Brillouin Zones

It has been indicated in the Ewald construction that all the **k**-values for which the reciprocal lattice point 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 side a. The primitive translation vectors of this lattice are

$$\vec{a} = a\hat{i}\,; \qquad \vec{b} = a\hat{j}$$

The corresponding translation vectors of the reciprocal lattice are

$$\vec{a}^* = \frac{2\pi}{a}\hat{i}\,; \qquad \vec{b}^* = \frac{2\pi}{a}\hat{j}$$

Therefore, the reciprocal lattice vector is written as

$$\vec{G} = \frac{2\pi}{a}\left(h\hat{i} + k\hat{j}\right)$$

where h and k are integers. The wave vector $\vec{k}$ can be expressed as

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

From the Bragg's condition, we have

$$2\vec{k}\cdot\vec{G} + G^2 = 0$$
$$\frac{4\pi}{a}\left[\left(k_x\hat{i} + k_y\hat{j}\right)\cdot\left(h\hat{i} + k\hat{j}\right)\right] + \frac{4\pi^2}{a^2}\left(h^2 + k^2\right) = 0$$
$$hk_x + kk_y = -\frac{\pi}{a}\left(h^2 + k^2\right)$$

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 figure 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 $hk_x + kk_y = -\frac{\pi}{a}\left(h^2 + k^2\right)$. For example, for $h = \pm 1$ and $k = \pm 1$, the condition gives the following set of four lines

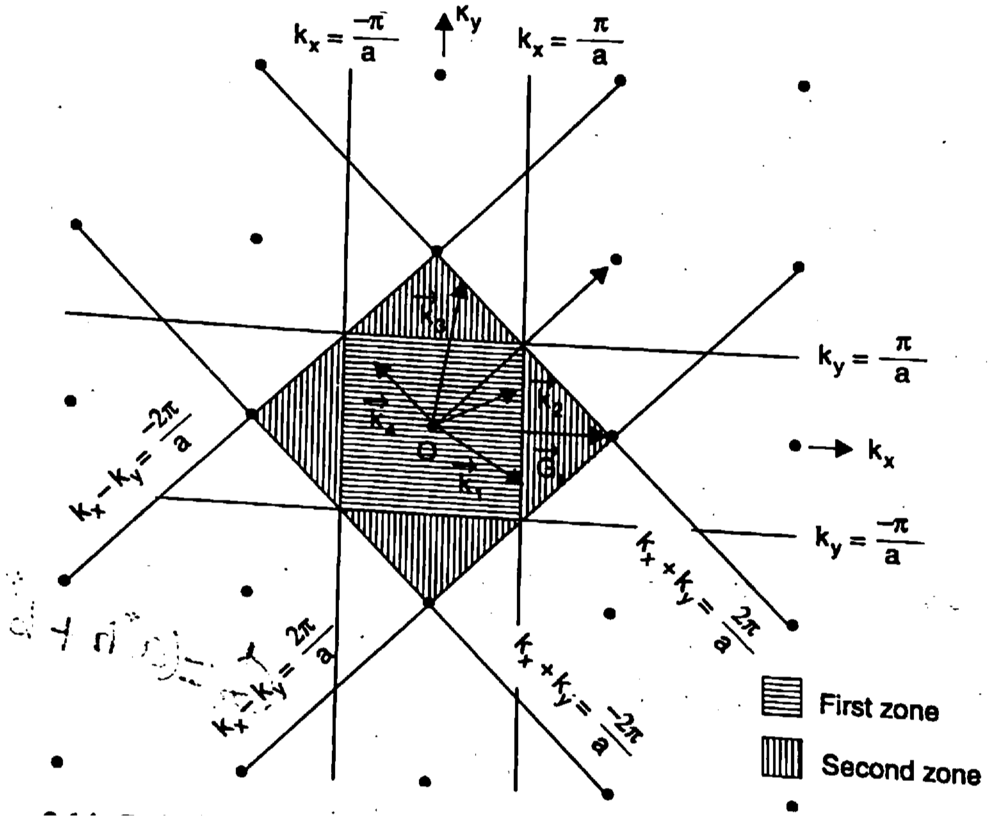
$$\pm k_x \pm k_y = 2\pi/a$$

These lines are also plotted in figure. The additional area bounded by these four lines is called 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

$$hk_x + kk_y + lk_z = -(\pi/a)\left(h^2 + k^2 + l^2\right)$$

where a is the length of the cube edge. It is clear from the equation 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 figure that the reciporcal lattice vector $\vec{G}$ which satisfy $2\vec{k}\cdot\vec{G} + G^2 = 0$ is a perpendicular bisector of the zone boundary and all the **k**-vectors lying on this boundary have the same $\vec{G}$ for reflection. Thus it is sufficient to consider only the allowed $\vec{G}$-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 $\vec{G}$-vectors, the second zone is the region bounded by the normal bisectors of the next larger $\vec{G}$-vectors and so on.