Brillouin Zones and their importance:

The different Brillouin zones correspond to primitive cells of a different type that come up in the theory of electronic levels in a periodic potential. The first Brillouin zone is considered as the Wigner-Seitz (WS) primitive cell in the reciprocal lattice. In other words, the first Brillouin zone is a geometrical construction to the WS primitive cell in the k-space.

In a direct lattice, the procedure of drawing a WS cell is as follows:

i) Draw lines to connect a given lattice points to all nearby lattice points.

ii) Draw new lines or plane at the mid point and normal to the lines in (*i*).

iii) The smallest volume enclosed in this way is the WS primitive cell. [See figure 29].

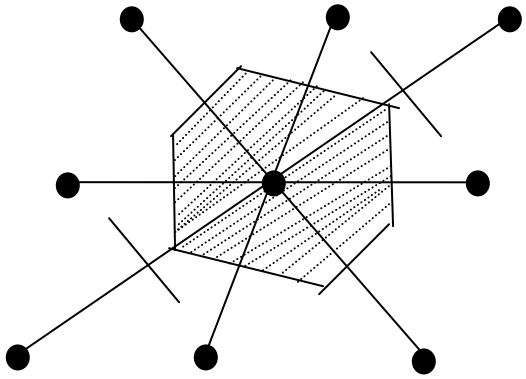


Figure 29: Construction of primitive Wigner-Sietz cell in 2-D direct space lattice.

Construction of a Wigner-Seitz cell in the reciprocal lattice (called first Brillouin zone):

To construct the first Brillouin zone, we need to find the link between the incident beam (like electron or neutron or phonon beam) of wave vector $\vec{k}$ and the reciprocal lattice vector $\vec{G}$. This relation may be found as $\vec{k} \bullet (\frac{\vec{G}}{2}) = (\frac{G}{2})^2$, [for example, an x-ray beam in the crystal will be diffracted if its wave vector $\vec{k}$ has the magnitude and direction required by this latter relation]. [See the proof in the next chapter]. Thus the procedure to build up the first Brillouin zone is as follows (see figure 30):

i) Select a vector $\vec{G}$ from the origin to a reciprocal lattice point.

ii) Construct a plane normal to the vector $\vec{G}$ at its mid point. This plane forms a part of the zone boundary.

iii) The diffracted beam will be in the direction $\vec{k} - \vec{G}$.

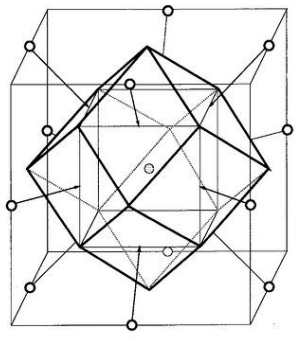
iv) Thus the Brillouin construction exhibits all the wave vectors $\vec{k}$ which can be Bragg-reflected by the crystal.

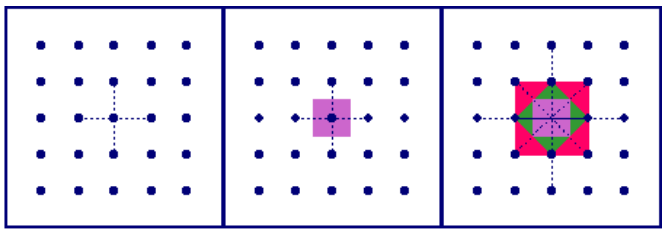
Important note:

A wave whose wave vector drawn from the origin terminates on any of the planes will satisfy the condition of diffraction. Such planes are the perpendicular bisectors of the reciprocal vectors.

Remarks:

- The planes divide the Fourier space of the crystal into fragments as shown for a square lattice.
- The central square is a primitive cell of the reciprocal lattice. It is a Wigner-Seitz cell of the reciprocal lattice (called the first Brillouin zone).(See figure 29).
- The first Brillouin zone is the smallest volume entirely enclosed by the planes.





Conclusion: Wigner-Seitz cell: smallest possible primitive cell, which consist of one lattice point and all the surrounding space closer to it than to any other point. The construction of the W-S cell in the reciprocal lattice delivers the first Brillouin zone (important for diffraction).

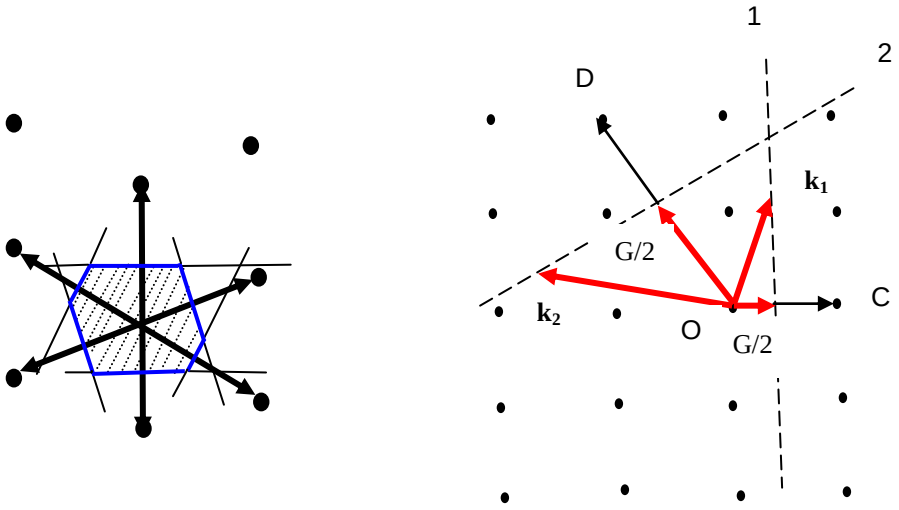
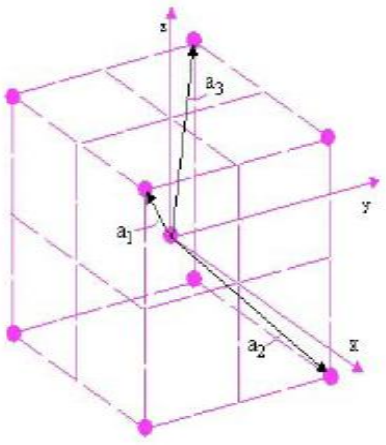


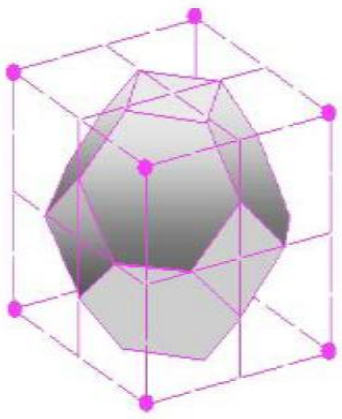
Figure 30: Construction of the first Brillouin zone for oblique lattice in 2-D reciprocal space lattice.

The importance of Brillouin zone:

The Brillouin zones are used to describe and analyze the electron energy in the band energy structure of crystals.



Body Centered Cubic Lattice



Wigner-Seitz Cell for Body Centered Cubic Lattice

Lattice planes and their importance:

The plane of points in the direct lattice may be represented by their intersection with the crystal axses $\vec{a}_1$, $\vec{a}_2$ and $\vec{a}_3$ as $x_1\vec{a}_1$, $x_2\vec{a}_2$ and $x_3\vec{a}_3$. The relations $x_1=n/h$, $x_2=n/k$ and $x_3=n/\ell$ give intercepts of planes that do not pass through lattice points. The integers h, k and ℓ are used to index a plane. Here n is any integer (which represents the common divisor used for a proper choice of the h, k and ℓ indices)*. When primitive vectors in reciprocal lattice are used to index a plane, no common divisor other than 1 is needed for the indices. However, a common factor other than one is needed to get h, k and ℓ indices and then finding the intercepts of all planes, when non-primitive lattice vectors are chosen instead.

*[Note: Here, the set of integers k_1, k_2 and k_3 is replaced from now on by a well-known set of integers the h, k and ℓ].

Definitions

A lattice plane in a Bravais lattice:

It is the plane that may contain at least three noncollinear Bravais lattice points. Actually such a plane may contain infinitely many lattice points which form a two-dimensional Bravais lattice. [See figure 31].

A family of lattice planes:

This represents the collection of parallel, equally spaced lattice planes which together contain the entire 3-D Bravais lattice. There are many different possible families of lattice planes.

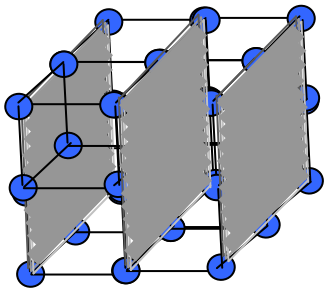


Figure 31: A family of lattice planes in a simple cubic lattice

If we consider the set of real space planes on which the plane wave $e^{i\vec{K}\bullet\vec{r}}$ has a value of one (where $\vec{r} = x_1\vec{a}_1 + x_2\vec{a}_2 + x_3\vec{a}_3$). These planes (one of which contains the point $\vec{r} = 0$) are perpendicular to a set of vectors $\vec{K}$ in reciprocal lattice. These set of vectors satisfy the relation $e^{i\vec{K}\bullet\vec{R}} = 1$(i.e. the plane wave is constant in planes perpendicular to $\vec{K}$ and has the same value in planes separated by d) for all Bravais lattice vectors $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$. The latter vectors must lie within a family of lattice planes. For nth plane in a family of planes that do not contain lattice points, the separation between plane is rather nd (where n is defined before as $n = hn_1 + kn_2 + \ell n_3$). [It must be noted here that $\vec{K}$ is redefined as $\vec{K} = h\vec{b}_1 + k\vec{b}_2 + \ell\vec{b}_3$]. Thus the reciprocal lattice vector normal to the nth plane and then its family of planes, is $\vec{K} = n\vec{G}$. This means that when the family of planes contain lattice points then the shortest reciprocal lattice vector $\vec{G} = \vec{K}$ will be used instead (*i.e.* n must be equal unity in this case).

Example: Consider a plane $h\ k\ \ell$ in a crystal lattice which intersects the crystal axis as $x_1\vec{a}_1$, $x_2\vec{a}_2$ and $x_3\vec{a}_3$.

a) Prove that the reciprocal lattice vector $\vec{G} = h\vec{b}_1 + k\vec{b}_2 + \ell\vec{b}_3$ is perpendicular to this plane.

b) Prove that the distance between the two adjacent parallel planes of the lattice is $d(hk\ell) = \dfrac{2\pi}{|\vec{G}|}$.

c) Show for a simple cubic lattice that $d = \dfrac{a}{\sqrt{h^2 + k^2 + \ell^2}}$.

Solution:

In figure 32 the plane $h\ k\ \ell$ intersecting the axis $\vec{a}_1$, $\vec{a}_2$ and $\vec{a}_3$ by $x_1\vec{a}_1$, $x_2\vec{a}_2$ and $x_3\vec{a}_3$, respectively. The small plane $hk\ell$ contains the two vectors $x_1\vec{a}_1 - x_2\vec{a}_2$ and $x_1\vec{a}_1 - x_3\vec{a}_3$. The reciprocal lattice vector $\vec{G} = h\vec{b}_1 + k\vec{b}_2 + \ell\vec{b}_3$ is in the direction of the unit vector $\hat{n}$ which is normal to the $hk\ell$ plane.

a) Taking the dot products $(x_1\vec{a}_1 - x_2\vec{a}_2) \bullet \vec{G}$ and $(x_1\vec{a}_1 - x_3\vec{a}_3) \bullet \vec{G}$, where each product gives zero. This result indicates that these vectors are perpendicular to the two vectors and also perpendicular to the $hk\ell$ plane.

b) The projection of the vector $x_1\vec{a}_1$ on the normal unit vector $\hat{n}$ is simply the distance $d(hk\ell)$ which separating the $hk\ell$ plane and another plane passing through the origin.
$\therefore d(hk\ell) = \hat{n} \bullet x_1\vec{a}_1$,

but $\hat{n} = \dfrac{\vec{G}}{|\vec{G}|}$.

$$\therefore d(hk\ell) = \frac{h\vec{b}_1 + k\vec{b}_2 + \ell\vec{b}_3}{|\vec{G}|} \bullet x_1\vec{a}_1 ,$$

where $\vec{b}_1 = 2\pi \dfrac{\vec{a}_2 \times \vec{a}_3}{V_{cell}}$, $\vec{b}_2 = 2\pi \dfrac{\vec{a}_3 \times \vec{a}_1}{V_{cell}}$ and $\vec{b}_3 = 2\pi \dfrac{\vec{a}_1 \times \vec{a}_2}{V_{cell}}$, and n is chosen to be one.

This gives $d(hk\ell) = \dfrac{2\pi}{|\vec{G}|}$.

c) For a simple cubic lattice $\vec{G} = (\dfrac{2\pi}{a})(h\hat{x} + k\hat{y} + \ell\hat{z})$, where

$\vec{b}_1 = (\dfrac{2\pi}{a})\hat{x}$, $\vec{b}_2 = (\dfrac{2\pi}{a})\hat{y}$ and $\vec{b}_3 = (\dfrac{2\pi}{a})\hat{z}$.

$$\therefore d(hk\ell) = \frac{a}{\sqrt{h^2 + k^2 + \ell^2}} .$$

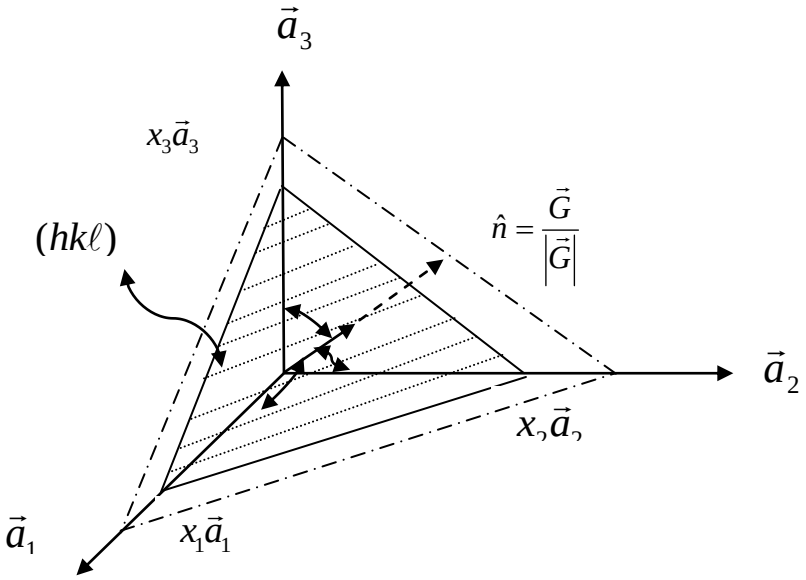


Figure 32: The interplanar distance of two parallel planes intersecting the crystal axis.

Indexing of lattice planes (Miller indices):

Miller indices are usually used to specify the crystal orientation of solids. It is shown above that a vector normal to a lattice plane may describe the orientation of this plane. This normal vector is obviously a reciprocal lattice vector. Therefore the unique choice of such a vector is the shortest reciprocal lattice vector $\vec{G} = h\vec{b}_1 + k\vec{b}_2 + \ell\vec{b}_3$.

Conclusions:

1. Miller indices of a lattice plane are the coordinates of the shortest reciprocal lattice vector normal to that plane, with respect to a specified set of primitive reciprocal lattice vectors. (*i.e.* A plane with Miller indices h, k, ℓ is normal to the reciprocal lattice vector $\vec{G} = h\vec{b}_1 + k\vec{b}_2 + \ell\vec{b}_3$).
2. Miller indices are set of integers that depend on the choice of primitive vectors.
3. If the shortest reciprocal lattice vector is chosen as the normal to a lattice plane, then the integers h, k, ℓ may have no common factor.

An alternative way of defining Miller indices:

It can be shown that the projection of the reciprocal lattice vector $\vec{G} = h\vec{b}_1 + k\vec{b}_2 + \ell\vec{b}_3$ on any of the direct lattice vectors $x_1\vec{a}_1$, $x_2\vec{a}_2$ and $x_3\vec{a}_3$, as shown in figure 32, give us the following equations: $\vec{G} \bullet (x_1\vec{a}_1) = C$; $\vec{G} \bullet (x_2\vec{a}_2) = C$; $\vec{G} \bullet (x_3\vec{a}_3) = C$, where C is any suitably chosen constant.

[Note: It can be easily concluded that the constant C may be defined as $C = 2\pi m$].

Conclusion:

The intercepts with the crystal axes of a lattice plane are inversely proportional to the Miller indices of the plane. However when lattices planes are considered such that no common factors for the Miller indices does exist, the Miller indices have the following proportionality relation: $h : k : \ell = \frac{1}{x_1} : \frac{1}{x_2} : \frac{1}{x_2}$.