2.4 RECIPROCAL LATTICE

As described earlier, the diffraction of x-rays occurs from various sets of parallel planes having different orientations (slopes) and interplanar spacings. In certain situations involving the presence of a number of sets of parallel planes with different orientations, it becomes difficult to visualize all such planes because of their two-dimensional nature. The problem was simplified by P.P. Ewald by developing a new type of lattice known as the *reciprocal lattice*. The idea underlying the development was that each set of parallel planes could be represented by a normal to these planes having length equal to the reciprocal of the interplanar spacing. Thus the direction of each normal represents the orientation of the corresponding set of parallel planes and its length is proportional to the reciprocal of the interplanar spacing.

The normals are drawn with reference to an arbitrary origin and points are marked at their ends. These points form a regular arrangement which is called a reciprocal lattice. Obviously, each point in a reciprocal lattice is a representative point of a particular parallel set of planes and it becomes easier to deal with such points than with sets of planes.

A reciprocal lattice to a direct lattice is constructed using the following procedure :

(a) Take origin at some arbitrary point and draw normals to every set of parallel planes of the direct lattice.

(b) Take length of each normal equal to the reciprocal of the interplanar spacing for the corresponding set of planes. The terminal points of these normals form the reciprocal lattice.

Consider, for example, a unit cell of monoclinic crystal in which $a \neq b \neq c$, $\alpha = \gamma = 90°$ and $\beta > 90°$ as shown in Fig. 2.8. For simplicity, we orient the unit cell in such a way that the b-axis is perpendicular to the plane of the paper; hence a and c-axes lie in the plane of the paper as shown in Fig. 2.9.

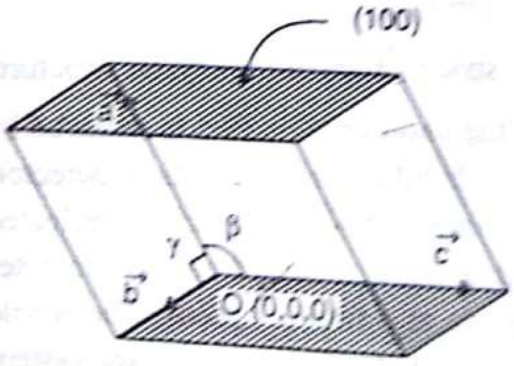

Fig. 2.8. *Unit cell of a monoclinic crystal.*

Consider planes of the type (*h0l*) which are parallel to b-axis, i.e., perpendicular to the plane of the paper. Hence normal to these planes lie in the plane of the paper. The planes (*h01*), being perpendicular to the plane of the paper, are represented by lines. Thus the line (101) in fact means the plane (101), and so on. Taking the point of intersection of the three axes as the origin, normals are drawn to the

planes (*h0l*) and their lengths are taken to be $1/d_{h0l}$, where d_{h0l} is the interplanar spacing for the planes (*h0l*). For example, since the planes (200) have half the interplanar spacing as compared to the plane (100), the reciprocal lattice point (200) is twice as far away as point (100) from the origin. If normals to all the (*hkl*) planes are drawn, a three-dimensional reciprocal lattice is obtained.

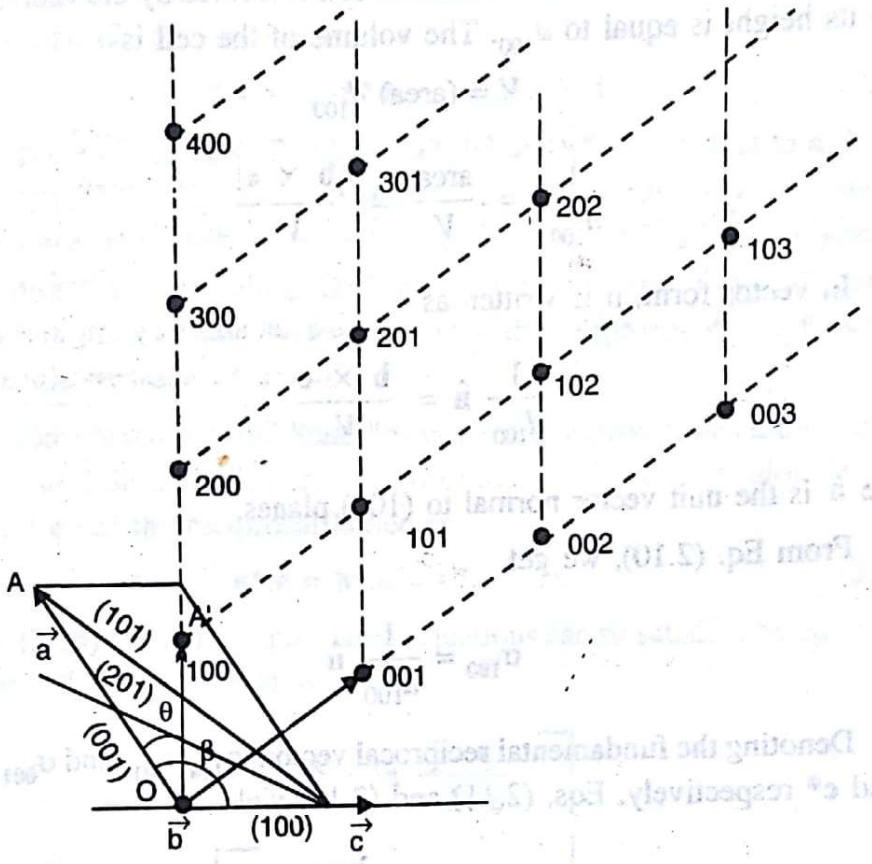

Fig. 2.9. *Two-dimensional reciprocal lattice to a monoclinic lattice. The* **b***-axis is perpendicular to the plane of the paper.*

2.4.1 Reciprocal Lattice Vectors

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

$$\sigma_{hkl} = \frac{1}{d_{hkl}} \hat{\mathbf{n}} \qquad (2.10)$$

where $\hat{\mathbf{n}}$ 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 which 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 σ_{100}, σ_{010} and σ_{001} which represent the *fundamental reciprocal lattice vectors.*

Let **a**, **b** and **c** be the primitive translation vectors of the direct lattice as shown in Fig. 2.8. The base of the unit cell is formed by the vectors **b** and **c** and its height is equal to d_{100}. The volume of the cell is

$$V = (\text{area})\, d_{100}$$

or

$$\frac{1}{d_{100}} = \frac{\text{area}}{V} = \frac{|\mathbf{b} \times \mathbf{c}|}{V}$$

In vector form, it is written as

$$\frac{1}{d_{100}} \hat{\mathbf{n}} = \frac{\mathbf{b} \times \mathbf{c}}{V} \tag{2.11}$$

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

From Eq. (2.10), we get

$$\sigma_{100} = \frac{1}{d_{100}} \hat{\mathbf{n}} \tag{2.12}$$

Denoting the fundamental reciprocal vectors σ_{100}, σ_{010} and σ_{001} by **a***, **b*** and **c*** respectively, Eqs. (2.11) and (2.12) yield

$$\left.\begin{aligned} \mathbf{a}^* = \sigma_{100} &= \frac{\mathbf{b}\times\mathbf{c}}{\mathbf{a}.\mathbf{b}\times\mathbf{c}} \\ \text{Similarly,} \\ \mathbf{b}^* = \sigma_{010} &= \frac{\mathbf{c}\times\mathbf{a}}{\mathbf{a}.\mathbf{b}\times\mathbf{c}} \\ \text{and} \\ \mathbf{c}^* = \sigma_{001} &= \frac{\mathbf{a}\times\mathbf{b}}{\mathbf{a}.\mathbf{b}\times\mathbf{c}} \end{aligned}\right\} \tag{2.13}$$

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

$$\left.\begin{aligned} &\mathbf{a}^* \text{ is normal to } \mathbf{b} \text{ and } \mathbf{c} \\ &\mathbf{b}^* \text{ is normal to } \mathbf{c} \text{ and } \mathbf{a} \\ &\mathbf{c}^* \text{ is normal to } \mathbf{a} \text{ and } \mathbf{b} \end{aligned}\right\} \tag{2.14}$$

In vector notation, it means

$$\left.\begin{aligned} \mathbf{a}^*.\mathbf{b} = 0 \qquad & \mathbf{a}^*.\mathbf{c} = 0 \\ \mathbf{b}^*.\mathbf{c} = 0 \qquad & \mathbf{b}^*.\mathbf{a} = 0 \\ \mathbf{c}^*.\mathbf{a} = 0 \qquad & \mathbf{c}^*.\mathbf{b} = 0 \end{aligned}\right] \tag{2.15}$$

Taking scalar product of **a***, **b*** and **c*** with **a**, **b** and **c** respectively and using Eqs. (2.13), we find

$$\mathbf{a}^*.\mathbf{a} = 1, \quad \mathbf{b}^*.\mathbf{b} = 1, \quad \mathbf{c}^*.\mathbf{c} = 1 \tag{2.16}$$

It appears from Eqs. (2.16) that **a***, **b*** and **c*** are parallel to **a**, **b** and **c** respectively. However, this is not always true. In non-cubic crystal systems, such as monoclinic crystal system, as shown in Fig. 2.8, **a*** and **a** point in different directions, i.e., along OA′, and OA respectively. Thus all that is meant by Eqs. (2.16) is that the length of **a*** is the reciprocal of $a\cos\theta$, where θ is the angle between **a*** and **a**.

In some texts on Solid State Physics, the primitive translation vectors **a**, **b** and **c** of a direct lattice are related to the primitive translation vectors **a***, **b*** and **c*** of the reciprocal lattice as

$$\mathbf{a}^*.\mathbf{a} = \mathbf{b}^*.\mathbf{b} = \mathbf{c}^*.\mathbf{c} = 2\pi \tag{2.17}$$

with Eqs. (2.15) still being valid. These equations can be satisfied by choosing the reciprocal lattice vectors as

$$\left.\begin{aligned} \mathbf{a}^* &= 2\pi \frac{\mathbf{b}\times\mathbf{c}}{\mathbf{a}.\mathbf{b}\times\mathbf{c}} \\ \mathbf{b}^* &= 2\pi \frac{\mathbf{c}\times\mathbf{a}}{\mathbf{a}.\mathbf{b}\times\mathbf{c}} \\ \mathbf{c}^* &= 2\pi \frac{\mathbf{a}\times\mathbf{b}}{\mathbf{a}.\mathbf{b}\times\mathbf{c}} \end{aligned}\right] \tag{2.18}$$

It is now obvious that every crystal structure is associated with two important lattices — the direct lattice and the reciprocal lattice. The two lattices are related to each other by Eqs. (2.13). The fundamental translation vectors of the crystal lattice and the reciprocal lattice have dimensions of [length] and $[\text{length}]^{-1}$ respectively. This is why the latter is called the 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 the **k**-space. The points of the crystal lattice are given by

$$\mathbf{T} = m\mathbf{a} + n\mathbf{b} + p\mathbf{c} \tag{2.19}$$

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

$$\mathbf{G} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* \tag{2.20}$$

where h, k and l are integers. Every point in the Fourier space has a meaning, but the reciprocal lattice points defined by Eq. (2.20) carry a special importance. In order to find the significance of G's, we take the dot product of G and T :

$$\mathbf{G.T} = (h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*) \,.\, (m\mathbf{a}+n\mathbf{b}+p\mathbf{c})$$

$$= 2\pi\,(hm+kn+lp) = 2\pi \text{ (an integer)}$$

or $$\exp\,(i\mathbf{G.T}) = 1$$

where we have used Eq. (2.17). Thus it is clear from Eq. (2.20) that h, k and l define the coordinates of the points of reciprocal lattice space. In other words, it means that a point (h,k,l) 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.

2.4.2 Reciprocal Lattice to SC Lattice

The primitive translation vectors of a simple cubic lattice may be written as

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

Volume of the simple cubic unit cell $= \mathbf{a.b\times c}$

$$= a^3\,(\hat{\mathbf{i}}.\hat{\mathbf{j}}\times\hat{\mathbf{k}}) = a^3$$

Using Eqs. (2.18), the reciprocal lattice vectors to the *sc* lattice are obtained as

$$\mathbf{a}^* = 2\pi\,\frac{\mathbf{b}\times\mathbf{c}}{\mathbf{a}.\mathbf{b}\times\mathbf{c}} = 2\pi\,\frac{a\hat{\mathbf{j}}\times a\hat{\mathbf{k}}}{a^3} = \frac{2\pi}{a}\hat{\mathbf{i}}$$

Similarly,

$$\mathbf{b}^* = 2\pi\,\frac{\mathbf{c}\times\mathbf{a}}{\mathbf{a}.\mathbf{b}\times\mathbf{c}} = \frac{2\pi}{a}\hat{\mathbf{j}} \tag{2.21}$$

and

$$\mathbf{c}^* = 2\pi\,\frac{\mathbf{a}\times\mathbf{b}}{\mathbf{a}.\mathbf{b}\times\mathbf{c}} = \frac{2\pi}{a}\hat{\mathbf{k}}$$

The Eqs. (2.21) 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 $2\pi/a$.

2.4.3 Reciprocal Lattice to BCC Lattice

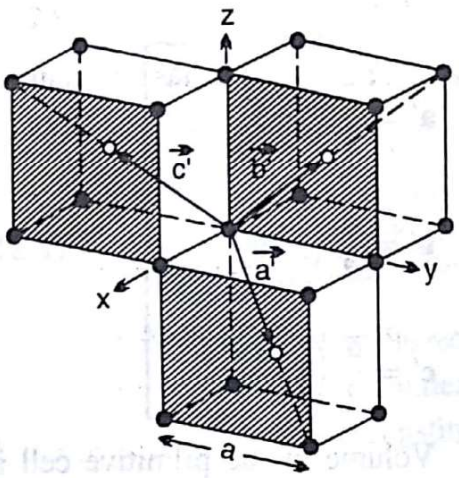

Fig. 2.10. *Primitive translation vectors of a bcc lattice.*

The primitive translation vectors of a body-centred cubic lattice, as shown in Fig. 2.10, are

$$\left.\begin{aligned} \mathbf{a}' &= \frac{a}{2}\left(\hat{\mathbf{i}}+\hat{\mathbf{j}}-\hat{\mathbf{k}}\right) \\ \mathbf{b}' &= \frac{a}{2}\left(-\hat{\mathbf{i}}+\hat{\mathbf{j}}+\hat{\mathbf{k}}\right) \\ \mathbf{c}' &= \frac{a}{2}\left(\hat{\mathbf{i}}-\hat{\mathbf{j}}+\hat{\mathbf{k}}\right) \end{aligned}\right\} \quad (2.22)$$

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

$$\mathbf{V} = \mathbf{a}'.\mathbf{b}'\times\mathbf{c}' = \frac{a}{2}\left(\hat{\mathbf{i}}+\hat{\mathbf{j}}-\hat{\mathbf{k}}\right) \cdot \left[\frac{a^2}{4}\left(-\hat{\mathbf{i}}+\hat{\mathbf{j}}+\hat{\mathbf{k}}\right)\times\left(\hat{\mathbf{i}}-\hat{\mathbf{j}}+\hat{\mathbf{k}}\right)\right]$$

$$= \frac{a}{2}\left(\hat{\mathbf{i}}+\hat{\mathbf{j}}-\hat{\mathbf{k}}\right) \cdot \frac{a^2}{2}\left(\hat{\mathbf{i}}+\hat{\mathbf{j}}\right)$$

$$= a^3/2$$

Using Eqs. (2.18), the reciprocal lattice vectors are obtained as

$$\left.\begin{aligned} \mathbf{a}^* &= 2\pi\frac{\mathbf{b}'\times\mathbf{c}'}{\mathbf{a}'.\,\mathbf{b}'\times\mathbf{c}'} = \frac{2\pi\left(a^2/2\right)}{a^3/2}\left(\hat{\mathbf{i}}+\hat{\mathbf{j}}\right) = \frac{2\pi}{a}\left(\hat{\mathbf{i}}+\hat{\mathbf{j}}\right) \\ \text{Similarly,} \quad \mathbf{b}^* &= 2\pi\frac{\mathbf{c}'\times\mathbf{a}'}{\mathbf{a}'.\,\mathbf{b}'\times\mathbf{c}'} = \frac{2\pi}{a}\left(\hat{\mathbf{j}}+\hat{\mathbf{k}}\right) \\ \text{and} \quad \mathbf{c}^* &= 2\pi\frac{\mathbf{a}'\times\mathbf{b}'}{\mathbf{a}'.\,\mathbf{b}'\times\mathbf{c}'} = \frac{2\pi}{a}\left(\hat{\mathbf{k}}+\hat{\mathbf{i}}\right) \end{aligned}\right\} \quad (2.23)$$

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

2.4.4 Reciprocal Lattice to FCC Lattice

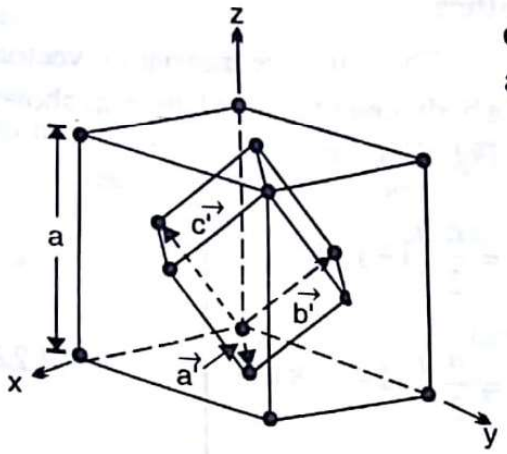

Fig. 2.11. *Primitive translation vectors of an fcc lattice.*

The primitve translation vectors of an *fcc* lattice, as shown in Fig. 2.11, are

$$\left.\begin{aligned} \mathbf{a}' &= \frac{a}{2}\left(\hat{\mathbf{i}}+\hat{\mathbf{j}}\right) \\ \mathbf{b}' &= \frac{a}{2}\left(\hat{\mathbf{j}}+\hat{\mathbf{k}}\right) \\ \mathbf{c}' &= \frac{a}{2}\left(\hat{\mathbf{k}}+\hat{\mathbf{i}}\right) \end{aligned}\right] \qquad (2.24)$$

Volume of the primitive cell is given by

$$V = \mathbf{a}' .\mathbf{b}' \times \mathbf{c}'$$

$$= \frac{a}{2}\left(\hat{\mathbf{i}}+\hat{\mathbf{j}}\right) \cdot \frac{a^2}{4}\left[\left(\hat{\mathbf{j}}+\hat{\mathbf{k}}\right)\times\left(\hat{\mathbf{k}}+\hat{\mathbf{i}}\right)\right]$$

$$= \frac{a}{2}\left(\hat{\mathbf{i}}+\hat{\mathbf{j}}\right) \cdot \frac{a^2}{4}\left(\hat{\mathbf{i}}+\hat{\mathbf{j}}-\hat{\mathbf{k}}\right)$$

$$= a^3/4$$

Using Eqs. (2.18), the primitive translation vectors of the reciprocal lattice are obtained as

$$\left.\begin{aligned} \mathbf{a}^* &= 2\pi \frac{\mathbf{b}'\times\mathbf{c}'}{\mathbf{a}'.\,\mathbf{b}'\times\mathbf{c}'} = 2\pi \frac{\left(a^2/4\right)\left(\hat{\mathbf{i}}+\hat{\mathbf{j}}-\hat{\mathbf{k}}\right)}{a^3/4} = \frac{2\pi}{a}\left(\hat{\mathbf{i}}+\hat{\mathbf{j}}-\hat{\mathbf{k}}\right) \\ \text{Similarly,} \quad \mathbf{b}^* &= 2\pi \frac{\mathbf{c}'\times\mathbf{a}'}{\mathbf{a}'.\,\mathbf{b}'\times\mathbf{c}'} = \frac{2\pi}{a}\left(-\hat{\mathbf{i}}+\hat{\mathbf{j}}+\hat{\mathbf{k}}\right) \\ \text{and} \quad \mathbf{c} &= 2\pi \frac{\mathbf{a}'\times\mathbf{b}'}{\mathbf{a}'.\,\mathbf{b}'\times\mathbf{c}'} = \frac{2\pi}{a}\left(\hat{\mathbf{i}}-\hat{\mathbf{j}}+\hat{\mathbf{k}}\right) \end{aligned}\right] \qquad (2.25)$$

Comparing Eqs. (2.25) with Eqs. (2.22), 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.

2.5 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 an arbitrarily fixed origin is inversely proportional to the interplanar spacing of the corresponding parallel planes of the direct lattice.
3. The volume of a unit cell of the reciprocal lattice is inversely proportional to the volume of the corresponding unit cell of the direct lattice.
4. The unit cell of the reciprocal lattice need not be a parallelopiped. It is customary to deal with Wigner-Seitz cell of the reciprocal lattice which constitutes the Brillouin 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.

2.6. 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 vectors in the reciprocal lattice. Consider a reciprocal lattice as shown in Fig. 2.12. 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 centre, draw a sphere of radius AO which may intersect some point B of the reciprocal lattice.

Let the coordinates of 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,

$$|\vec{OB}| = n/d_{hkl} \tag{2.26}$$

It follows from the geometry of Fig. 2.12. 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

$$OB = 2\,OE = 2\,OA\,\sin\theta = (2\,\sin\theta)/\lambda \tag{2.27}$$

From Eqs. (2.26) and (2.27), we get

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

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

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 nth order reflection from the planes (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 $1/\lambda$ drawn about the point A intersects a point of the reciprocal lattice. Such a construction is called *Ewald construction.*

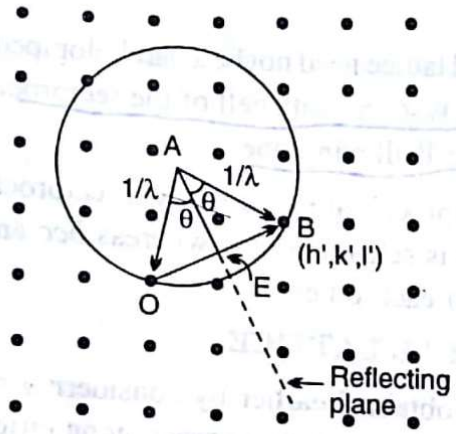

Fig. 2.12. *Ewald construction in the reciprocal lattice.*

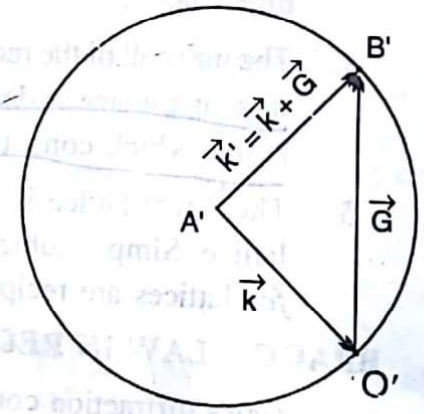

Fig. 2.13. *Magnified Ewald construction relating reciprocal lattice vector to the wave vectors of the incident and reflected radiation.*

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 $\overrightarrow{AO}$, $\overrightarrow{OB}$ and $\overrightarrow{AB}$ such that each is magnified by a constant factor of 2π. Let the new vectors be $\overrightarrow{A'O'}$, $\overrightarrow{O'B'}$ and $\overrightarrow{A'B'}$ respectively as shown in Fig. 2.13. Since

$$A'O' = 2\pi\,(AO) = 2\pi/\lambda,$$

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

$$|\overrightarrow{A'B'}| = |\overrightarrow{A'O'}|$$

or $$(\mathbf{k} + \mathbf{G})^2 = k^2$$

or $$k^2 + 2\mathbf{k}.\mathbf{G} + G^2 = k^2$$

or $$2\mathbf{k}.\mathbf{G} + G^2 = 0 \qquad (2.28)$$

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

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

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

which gives

$$k'^2 = k^2 \tag{2.29}$$

and

$$\mathbf{k}' - \mathbf{k} = \Delta\mathbf{k} = \mathbf{G} \tag{2.30}$$

This indicates that the scattering does not change the magnitude of wave vector **k**; only its direction is changed. Also, the scattered wave differs from the incident wave by a reciprocal lattice vector **G**.

2.7 BRILLOUIN ZONES

It has been indicated in the Ewald construction that all the **k**-values for which the reciprocal lattice points intersect the Ewald sphere are Bragg reflected. A *Brillouin zone* is the locus of all those **k**-values in the reciprocal lattice which are Bragg reflected. We construct the Brillouin zones for a simple square lattice of s.de a. The primitive translation vectors of this lattice are

$$\mathbf{a} = a\hat{\mathbf{i}}; \quad \mathbf{b} = a\hat{\mathbf{j}}$$

The corresponding translation vectors of the reciprocal lattice are

$$\mathbf{a}^* = (2\pi/a)\,\hat{\mathbf{i}}\,; \mathbf{b}^* = (2\pi/a)\hat{\mathbf{j}}$$

Therefore, the reciprocal lattice vector is written as

$$\mathbf{G} = (2\pi/a)\,(h\hat{\mathbf{i}} + k\hat{\mathbf{j}})$$

where h and k are integers. The wave vector **k** can be expressed as

$$\mathbf{k} = k_x\hat{\mathbf{i}} + k_y\hat{\mathbf{j}}$$

From the Bragg's condition (2.28), we have

$$2\mathbf{k}.\mathbf{G} + G^2 = 0$$

or $$\frac{4\pi}{a}\,[(k_x\hat{\mathbf{i}} + k_y\hat{\mathbf{j}}) \,.\, (h\hat{\mathbf{i}} + k\hat{\mathbf{j}})] + \frac{4\pi^2}{a^2}\,(h^2 + k^2) = 0$$

or $$hk_x + kk_y = -(\pi/a)\,(h^2 + k^2) \tag{2.31}$$

The **k**-values which are Bragg reflected are obtained by considering all possible combinations of h and k.

For $h = \pm 1$ and $k = 0$, $k_x = \pm\pi/a$ and k_y is arbitrary;

Also, for $h = 0$ and $k = \pm 1$, $k_y = \pm\pi/a$ and k_x is arbitrary.

These four lines, i.e., $k_x = \pm\pi/a$ and $k_y = \pm\pi/a$, are plotted in Fig. 2.14. Taking origin as shown, all the **k**-vectors originating from it and terminating on these lines will produce Bragg reflection. The square bounded by these four lines is called the *first Brillouin zone*. Thus the first zone of a square lattice of side a is a square of side $2\pi/a$. In addition to this set of lines, some other sets of lines are also possible which satisfy (2.31). For example, for $h = \pm 1$ and $k = \pm 1$, the condition (2.31) gives the following set of four lines.

$$\pm k_x \pm k_y = 2\pi/a$$

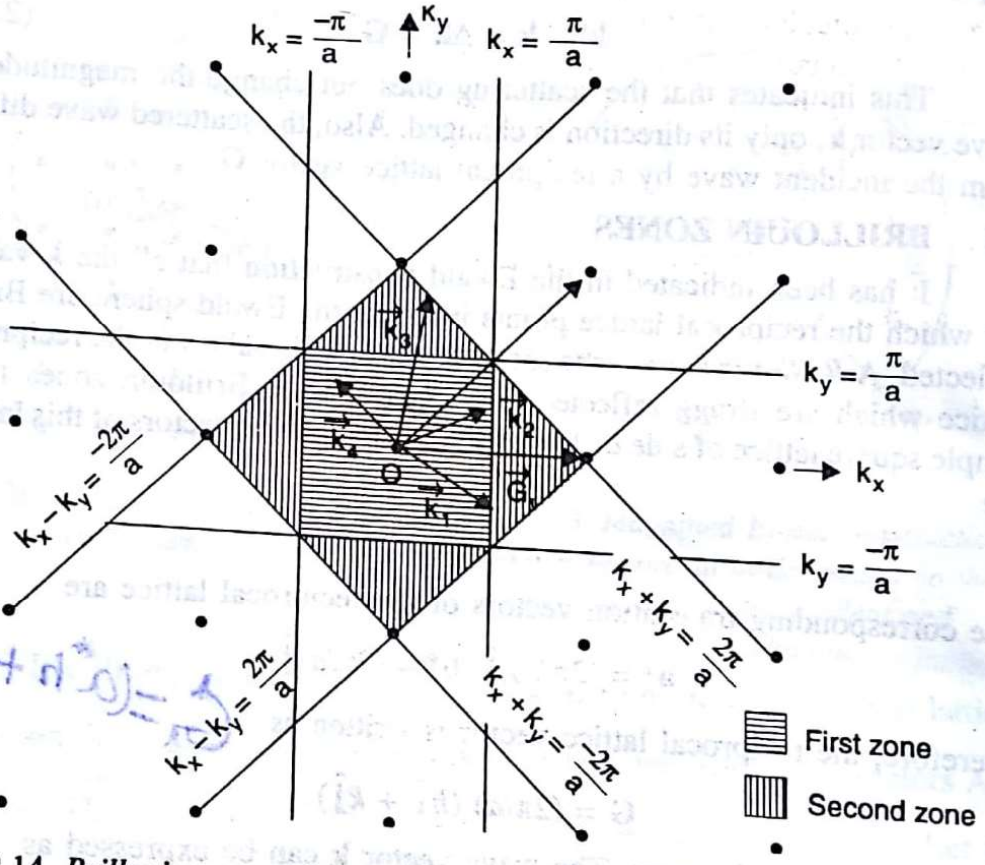

Fig. 2.14. *Brillouin zones of a square lattice in its reciprocal lattice. The vectors* $\mathbf{k}_1$, $\mathbf{k}_2$, *and* $\mathbf{k}_3$ *are Bragg reflected whereas* $\mathbf{k}_4$ *is not. The vectors* $\mathbf{k}_1$ *and* $\mathbf{k}_2$ *have the same reciprocal lattice vector* $\mathbf{G}_1$, *while* $\mathbf{G}_2$ *is the reciprocal vectors of* $\mathbf{k}_3$.

These lines are also plotted in Fig. 2.14. The additional area bounded by these four lines is the *second Brillouin zone*. Similarly the other zones can be constructed. The boundaries of the Brillouin zones represent the loci of **k**-values that are Bragg reflected and hence may be considered as the reflecting planes. The boundaries of the first zone represent the reflecting planes for the first order reflection, those of the second zone represent the reflecting planes for the second order reflection, and so on. A **k**-vector that does not terminate at a zone boundary cannot produce Bragg reflection. Thus the Brillouin zone pattern can be employed to determine the x-ray diffraction pattern of a crystal and vice versa.

The Brillouin zones for a three-dimensional cubical lattice are constructed using the generalized equation

$$hk_x + kk_y + lk_z = -(\pi/a)\,(h^2 + k^2 + l^2) \qquad (2.32)$$

where a is the length of the cube edge. It is clear from Eq. (2.32) that the first zone is a cube having side equal to $2\pi/a$. The second zone is formed by adding pyramids to each face of the cube (first zone) as triangles are added to the square in two dimensions, and so on.

There is another simple method to determine Brillouin zones. We note from Fig. 2.14 that the reciprocal lattice vector **G** which satisfies Eq. (2.28) is a perpendicular bisector of the zone boundary and all the **k**-vectors lying on this boundary have the same **G** for reflection. Thus it is sufficient to consider only the allowed **G**-values and their normal bisectors to construct the Brillouin zones. The first Brillouin zone is the region bounded by the normal bisectors of the shortest possible **G**-vectors, the second zone is the region bounded by the normal bisectors of the next larger **G**-vectors, and so on. This method will be used to determine the Brillouin zones of the *bcc* and *fcc* lattices as given below.

2.7.1 Brillouin Zone of BCC Lattice

The primitive translation vectors of a *bcc* lattice are

$$\mathbf{a} = (a/2)\,(\hat{\mathbf{i}}+\hat{\mathbf{j}}-\hat{\mathbf{k}})$$

$$\mathbf{b} = (a/2)\,(-\hat{\mathbf{i}}+\hat{\mathbf{j}}+\hat{\mathbf{k}})$$

$$\mathbf{c} = (a/2)\,(\hat{\mathbf{i}}-\hat{\mathbf{j}}+\hat{\mathbf{k}})$$

The primitive translation vectors of its reciprocal lattice are (Sec. 2.4.3)

$$\mathbf{a}^* = (2\pi/a)\,(\hat{\mathbf{i}}+\hat{\mathbf{j}})$$

$$\mathbf{b}^* = (2\pi/a)\,(\hat{\mathbf{j}}+\hat{\mathbf{k}})$$

$$\mathbf{c}^* = (2\pi/a)\,(\hat{\mathbf{k}}+\hat{\mathbf{i}})$$

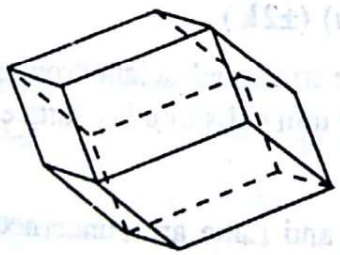

Fig. 2.15. *First Brillouin zone of a bcc lattice.*

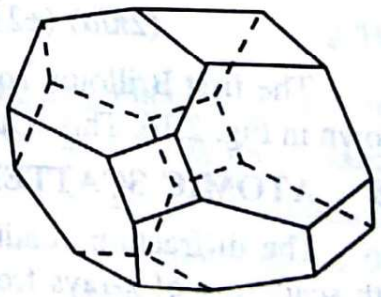

Fig. 2.16. *First Brillouin zone of an fcc lattice.*

The G-type reciprocal lattice vector is

$$\mathbf{G} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$$
$$= (2\pi/a)\,[(h + l)\,\hat{\mathbf{i}} + (h + k)\,\hat{\mathbf{j}} + (k + l)\,\hat{\mathbf{k}}] \quad (2.33)$$

The shortest non-zero G's are the following twèlve vectors

$$(2\pi/a)\,(\pm\hat{\mathbf{i}} \pm \hat{\mathbf{j}});\ (2\pi/a)\,(\pm\hat{\mathbf{j}} \pm \hat{\mathbf{k}});\ (2\pi/a)(\pm\hat{\mathbf{k}} \pm \hat{\mathbf{i}})$$

The first Brillouin zone is the region enclosed by the normal bisector planes to these twelve vectors. This zone has the shape of a regular twelve-faced solid as shown in Fig. 2.15 and is called rhombic dodecahedron.

2.7.2 Brillouin Zone of FCC Lattice

The primitive translation vectors of an *fcc* lattice are

$$\mathbf{a} = (a/2)\,(\hat{\mathbf{i}} + \hat{\mathbf{j}})$$
$$\mathbf{b} = (a/2)\,(\hat{\mathbf{j}} + \hat{\mathbf{k}})$$
$$\mathbf{c} = (a/2)\,(\hat{\mathbf{k}} + \hat{\mathbf{i}})$$

The primitive translation vectors of its reciprocal lattice are (Sec. 2.4.4)

$$\mathbf{a}^* = (2\pi/a)\,(\hat{\mathbf{i}}+\hat{\mathbf{j}}-\hat{\mathbf{k}})$$
$$\mathbf{b}^* = (2\pi/a)\,(-\hat{\mathbf{i}}+\hat{\mathbf{j}}+\hat{\mathbf{k}})$$
$$\mathbf{c}^* = (2\pi/a)\,(\hat{\mathbf{i}}-\hat{\mathbf{j}}+\hat{\mathbf{k}})$$

The G-type vector is

$$\mathbf{G} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$$
$$= (2\pi/a)\,[(h - k + l)\,\hat{\mathbf{i}} + (h + k - l)\,\hat{\mathbf{j}} + (-h + k + l)\,\hat{\mathbf{k}}] \quad (2.34)$$

The shortest non-zero G's are the following eight vectors

$$(2\pi/a)\,(\pm\hat{\mathbf{i}} \pm \hat{\mathbf{j}} \pm \hat{\mathbf{k}})$$

The boundaries of the first Brillouin zone are determined mostly by the normal bisector planes to the above eight vectors. However, the corners of the octahedron obtained in this manner are truncated by the planes which are normal bisectors to the following six reciprocal lattice vectors

$$(2\pi/a)\,(\pm2\hat{\mathbf{i}});\ (2\pi/a)\,(\pm2\hat{\mathbf{j}});\ (2\pi/a)\,(\pm2\hat{\mathbf{k}})$$

The first Brillouin zone has the shape of the truncated octahedron as shown in Fig. 2.16. This is also one of the primitive unit cells of a *bcc* lattice.

2.8 ATOMIC SCATTERING FACTOR

The diffraction conditions given by Bragg and Laue are concerned with scattering of x-rays from point scattering centres arranged on a space lattice. Since an electron is the smallest scattering centre, the diffraction conditions would ideally be applicable to a lattice in which every lattice point is occupied by an electron. This is, however, not a realistic situation. Lattice