ENTRI

HSST PHYSICS

MODULE 7: SOLID STATE PHYSICS

- A crystal is a solid composed of atoms or other microscopic particles arranged in an orderly repetitive array.
- The atomic arrangement in a crystal is called crystal structure.
- In a perfect crystal, there is a regular arrangement of atoms. This periodicity in the arrangement generally varies in different directions. It is very convenient to imagine points in space about which these atoms are located. Such points in space are called **lattice points** and the totality of such points forms a **crystal lattice or space lattice**. If all the atoms at the lattice points are identical, the lattice is called a **Bravais lattice**.
- For a lattice to represent a crystal structure we associate every lattice point with one or more atoms called the **Basis** or the pattern.
- **Lattice + Basis = Crystal structure**
- In every crystal some fundamental grouping of particles is repeated. Such fundamental grouping of particles is called a **unit cell**.
- The crystal lattice may be regarded as made up of an aggregate of a set of parallel equidistant planes, passing through the lattice points, which are known as **lattice planes**.

Miller Indices

- A crystal lattice may be considered as a set of parallel planes passing through the lattice points.
- The orientation of a crystal plane is specified by a set of indices known as Miller indices.

The Miller indices of a plane can be determined using the following procedure;

1. First determine the intercepts of the plane with the coordinate axes along the basis vectors a,b and c. Let these intercepts be x,y and z respectively.

Using x is a fractional multiple of a, y is a multiple of b and z is a multiple of c.

Now, we form a fractional triplet by dividing by unit vectors **â, b̂ and ĉ** to get x/a, y/b and z/c.

2. Take the reciprocal of this triplet, thereby bringing all the planes inside a single unit cell.
3. Finally reduce these fractions to 3 smallest integers having the same ratio by multiplying by the lowest common denominator and enclose them in brackets.

The set so obtained is called Miller indices of the plane and is denoted as (h,k,l)

❖ Example : Determine the Miller indices of a plane parallel to z –axes and cut intercepts of 2 and 3/2 along the x and y axes respectively.

Solution : Intercepts are 2a, $\frac{3b}{2}$,∞

- Dividing by unit translation: $\frac{2a}{a},\frac{3b}{2b},\frac{\infty}{c}$ = 2, $\frac{3}{2}$, ∞
- Taking reciprocals : ½ , $\frac{2}{3},\frac{1}{\infty}$
- Multiplying by the common denominator : 3,4,0
- Therefore the miller indices are (3,4,0)

RECIPROCAL LATTICE

- Every crystal has two types of lattices (i) A direct lattice and (ii) A Reciprocal Lattice. The is a microscopic image of the crystal and the reciprocal lattice is an x-ray diffraction pattern of the crystal.
- Just as the direct lattice is defined by the direct lattice translation vector:

T = ua + vb +wc, a, b, c being the primitive vectors of the direct lattice and *u*, *v*, *w* being integers, the reciprocal lattice is defined by the reciprocal lattice vector: **G = ha* + kb* + lc***

A real lattice consists of planes of different slopes. Therefore its structural studies using Bragg condition are different. The situation can be simplified by introducing the concept of reciprocal lattice. The formulation of reciprocal lattice is based on the following facts.

The orientation of a plane is determined by its normal which has only one dimension. Thus, one normal corresponds to a set of parallel planes. Now, if the length of each normal is proportional to the reciprocal of the inter-planar spacing of those planes, the points at the end of the normal drawn from a common origin form a lattice. This lattice is called Reciprocal lattice. The reciprocal lattice in 3 dimensions is called reciprocal lattice or k- space.

The points in the reciprocal lattice are called reciprocal lattice points.

The reciprocal lattice is constructed using the following procedure:

1. Fix up some point in the direct lattice as a common origin
2. From this common origin draw normal's to each and every set of parallel planes in the direct lattice.
3. Fix the length of each normal as equal to the reciprocal of the interplanar spacing for that set of planes.
4. Place a point at the end of each normal.

The collection of all such points gives us the reciprocal lattice. For the primitive translation vectors a,b and c of the direct lattice, the corresponding reciprocal lattice vectors, denoted by a*, b* and c* respectively, are given by;

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

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

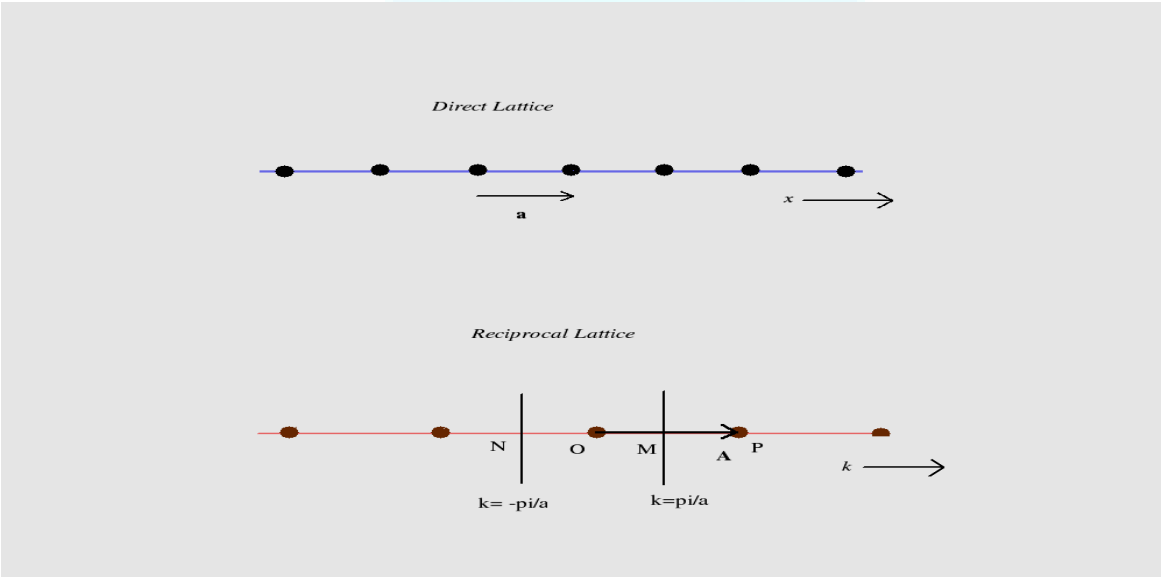
$$c^* = 2\pi \frac{a \times b}{a.(b \times c)}$$

Brillouin Zones

The concept of a Brillouin zone was first developed by Léon Brillouin (1889-1969), a French physicist.

- A Brillouin zone is defined as a Wigner-Seitz primitive cell in the reciprocal lattice.
- The first Brillouin zone is the smallest volume entirely enclosed by planes that are the perpendicular bisectors of the reciprocal lattice vectors drawn from the origin.
- The concept of Brillouin zone is particularly important in the consideration of the electronic structure of solids. There are also second, third, etc., Brillouin zones, corresponding to a sequence of disjoint regions (all with the same volume) at increasing distances from the origin, but these are used more rarely. As a result, the first Brillouin zone is often called simply the Brillouin zone. (In general, the n-th Brillouin zone consist of the set of points that can be reached from the origin by crossing n − 1 Bragg planes.)

Let us see how we to construct the Brilloin zones of a one dimensional linear lattice for which the direct lattice translational vector T = a where a is the only basis vector of the direct lattice. The reciprocal lattice for this linear direct lattice would also be linear as shown below.



Then the reciprocal lattice vector G equals A where A is the only basis vector for the one dimensional reciprocal lattice. In the figure OP = A. The two normal's bisecting A on either side of the origin at the points M and N specify the boundaries of the brillouin zone.

From the equations relating the basis vectors in the two lattices, we find that

$$\begin{aligned} \mathbf{k} \cdot (\frac{1}{2}\mathbf{G}) &= (\frac{1}{2}G)^2 \\ \mathbf{k} \cdot (\frac{1}{2}\mathbf{A}) &= (\frac{1}{2}A)^2 \end{aligned}$$

K : Wave vector and G : Reciprocal lattice vector

Since **k** can occur on both sides of the origin

$$\begin{aligned} \pm\frac{1}{2}kA &= \frac{A^2}{4} \\ k &= \pm\frac{A}{2} \\ &= \pm\frac{2\pi}{2a} \\ &= \pm\frac{\pi}{a} \end{aligned}$$

Thus the Brillouin zone of a one dimensional linear lattice is specified by two points, $\pm\pi/a$.

- Any diffraction pattern of a crystal is a map of the reciprocal lattice of the crystal whereas the microscopic image is a map of the direct lattice.
- When a crystal is made to rotate both the direct lattice and reciprocal lattice rotate.
- Direct lattice is a lattice in ordinary space while Reciprocal lattice is in reciprocal space or k- space or fourier space.
- The direct lattice is the reciprocal of its own reciprocal lattice.