We have looked at diffraction in real space and in reciprocal space, and seen examples of what happens when real space structures are represented in reciprocal space. We have also noted that such transformations are carried out primarily for our convenience, the material retains its structure regardless of how we choose to look at it.

In this class, let us introduce a few new terms which we will use extensively later. The first is a ‘Wigner-Seitz cell’. Stated in words, a Wigner-Seitz cell, about a lattice point, is the region in space that is closest to that lattice point than to any other lattice point. While the definition may not be easy to visualize at first glance, it is actually quite easy to determine. As shown in the Figure 30.1 below, Take any two points in space and draw a straight line joining them. Draw a plane that perpendicularly bisects the line joining these two points. All of the points on one side of the perpendicular bisector are by definition closer to the point on the same side of the perpendicular bisector than to the other point. This is illustrated in the figure below.

![Diagram of Wigner-Seitz cell](image)

**Figure 30.1:** Identifying a region closest to a given lattice point than to its neighbor

A lattice, as we have seen, is an array of points. In the most general case it is a three dimensional array of points. To identify the region in space closest to a single lattice point than to any other lattice point, we merely extend the approach we have adopted above. As a first step we identify all of the nearest neighbors of the point we are examining. Lines are then drawn from the point to all of its nearest neighbors. Perpendicular bisectors are drawn to each of the lines. Once these steps are completed, it will be possible to identify the innermost region bounded by these perpendicular bisectors. That innermost region then consists of all of the points in space that are closest to the lattice point in that region than to any other lattice point. This region, bounded by the perpendicular bisectors, is then the Wigner-Seitz cell about that lattice point. The procedure described above is shown in Figure 30.2 below.
Consider a two dimensional square lattice, as drawn below and see how its Wigner-Seitz cell is identified.

![Two dimensional square lattice](image)

**a) Two dimensional square lattice**

**b) Draw lines from a given lattice point to all of its nearest neighbors**

![Lines drawn from lattice points](image)

**c) Draw perpendicular bisectors to the lines joining the point to its nearest neighbors**

![Perpendicular bisectors](image)

**d) The Wigner-Seitz cell is identified as the innermost region bounded by the perpendicular bisectors. It is shown in the figure as the shaded region.**

![Wigner-Seitz cell](image)

**Figure 30.2:** The steps to identify the Wigner-Seitz cell about a lattice point in a two dimensional square lattice.

The procedure described above can easily be extended to three dimensions. The primary difference will be that the perpendicular bisectors will now be planes instead of lines. So for a three dimensional cubic lattice, the two dimensional lattice shown in Figure 30.2 above will form a section of the lattice, and the perpendicular bisectors shown in the figure, will be planes instead of lines. Additionally, there will be a perpendicular bisector above the plane of the paper and one below the plane of paper corresponding to the lines joining the central point to the lattice points above and below the plane of the paper. The Wigner-Seitz cell for the three dimensional cubic
lattice, will therefore be a cube about the lattice point chosen. In the case of the two dimensional square, and the three dimensional cube, the Wigner-Seitz cells also have similar structures, but for other lattices, the shape of the lattice and the shape of the corresponding Wigner Seitz cell may not display such immediate equality.

In two dimensions, a square lattice displays a square Wigner-Seitz cell, and a rectangular lattice displays a rectangular Wigner-Seitz cell. Consider the lattice shown in Figure 30.3 below, which is a more general case of a two dimensional lattice, and its Wigner-Seitz cell.

![Figure 30.3: A general two dimensional lattice and its Wigner-Seitz cell. In the most general case, a two dimensional Wigner Seitz cell will be a hexagon.](image)

In the most general case, the two dimensional Wigner-Seitz cell will be a hexagon. Due to symmetry, in specific cases it reduces to a rectangle or a square based on the lattice chosen, as discussed above.

The second term we will define is a ‘Brillouin Zone’. Given that we now understand how a Wigner Seitz cell is defined, it is easy to see what a Brillouin zone is. We shall first define and look at what a ‘First’ Brillouin zone is, and then subsequently look at the second, third, and higher Brillouin zones. The first Brillouin zone is defined as the Wigner-Seitz primitive cell about a lattice point in reciprocal space. In other words, to identify the first Brillouin zone for a lattice, we first draw the reciprocal lattice corresponding to the given lattice, and then identify the Wigner-Seitz cell about a point in that reciprocal lattice. This specific Wigner-Seitz cell is then the first Brillouin zone corresponding to the original real space lattice.

At this stage it is relevant to note that Wigner Seitz cell is a more general concept and can be defined both with respect to real space as well as with respect to reciprocal space. However, Brillouin Zones are defined only with respect to reciprocal space. Further, Brillouin Zones have greater significance in terms of the electronic properties of the materials and hence are treated as
a concept worthy of independent recognition over and above their relationship to Wigner Seitz cells.

While describing Wigner Seitz cells, we considered planes that perpendicularly bisect lines joining a lattice point to its nearest neighbors. In reciprocal space, planes bisecting lines joining reciprocal lattice points have special significance with respect to diffraction phenomena displayed by that lattice. Planes that are perpendicular bisectors of lines joining the origin to lattice points in reciprocal space, therefore have a special name – they are referred to as ‘Bragg planes’—this is the third term that we are defining in this class. It is important to recognize that Bragg planes bisect lines joining a reciprocal lattice point, chosen as the origin, to all of the other points in the reciprocal lattice, and are not restricted to just lines joining the reciprocal lattice point to its nearest neighbors. The first Brillouin Zone is thus the region bounded by the nearest collection of Bragg planes around a reciprocal lattice point.

To identify the second, third and higher Brillouin Zones, we extend the procedure we have followed thus far. The second Brillouin zone is identified as the region in reciprocal space that extends beyond the nearest (first) Bragg plane in all directions, but not beyond the very next (second) Bragg plane in each of those directions. Generalizing further, the n\textsuperscript{th} Brillouin zone is all of the points between the (n-1)\textsuperscript{th} Bragg plane and the n\textsuperscript{th} Bragg plane in all directions. Stated differently, if we start from each of the points in the (n-1)\textsuperscript{th} Brillouin zone and continue to move outward from the central point, the n\textsuperscript{th} Brillouin zone consists of all of the points that can be reached by crossing just one more Bragg plane.

The process of identifying various Brillouin zones is illustrated in Figure 30.4 below. The points in the figure represent reciprocal lattice points (in this case corresponding to a square real lattice). The lines drawn are various Bragg planes with respect to the central point. The numbers indicate the Brillouin zone to which each region belongs.
Figure 30.4: Identification of the first and higher order Brillouin Zones for a two dimensional square lattice. Although all of the Bragg planes have been drawn in the context of the figure, for clarities sake in (a) Only the first Brillouin Zone is identified; in (b) First, second and third Brillouin zones are identified; and in (c) First second, third, fourth, fifth and sixth Brillouin zones have been identified. All the zones identified are only within the context of the figure drawn, i.e. there are other regions which will correspond to the fourth, fifth, and sixth Brillouin zones, which do not show up in the region shown above.

The first Brillouin zone for a two dimensional square lattice is a square, and this is easy to see in the figures we have drawn. The second Brillouin zone consists of four parts. As can be seen from the figure above, if these four parts are cut and rearranged, a square will emerge once again. Or,
conceptually, if they are moved by one lattice vector, into the first Brillouin zone, they will reassemble into a square. Higher order Brillouin zones get more fragmented and appear at various places in the diagram. However, these fragments too can be reassembled to obtain a square just the way we did with the second Brillouin zone. This process is possible as a direct result of the symmetry of the lattice.

In summary, in this class we have seen what is a Wigner Seitz cell, what is a Bragg plane, and what are Brillouin zones. We have seen examples of these in two dimensions. In three dimensions the corresponding diagrams can begin to look complicated. However the concept is the same. In the next class we will see the three dimensional versions of the first Brillouin zone and later see how it helps us understand the behavior of electrons in solids.

Animation of figure 30.4: 2D Brillouin Zones