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Lecture - 29 Bravais Lattice Types Part-I

So, while describing the crystalline solid, we saw that we have to break up the crystalline solid into first a geometrical structure namely a lattice and that lattice has to be a Bravais lattice and a basis, which is the atoms that you will put at every point on the Bravais lattice.

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And what is the requirement for the Bravais lattice? First is that the orientation and arrangement of atoms at any point has to be exactly the same, the arrangement of points around any point in the lattice has to look exactly identical. So, these are examples of Bravais lattice in two dimensions. There if you go to three dimensions, there are other examples also.

(Refer Slide Time: 00:59)

And one other example which I showed you which looks like a Bravais lattice, but is actually not is the honeycomb lattice, where you have these vertices at the corners of a hexagon. And if you look at the points P and Q and if you look at the distribution of atoms around P and Q, they of course, look exactly identical, but if you look at the distribution of points around R, it looks exactly 180 degrees. As if you have rotated it to 180 degrees and from here you get this sort of a configuration. So, the point R is not equivalent to point p and q. this is not a Bravais lattice the arrangement of atoms is not identical.

(Refer Slide Time: 01:37)

(Refer Slide Time: 01:43)

The second requirement is that if you do a translation operation, which is that if you go from any point in the lattice to any other point ok, then these two points are connected by a translation vector which is of the form n 1 a 1 plus n 2 a 2 plus n 3 a 3 in general for a three-dimensional lattice. For a two dimension, it will just be n 1 a 1 plus n 2 a 2. And this is an example of this translation vector that any two points in the lattice for any of these two points you can describe these two fundamental translation vectors a 1 and a 2. And then you can go from this point to this point using this translation vector which is in this example it is twice of a 1 plus twice of a 2.

So, this is now R a 1 and a 2 a unique choice is this a 1 and a 2 has chosen a unique choice it is not, because I can also choose if I can show you another example where this condition is still satisfied with another choice of a 1 and a 2. One other choice I can do for a 1 and a 2 is this; I can choose my a 1 and a 2 like this. So, this is my a 1 vector, and this is my a 2 vector. And then from this point, I can move to any other point in the lattice by choosing combinations of a 1 and a 2. For example, if I want to move from this point to this point here in the lattice, my R vector which will join this will be thrice of a 1 plus a 2. So, n 1 is equal to 3 and integer and n 2 is equal to 1.

So, I can move from any point in the lattice to any other point using these a 1 and a 2. So, it is important to have these fundamental vectors that fundamental vectors that fundamental translation vectors a 1 and a 2, but by no means given a lattice they are unique. You can have different combinations of a 1 and a 2, you can have different choices of a 1 and a 2 to be more precise for a given Bravais lattice. This is a clear example of it. They do not have to be exactly perpendicular to each other as such.

So, given a Bravais lattice we can define the fundamental translation vectors and then any point in the lattice to any other point can be joined by the translation operation, which is the translation vector namely I can go from point A which is a lattice point to a point B, which is another lattice point by using the translation vector R which has a particular form which has shown you. Once these conditions are satisfied, I had a Bravais lattice ok.

(Refer Slide Time: 04:47)

I am just to illustrate to you this thing about moving from one point to another. If I have these set of points, the Bravais lattice is one where I can move from this point to any other point using the translation vector r. So, if this is my coordinate system somewhere outside x, y and z, this is my small vector r, then I can move from this point to this other point, which is my r bar prime by using.

So, r prime minus r bar should be equal to the translation vector R, where R should be of the form n 1 a 1 plus n 2 a 2 plus n 3 a 3. Where a 1, a 2, a 3 are some choice of fundamental translation vectors and n 1, n 2, n 3 are here integers. And this is the basic requirement. And this is the translation vector R which will take you from one point in the lattice to another.

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-------*<u>BREES</u>* Primitive Pattice cell: Is the nuinimum volume (area) cell when traslated agross the (translation opening) will cover entire lattice

Now, we come to the concept so along with the lattice there are some other concepts that we bring in. And another very important concept is that of a primitive cell, lattice cell, which is associated with any Bravais lattice. The primitive lattice cell associated with any Bravais lattice is the minimum volume or area cell which when translated across the lattice using the translation operation or vector will cover the entire lattice. So, it is the minimum volume or area cell in the lattice which if you translated across the lattice, it will cover an entirely cover your entire lattice without leaving any gaps in the lattice.

So, one typical example is given this lattice of points, one example of my primitive a 1 and a 2, this is of course an example in two dimension. So, instead of a volume, we have an area. And this now if I move it if I translated by the translation vector across my entire lattice, I will cover each and every point inside the lattice without leaving any gaps. So, this is one example of a primitive lattice cell.

Another example is this, this is another choice, I can also choose this as my primitive cell this is my a 1 vector, this is my a 2 vector. And my primitive cell is now this; this also I can translated across the entire cell and cover my lattice. So, a 1 and a 2 are again another choice of fundamental translation vector. And this volume or this area I can translated across the entire cell you can show that if I move it from here to here, I can cover every area and every point in this lattice by translating this.

Another choice of my primitive cell is the following. This is another choice; I am just showing you different examples of ways of choosing a 1 and a 2. This is another example of a choice of a 1 and a 2, which again can map every point in the lattice. And what is the primitive cell associated with this; this is my primitive cell, this is also equivalent. This is also equally valid choice of fundamental translation vectors giving you a primitive cell which will cover the entire lattice. This is the smallest, you cannot get smaller than this. These are the minimum volume area cells, which you can define for a lattice which when translated across the lattice will cover the entire lattice.

So, this is one example; this is another example; this is another example. These will all cover and uniformly cover the entire lattice. So, these are different choices of this primitive lattice cell that you can do when they are bounded by these lattice vectors this fundamental translation vectors a 1 and a 2 the choice is by no means unique. So, given a set of lattice, given a set of this geometric collection of points you can also define a primitive lattice cell. And it is important to do so, it gives you this minimum volume which is associated with this lattice

Now, an important point which is associated with this primitive cell is there is only one lattice point per primitive cell, then important point which is associated with this primitive lattice cell is that you have only one lattice point per primitive cell, can one show this a little bit more easily. For example, again I am just restricting myself for drawing to two dimensions, you this entire thing is also carried forward in three dimensions ok.

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But suppose I want to consider the lattice points, I exaggerate my lattice points and show as these circles. These are not atoms, these are again lattice points. And what is my primitive cell in this, one example of a primitive cell is this. This is my primitive lattice cell and a 1 and a 2, which form the sides of this primitive lattice cell are called the primitive translation vectors. So, the smallest or the minimum volume that I can have inside, this lattice cell which is defined by these a 1 and a 2 from the primitive lattice cell and these are called the primitive lattice vectors.

Now, if you look at this primitive cell that you can see that out of this circle only a quarter of each of the circle actually belongs to so this is one quarter, this is another quarter, this is another quarter and this is another quarter ok. One quarter of each point lattice point belongs to the primitive lattice cell, you can clearly see that is only a quarter of it which belongs to the primitive lattice cell. And there are four such points which are there inside this which are contributing to and there are 4 such points. So, therefore, the total point per primitive lattice cell is 4 into one -fourth of a point which is 1 point. So, there is only 1 lattice point that you can define per primitive lattice cell.

And that is the characteristic of this primitive lattice cell that you have one lattice point per primitive lattice cell. So, often in crystal structures while analysing crystals structures once you have made a lattice, you would like to define the primitive lattice for the cell.

And it makes things simple, because then you have only one point, which you need to describe per lattice cell. You can also look at it for a cube.

(Refer Slide Time: 14:41)

So, for a cube just to show you that this is also valid in three dimensions. And this is a lattice of cube, which are going to repeated itself in 3D space. And if you look at each point is like now is sphere at the corners of the cube and how many points are there, there are 8 points per primitive lattice cell. In this case, my primitive lattice cell now is a 1, a 2, a 3, this a 1, a 2 and a 3; a 1 is this a 2 is the vertical and a 3 is going along the other corner of the cube.

There are 8 lattice points and this is my whatever is a shaded this is my primitive lattice cell. And there are 8 such points associated on each vertex of the cube, but only oneeighth of each point belongs to the primitive lattice cell. Therefore, the total number of points per primitive cell is 8 into one-eighth which is nothing else but 1 point per cell. And this gives you again 1 point per cell.

(Refer Slide Time: 16:49)

............... Given primitive Lattice vectors
 $\overline{a}_1, \overline{a}_2, \overline{a}_3$

(20) Vélume of the cell = V= (\overline{a}_1 . ($\overline{a}_2 \times \overline{a}_3$)

(20) Area of the primitive = A= $\overline{a}_1 \times \overline{a}_2$)

cell

S Wigner - Seitz cell for enstructing

Given the primitive lattice vectors a 1, a 2, a 3 which enclose the minimum volume of the cell, which when translated will entire cover, the entire cell given the primitive lattice vectors a 1, a 2, a 3. The volume of the cell V is the magnitude of a 1 dot a 2 cross a 3, this you know from a vector analysis that the volume of the cell given these three vectors is defined like this.

And if you have two dimensions of course you have the n area of the primitive cell. The area of the primitive cell is nothing else, but a 1 cross a 2 the magnitude of a 1 cross a 2. So, if you have 3D, you have a volume of the primitive unit cell which has to be minimum ok and that you translate across the entire cell. If you have two dimension you can also define the area of the primitive cell. So, these are the concepts associated with the primitive cell.

And given a lattice you have to figure out what is the primitive lattice and you have to choose your a 1, a 2 and a 3, so that you can get your primitive lattice vectors and the primitive cell for your Bravais lattice. But there is another way to also do it and there is a standard procedure and that is called as the Wigner-Seitz cell for constructing of primitive lattice cell. And actually this construction will immediately show, you that there is going to be 1 point per primitive cell.

So, what is the Wigner-Seitz construction this is a procedure given to construct the primitive cell is just one of the ways for constructing the primitive lattice cell given a collection of points in the Bravais lattice. And the way to do it is the following, I will use again two dimensions to illustrate the point.

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So, let us take a collection of points. This is my set of points ok. And of course, they are extending out in both directions; I am just drawing a finite set of points. And now I would like to draw the Wigner-Seitz cell which is the primitive lattice cell for this Bravais lattice. So, how does one construct it one first constructs from any point you first join all the nearest neighbour by lines. All the nearest neighbours you join by the lines ok. From any point if you want to construct, the primitive cell associated with this point, then you take the midpoint of this line. For each of these lines, you take the midpoint ok, you first find out the midpoint of the line.

And what you start doing is that you start drawing normals which are perpendicular passing through this midpoint of this line, you draw perpendicular. So, this is the perpendicular bisector. So, you start drawing this perpendicular bisectors which are passing through these points. And what you will end up with is what is known as the Wigner-Seitz cell.

The intersection of all of these gives you an area which is enclosed by these perpendicular bisectors. And intersection of all these perpendicular bisectors gives you an area which is enclosed ok. And this is the minimum area which encloses 1 point. And

around each of these points you can draw a Wigner-Seitz cell. And this Wigner-Seitz cell can be of course, replicated across very point and they will cover the entire space.

So, this is the Wigner-Seitz cell construction around a given lattice point. And this defines your primitive lattice cell associated with the lattice point where now, you can see that the minimum area, which is bounded around this lattice point is your Wigner-Seitz cell and there is one lattice point per cell.