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Lecture - 28 Understanding crystal structure using concepts of Bravais Lattice

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We came across the concept of a lattice associated with a crystalline solid. A crystalline solid has these atoms or collection of items which are organized periodically in the crystal and we replace this with a lattice of points.

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And we had shown one of the ways is to say take the points in between these two atoms, and you will get a lattice which is a geometric collection of points in space ok, that is one way of doing it. And on of each of these geometric points, then you can put this collection of atoms and you will generate the crystalline solid that is one way of defining the lattice.

However, as I said that is not a unique way to get from the crystalline solid to the lattice of points, another way for this in this particular example another way to do it would be the following; that I can choose my lattice point as a point in between this four set of atoms, this four set of collection. And this I can do it infinitely, because I am assuming this is an infinite set though, I have not drawn it like that this I am assuming this is an infinite set.

So, therefore, I can get from here I can get my lattice, another choice of my lattice are these points, where now on each of these lattice points which is this geometric collection of points, I can put a configuration of atoms which is like this that I can put this configuration of atoms such that the centre of this configuration of atoms it is say these lattice points and then I will land up with this combination of the lattice plus this is called as the basis. The atom configuration which you will put one the each lattice point that is called the basis. So, the lattice plus basis these two together give you your crystalline solid. So, this gave us an important concept of the lattice that forms a collection of atoms which are periodically arranged I can construct a lattice.

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So, what is the requirement of a lattice is any point any geometrical configuration lattice or more specifically Bravais that from a crystalline solid I want to first get something called as a Bravais lattice. It is not any collection of points, but there is should be some particular requirement of the geometric the geometric collection of these points should satisfy something.

So, the two conditions which they have to satisfy to form a Bravais lattice is first the arrangement and orientation of the points in the lattice around any point in the lattice should look the same. Namely if I go to any lattice point in the lattice, then if I look at the distribution of my points or the arrangement and configuration of the points around that point, it should look identical whichever point I go to.

For example, let us take this lattice for example. Now, if I go to this point and I look at the arrangement of the lattice points around it looks exactly identical compared to this point or to this point. If I go further, if I keep on extending it, these are considered to be infinite lattices. So, I will really have to draw it as an infinite collection of these points which are periodically spaced, but the requirement of these geometric set of points is that to form a Bravais lattice they have to have the same configuration of points around it.

Remember these are not atoms, when I am talking of a lattice or the Bravais lattice these are not the atoms; the atoms are the bases ok.

On these lattice points if I put collection of atoms, then I will form the crystalline solid; at the moment these are just geometrical entities. So, from the crystalline lattice, I have generated crystalline solid, I have generated a lattice which is the geometrical arrangement of points. And these have to satisfy they have to be a Bravais lattice, namely the configuration and distribution of the points around any point should be identical.

Another example could be this. Here also if I go to any point and look at the distribution of points around a given point, it looks exactly identical. Whether I choose this or this or this or this any point in this lattice, we will look exactly identical. So, these are examples of Bravais lattice; I am drawing periodic two-dimensional structures, but you can also draw three-dimensional structures like cubes and so on.

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Points which are organised on the corners of a cube for example, a lattice which is formed by points at the corners of the cube. I can consider this arrangement of atoms which are at the corners of a cube. And similarly this will also be a lattice. This will also be a Bravais lattice. This is a example of a three-dimensional Bravais lattice, which I have drawn here. Where if I go to any point in this lattice, if I look at the arrangement of atoms around this point, then I will see that the orientation and the configuration of

atoms and the arrangement of atoms is exactly identical. So, the points of the lattice have to satisfy this condition to be a Bravais lattice.

One example which I would like to give you which is very contemporary is a material which is currently known is graphene. And it is very important in modern times, it is very important for the electronic industry this material is called graphene and this is finding large number of applications across the electronics industry. What is this graphene, this graphene is just a single layer of carbon atoms. It is just a single atomic layer of carbon atoms, it is called a monolayer of carbon atoms a monolayer of carbon atoms, where the material is only one atom thick. The graphene is just a layer of these one atom thick carbon atoms.

And what is the structure of this graphene; the structure of this graphene is that these carbon atoms are arranged in what is called as a honeycomb lattice. These are the carbon atoms which are actually bonded to each other. So, there is a bonding between them, covalent bonding between the carbon atoms. And these carbon atoms are arranged in a honeycomb structure. And this structure is very I mean this system is very important has some amazing properties. And this entire structure sort of periodically repeats itself over space. So, these are carbon atoms which are arranged in as one single layer of atoms of carbon which are connected to each other by these bonds and this is known as graphene structure.

So, what is it, you have now a lattice. So, this is the collection of atoms; this is a crystalline solid formed by atoms. So, if you want to make a lattice out of it, I can break it up into points; let us say which are sitting at each carbon atom. So, the lattice will be this. So, I will form this lattice of points and then on each of them I can put a carbon atom and then I will get the if each of these lattice points, I put this carbon atom, then I will get my graphene structure.

The question is that whatever I have formed out here, this lattice of points that I have formed is this a Bravais lattice. Namely if I go to each of these points in the lattice and I look at the distribution of points around it or the configuration of points which are present around it, is it identical to every other point in the lattice?

And if it is identical, then of course I have a Bravais lattice; but if it is not identical, then this cannot be a Bravais lattice. So, you can choose actually three points you can look at the distribution of the other atoms or the other lattice points around these three points P, Q and R ok. So, I can choose three points, three lattice points in this lattice. And around each of these points, I can find what is the distribution of other points around these three points and do they look exactly identical. And if it does, then of course you have a Bravais lattice; but if it does not, then of course there is some problem.

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So, to show you that let us look at the following example. So, this is your honeycomb lattice, where you have these lattice points which are sitting on the edges of this at the vertices of this honeycomb or at the vertices of this hexagon. And you have these three points P, Q and R; P, Q and R. And we would like to see if the distribution of points of the other lattice points is exactly identical as you see from P, if you were to sit on Q, what is the distribution and if you were to sit on R, what is the distribution.

So, I first go and sit on my point P, and here as red circles are the lattice points which I see around point P. So, this is how the distribution of the lattice points looks around point P. Now, I will go to another point say Q. If I go to Q and look at the distribution of the lattice points around Q, they look exactly identical exactly similar. I have just drawn it in different colours to show the red is the lattice points I am seeing when I go around point P. The green are the lattice points I am seeing when I go around Q. So, this is the distribution of lattice points around Q, and they look exactly identical to the distribution of points around P, so, all well and good.

But now let us go to point R and let us look at the distribution of points around R. If I just look at the distribution of points around R, now something look slightly different. It looks as if I have rotated my structure. The distribution of points around R is no longer like this, it does not have this sort of a symmetry, but it looks to have gotten rotated I seem to have rotated the structure if I look at the distribution around point R.

So, whereas, P and Q the distribution or the orientation of these atoms which are distributed around these points P and Q are identical, if I look at the distribution of points around R they are not the same as point P and Q. And therefore, this structure of just the lattice points arranged on the vertices of the honeycomb do not form a Bravais lattice. This honeycomb structure is not a Bravais lattice. There are different ways of handling it when one studies graphene one actually comes across how to handle these sort of structures.

But typically the honeycomb lattice is not a Bravais lattice, although it may seem like a Bravais lattice the distribution of points whereas the arrangement of atoms looks approximately the same. It is also important to see the orientation of the atoms, how are the atoms actually oriented along if you look at the orientation of the atoms then that turns out to be different. And therefore, this is an example, where, although it looks like a Bravais lattice, it is not a Bravais lattice. So, let us go back to our discussion of Bravais lattice. So, one important consideration while discussing the Bravais lattice is the distribution of atoms around a given point they have to be identical from point to point.

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All points in the lattice can be reached from any point on the lattice winy the relation R = n, a, + n, a, + N, a3 where $\overline{a_1}$, $\overline{a_2}$, $\overline{a_3}$: are called the fundamental translation vectors and m, N2, M2 are integer's

The second requirement of the Bravais lattice is that all points in the lattice can be reached from any point on the lattice using the relation R bar is equal to n 1, a 1 plus n 2 a 2 plus n 3 a 3. Where a 1, a 2 and a 3 are called the fundamental translation vectors; and n 1, n 2, n 3 are integers, they can be positive, negative, zero integers, does not matter. The idea is that if you have a Bravais lattice, then you can go from any point on the Bravais lattice and you can reach any other point on the Bravais lattice by using this relation. To give you a simple example in two dimensions what this relation means in two dimensions.

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Let us take a simple Bravais lattice. First condition is satisfied namely if you look at any point if you look at the distribution of atoms a distribution of points around any given point in this lattice, it is exactly identical. Now, if I take this point and if I define two vectors a 1 and a 2 around this point ok, then if I want to reach say this point in my lattice, can I reach it. If I want to describe this point, if I want to reach this point from this, then I can may write my vector R which will be taking me from this point A to this point B on the lattice as twice of this a 1 twice of a 2.

So, if I take twice of this, then I can reach the lattice. So, these are two integers and a 1 and a 2 are called as the fundamental translation vector. So, I can reach any point in the lattice and reach any other point in the lattice by using this relation ok and this is my translation vector. R is my translation vector because I can take you from one point in the lattice to another point when I apply this translation vector to it. So, if I apply a translation vector to this point R, I can take you to a another point R ok.

And this is the other condition on the Bravais lattice that I should have a 1 and a 2 associated with the lattice such that I can move from one point in the lattice to any other point using a relation which is like this. This is for two dimensions, but for three dimensions of course, I will have another direction a 3 for example. And then I can go from one point in the three-dimensional lattice to any other point in the three-dimensional lattice.