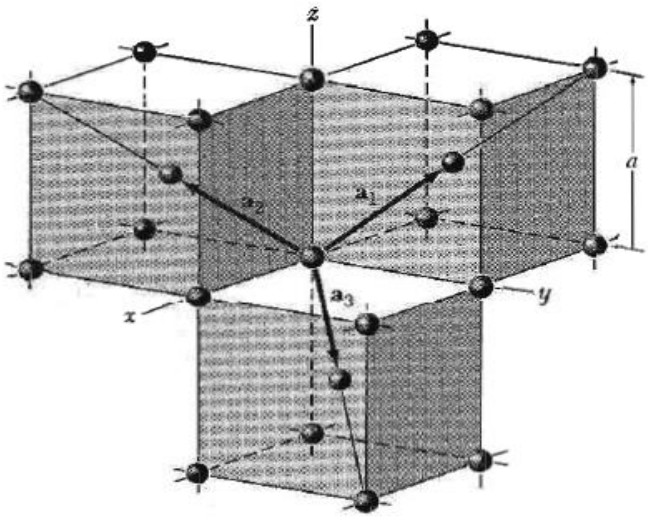
$$b^* = 2\pi \frac{c \times a}{b.(c \times a)} = 2\pi \frac{c \times a}{V} \qquad (16)$$

$$c^* = 2\pi \frac{a \times b}{c.(a \times b)} = 2\pi \frac{a \times b}{V} \qquad (17)$$

Where the V is the volume of the primitive lattice. Equations (15,16, and 17) represent the reciprocal lattice vectors, where

$$G_{hkl} = ha^* + kb^* + lc^*$$

Example: **Find the reciprocal lattice vectors to the body centered cubic lattice (bcc).**



The primitive translation vectors of the (bcc) lattice are:

$$\vec{a} = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z}), \qquad \vec{b} = \frac{a}{2}(-\hat{x} + \hat{y} + \hat{z}) \qquad \vec{c} = \frac{a}{2}(\hat{x} - \hat{y} + \hat{z})$$

The volume of the (bcc) lattice is;

$$V = \vec{a}.(\vec{b} \times \vec{c}) = \vec{a}. \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ -\frac{a}{2} & \frac{a}{2} & \frac{a}{2} \\ \frac{a}{2} & -\frac{a}{2} & \frac{a}{2} \end{vmatrix} = \frac{a^3}{8}(\hat{x} + \hat{y} - \hat{z}).(2\hat{x} + 2\hat{y}) = \frac{a^3}{2}$$

The primitive translation vectors of the reciprocal lattice are

$$\vec{a}^* = 2\pi \frac{(\vec{b} \times \vec{c})}{\vec{a}.(\vec{b} \times \vec{c})} = \frac{2\pi}{a^3/2} \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ -\frac{a}{2} & \frac{a}{2} & \frac{a}{2} \\ \frac{a}{2} & -\frac{a}{2} & \frac{a}{2} \end{vmatrix} = \frac{2\pi}{a}(\hat{x} + \hat{y})$$

$$\vec{b}^* = 2\pi \frac{(\vec{c} \times \vec{a})}{\vec{a}.(\vec{b} \times \vec{c})} = \frac{2\pi}{a^3/2} \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \frac{a}{2} & -\frac{a}{2} & \frac{a}{2} \\ \frac{a}{2} & \frac{a}{2} & -\frac{a}{2} \end{vmatrix} = \frac{2\pi}{a}(\hat{y} + \hat{z})$$

$$\vec{c}^* = 2\pi \frac{(\vec{a} \times \vec{b})}{\vec{a}.(\vec{b} \times \vec{c})} = \frac{2\pi}{a^3/2} \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \frac{a}{2} & \frac{a}{2} & -\frac{a}{2} \\ -\frac{a}{2} & \frac{a}{2} & \frac{a}{2} \end{vmatrix} = \frac{2\pi}{a}(\hat{x} + \hat{z})$$

Not that the primitive translation vectors of the reciprocal lattice are just the primitive vectors of an (fcc) lattice. So that the (fcc) lattice is the reciprocal lattice of the (bcc) lattice.

The general reciprocal lattice vector is;

$$G(hk\ell) = h\vec{a}^* + k\vec{b}^* + \vec{c}^*\ell = \frac{2\pi}{a}[(k+\ell)\hat{x} + (h+\ell)\hat{y} + (h+k)\hat{z}]$$

The volume of the primitive cell of the reciprocal lattice is:

$$V_R = \vec{a}^*.(\vec{b}^* \times \vec{c}^*) = 2(2\pi/a)^3$$

3-4. Diffraction condition

Let an X-ray be incident from very far away, along a direction $\hat{n}$,with wavelength λ and wave vector $\vec{k} = (2\pi/\lambda)\hat{n}$. A scattered ray will be observed in direction $\hat{n}'$,with wavelength λ and wave vector $\vec{k}' = (2\pi/\lambda)\hat{n}'$,provided that the path difference between the rays scattered by each of the two ions separated by displacement vector $\vec{d}$ is an integral number of wavelengths

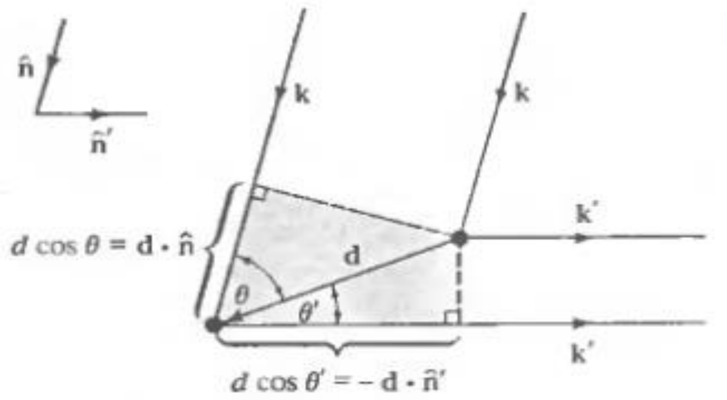


Figure (2) Illustrated that the path different for rays scattered from two point separated by displacement vector $\vec{d}$ is given by equations (18,19).

from figure (2) ,it can be seen that the path difference is just

$$d\cos\theta + d\cos\theta' = \vec{d}.(\vec{n} - \vec{n}') \qquad (18)$$

The condition for constrictive interference is thus

$$\vec{d}.(\vec{n} - \vec{n}') = m\lambda \qquad (19)$$

For integral m. Multiplying both side of equation (19) by ($2\pi/\lambda$), yield a condition on the incident and scattered wave vector.

$$\vec{d}.[(\frac{2\pi}{\lambda})\vec{n} - (\frac{2\pi}{\lambda})\vec{n}'] = 2\pi m$$

$$\vec{d}.(\vec{k}_i - \vec{k}_f) = 2\pi m$$

$$\vec{d}.(-\Delta\vec{k}) = 2\pi m \qquad (20)$$

Where

$$\Delta\vec{k} = \vec{k}_f - \vec{k}_i \tag{21}$$

In the other word , the amplitude of the electronic or magnetic field vectors in the scattered electromagnetic wave is proportional to the following integral which defines the quantity F that we <u>called the scattering amplitude</u>:

$$F = \int dV\, n_G\, e^{i(\vec{G}-\Delta\vec{k}).\vec{r}} \tag{22}$$

When $\Delta\vec{k}$ differs significantly from any reciprocal lattice vector $\vec{G}$, the scattering amplitude F is negligibly small, but if $\Delta\vec{k}$ is equal to particular reciprocal lattice vector $\vec{G}$,the scattering amplitude F is large and equal to $F = Vn_G$. This mean that occurrence of diffraction requires that:

$$\vec{G} = \Delta\vec{k} \tag{23}$$

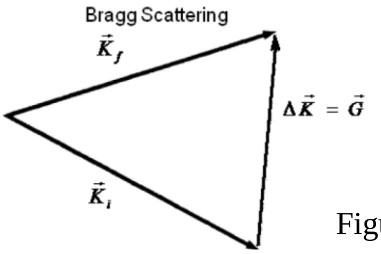


Figure (3)

From equation (20) we find:

$$\left|\Delta\vec{k}\right| = \frac{2\pi m}{d} = \left|\vec{G}\right| \tag{24}$$

Equation (24) is <u>called Von Laue condition</u>. In elastic scattering of X- ray, the energy is conserved , so that the magnitudes $k_i = k_f$ are equal, and $k_i^2 = k_f^2$, so that the diffraction condition reciprocal lattice is written as:

$$\vec{G} = \Delta\vec{k} \Rightarrow \vec{G} = \vec{k}_f - \vec{k}_i \Rightarrow \vec{G} + \vec{k}_i = \vec{k}_f \Rightarrow (\vec{G} + \vec{k}_i)^2 = k_f^2 \Rightarrow G^2 + 2\vec{G}.\vec{k}_i + k_i^2 = k_f^2$$

$$G^2 + 2\vec{k}.\vec{G} = 0 \tag{25}$$

Equation (25) is also The Bragg diffraction Low in reciprocal lattice.

3-5 The Ewald construction

A beautiful construction , The Ewald construction, is exhibited in figure (4). This help us visualize the nature of the accident that must occur in order to satisfy the diffraction condition in three dimensions.

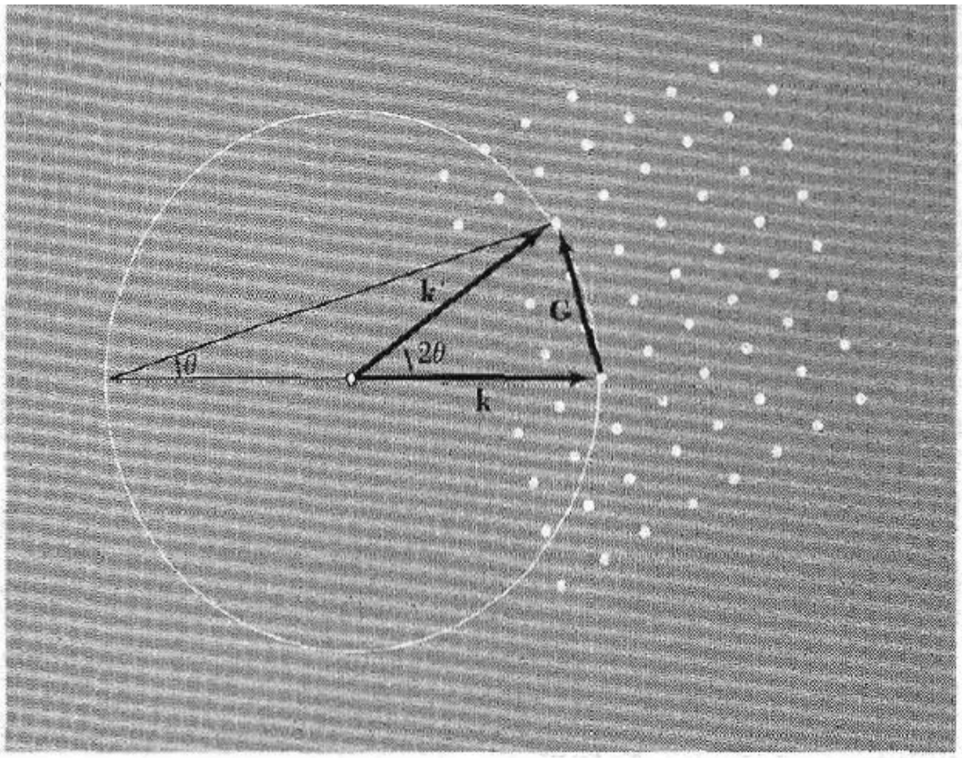


Figure 8 The points on the right-hand side are reciprocal-lattice points of the crystal. The vector **k** is drawn in the direction of the incident x-ray beam, and the origin is chosen such that **k** terminates at any reciprocal lattice point. We draw a sphere of radius $k = 2\pi/\lambda$ about the origin of **k**. A diffracted beam will be formed if this sphere intersects any other point in the reciprocal lattice. The sphere as drawn intercepts a point connected with the end of **k** by a reciprocal lattice vector **G**. The diffracted x-ray beam is in the direction $\mathbf{k}' = \mathbf{k} + \mathbf{G}$. The angle θ is the Bragg angle of Fig. 2. This construction is due to P. P. Ewald.

From the figure;

$$\sin\theta = \frac{|\vec{G}|}{2|\vec{k}|} = \frac{2\pi m / d}{2 \times 2\pi / \lambda} = \frac{m\lambda}{2d} \Rightarrow\Rightarrow \qquad 2d\sin\theta = m\lambda$$

3-6 Brillouin Zones

The Brillouin zone is defined as the smallest volume in the reciprocal space (k-space) contains one reciprocal lattice point in his center, this volume bounded by a set of planes which are perpendicular on mid-displacement that connect the centered reciprocal lattice point with the neighbors reciprocal lattice points in the k-space,. so the Brillouin Zone gives a geometrical interpretation of the diffraction condition $G^2 + 2\vec{k}.\vec{G} = 0$, of equation (25) , which is can be written as:

$$\vec{k}.\vec{G} = \frac{1}{2}G^2 \qquad \textbf{(26)}$$

We now work in reciprocal space the space of $\vec{k}$ and $\vec{G}$. Select a vector $\vec{G}$ from the origin to a reciprocal lattice point. Construct a plane normal to this vector $\vec{G}$ at its midpoint. This plane forms a part of a zone boundary .

From the figure (5), and equation (26): we find that:

$$\vec{k}.\vec{G} = \frac{1}{2}G^2 \Longrightarrow\Longrightarrow |k||G|\cos\phi = \frac{1}{2}G^2$$

$$|k|\cos\phi = \frac{1}{2}|G|$$

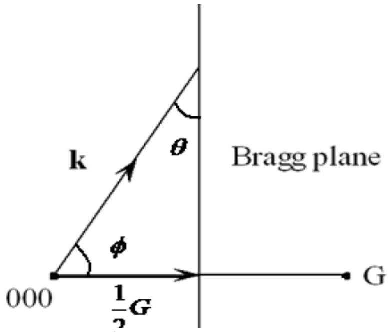
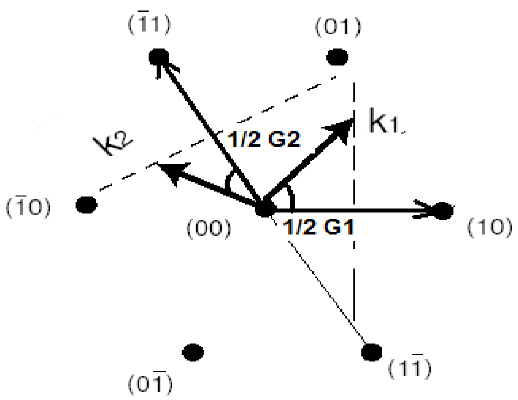


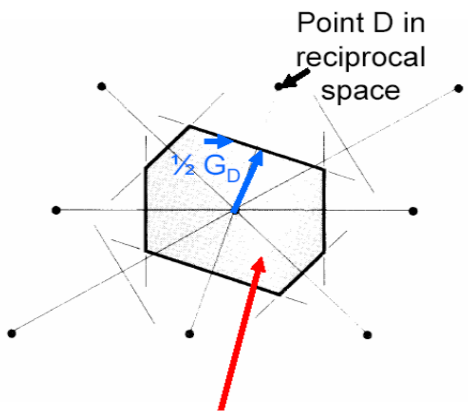
Figure (5)

But $\cos\phi = \sin\theta$, **so that**

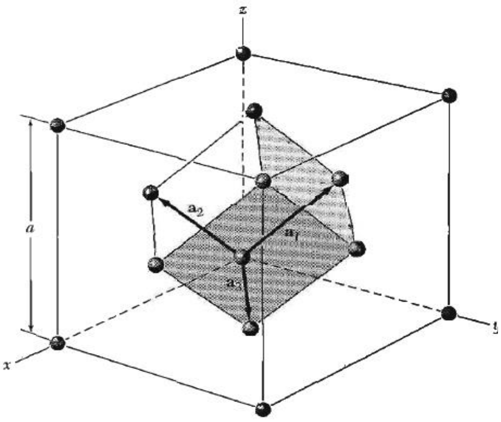
$$|k|\sin\theta = \frac{1}{2}|G| \Longrightarrow\Longrightarrow \frac{2\pi}{\lambda}\sin\theta = \frac{1}{2}\frac{2\pi m}{d} \Longrightarrow\Longrightarrow 2d\sin\theta = m\lambda$$

An x- ray beam in the crystal will be diffracted if its wave vector $\vec{k}$ has the magnitude and direction required by equation (25), which satisfies The Bragg diffraction low.





Example 2: By using the general reciprocal lattice vector $G(hkl)$,drive a relationship between $d_{hk\ell}$ and direct primitive translation vectors of the (fcc) lattice.



The primitive translation vectors of the (fcc) lattice are:

$$\vec{a} = \frac{a}{2}(\hat{x} + \hat{y}), \qquad \vec{b} = \frac{a}{2}(\hat{y} + \hat{z}) \qquad \vec{c} = \frac{a}{2}(\hat{x} + \hat{z})$$

The volume of the (fcc) lattice is;

$$V = \vec{a}.(\vec{b} \times \vec{c}) = \vec{a} \ .\frac{a^2}{4} \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{vmatrix} = \frac{a^3}{8}(\hat{x} + \hat{y}).(\hat{x} + \hat{y} - z) = \frac{a^3}{4}$$

The primitive translation vectors of the reciprocal lattice are;

$$\vec{a}^* = 2\pi \frac{(\vec{b} \times \vec{c})}{\vec{a}.(\vec{b} \times \vec{c})} = 2\pi \frac{(a^2/4)}{a^3/4} \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{vmatrix} = \frac{2\pi}{a}(\hat{x} + \hat{y} - \hat{z})$$

$$\vec{b}^* = 2\pi \frac{(\vec{c} \times \vec{a})}{\vec{a}.(\vec{b} \times \vec{c})} = 2\pi \frac{(a^2/4)}{a^3/4} \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{vmatrix} = \frac{2\pi}{a}(-\hat{x} + \hat{y} + \hat{z})$$

$$\vec{c}^* = 2\pi \frac{(\vec{a} \times \vec{b})}{\vec{a}.(\vec{b} \times \vec{c})} = 2\pi \frac{(a^2/4)}{a^3/4} \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 1 & 1 & 0 \\ 0 & 1 & 1 \end{vmatrix} = \frac{2\pi}{a}(\hat{x} - \hat{y} + \hat{z})$$

Not that the primitive translation vectors of the reciprocal lattice are just the primitive vectors of an (bcc) lattice. So that the (bcc) lattice is the reciprocal lattice of the (fcc) lattice.

The volume of the primitive cell of the reciprocal lattice is:

$$V_R = \vec{a}^*.(\vec{b}^* \times \vec{c}^*) = \vec{a}^*.(\frac{2\pi}{a})^2 \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ -1 & 1 & 1 \\ 1 & -1 & 1 \end{vmatrix} = (2\pi / a)^3 (\hat{x} + \hat{y} - \hat{z}).(2\hat{x} + 2\hat{y})$$

$$V_R = 4(2\pi / a)^3 = \frac{(2\pi)^3}{a^3 / 4} = \frac{(2\pi)^3}{V}$$

The general reciprocal lattice vector is

$$G(hk\ell) = h\vec{a}^* + k\vec{b}^* + \vec{c}^* = \frac{2\pi}{a}[(h-k+\ell)\hat{x} + (h+k-\ell)\hat{y} + (-h+k+\ell)\hat{z}]$$

$$G(hk\ell) = h\vec{a}^* + k\vec{b}^* + \vec{c}^* = \frac{2\pi}{a}[(h-k+\ell)\hat{x} + (h+k-\ell)\hat{y} + (-h+k+\ell)\hat{z}]$$

So that

$$\left|\vec{G}_{hkl}\right| = \frac{2\pi}{a}[3(h^2 + k^2 + l^2) - 2(hk + hl + kl)]^{1/2}$$

$$d_{hkl} = \frac{2\pi}{\left|\vec{G}_{hkl}\right|} = \frac{a}{\sqrt{3(h^2 + k^2 + l^2) - 2(hk + hl + kl)}}$$