Solid State Chemistry
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Lecture – 07
Conventional Unit Cell, Primitive Unit Cell

Now, we will go to the second lecture of week 2 of this course. In this lecture, I will be talking about a little bit more about unit cells, I will be talking about what is a conventional unit cell and what is a primitive unit cell.

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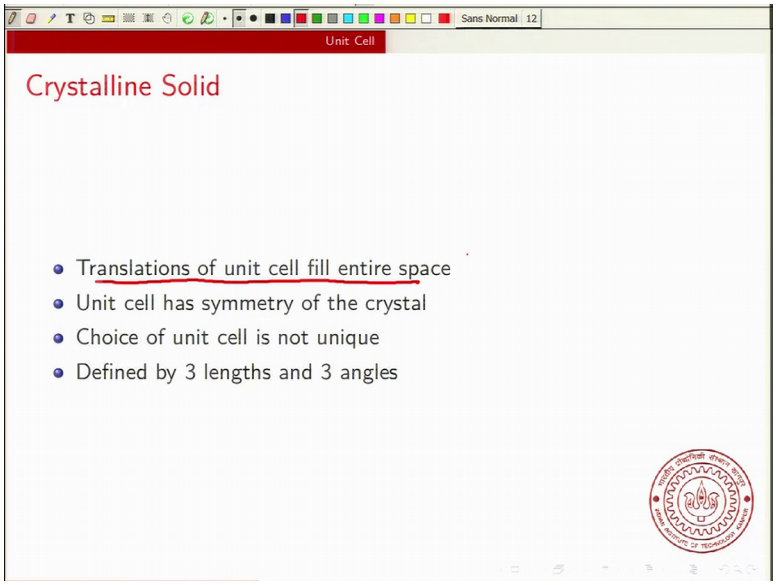

So, as we saw in the last class unit cell is repeating unit of the crystal.

So, now let us talk about what is the conventional unit cell and what is the primitive unit cell. So, as we saw in the last class a Crystalline Solid is consists of some repeating unit and that repeating unit roughly we called it the unit cell. And what we said is that this unit cell is the repeating unit of the crystal and translations of the unit cell have to fill the entire space without voids ok. And where this was very important we said that the translations of the unit cell should fill the entire space without any voids ok.

Further we said that, the unit cell is chosen to have the symmetry of the crystal. And we also saw that the choice of the unit cell is not unique in what we mean by that is, there

are several choices for unit cell and at the end we saw that you can define the unit cell using three lengths and three angles ok. So, this was what we learnt in the last class ok.

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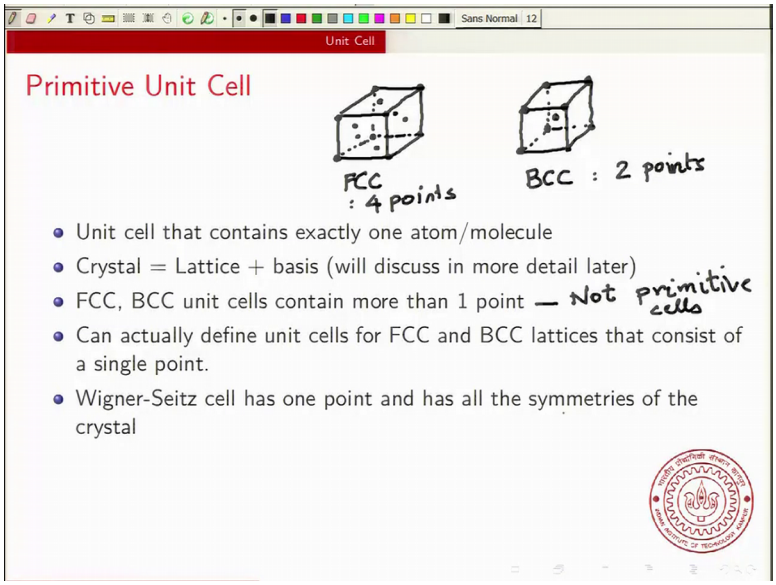

Now let us talk now about what is the primitive unit cell.

So, now in order to understand the primitive unit cell you really need to think of the repeating units as either atoms or molecules ok. So, unit cell that contains exactly one atom or molecule would is called a primitive unit cell. And I have sort of gone a little ahead of what we are discussing now in the sense that we should keep in mind that when we referred to a crystal, its composed of both a lattice and a basis and we will come to this a little later ok, but let us just try to go ahead with this unit cell ok. So, notice that if you take the FCC or BCC unit cells they contain more than one point.

So, many of you all of you would have heard of an of an FCC, which is actually a Lattice ok. So, so if you had a face centered cube then we would think that there are these points which could be atoms if it is an FCC crystal and we say that these points are also located at the face centers and so, so this is an FCC whereas, the BCC will exactly like this, only thing the additional there is one additional point at the body center.

So, now the BCC as you are aware this contains two points and I am deliberately leaving at points I am just calling this points as a suppose to atoms or molecules and this distinction will be will become clear as we go along and this contains four points ok.

And let me emphasize what you have already learnt in your high school, that each of the corner points contributes one-eighth to this unit cell ok. So, the eight you have eight corner points. So, the total you have one effectively one point per corner atom then each of these face center each of the six face centers contributes half. So, you have 6 into half that is 3. So, you have 3 plus 1 4 points. And here in this case you have you have one from the corner and one from the body centers.

So, you have to points ok. So, so what you see is that if you choose this as the unit cell for FCC then you will have four points. Similarly if you choose this cube as the unit cell for BCC you will have two points. So, does that mean that if you have an FCC or BCC you cannot have a primitive cell? And the answer is no you it is possible to define primitive unit cells that contain exactly one point in FCC and BCC ok. Now let us just step back and say again that if you take this unit cell of FCC and you translate it in all directions, you will get the entire crystal and you would not have any voids.

Similarly, if you take this BCC unit cell and you translate it in all directions, you will get a crystal without any voids. However, both these unit cells have more than one point FCC has four points BCC has two points. So, these are not primitive cells ok. So, these are not primitive. Notice that it is the cells it is the unit cells that are not primitive now. So, the question is can we suppose you have an FCC lattice, is it possible to define a unit cell for an FCC lattice that has exactly one point? And the answer is yes, the answer is that there is a construction called a Wigner Seitz cell that allows you to construct a primitive unit cell for any lattice ok.

So, and this Wigner Seitz cell is a unit cell that contains exactly one atom or molecule and it has all the symmetries of the crystal. So, so I will just illustrate what a Wigner Seitz cell is ok.

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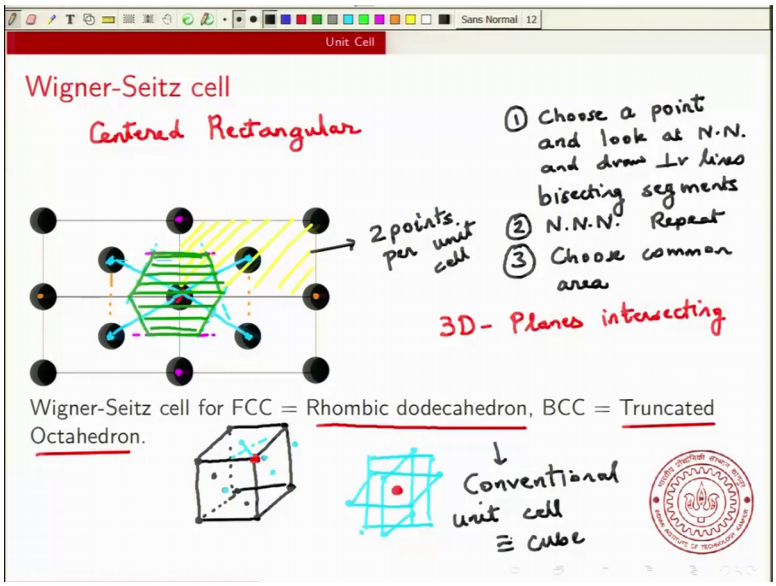

And let us take an examples again we will we will start with 2 D example of how to construct a Wigner Seitz cell. So, so here I have a 2 D this is a 2 D lattice it is referred to as a Centered Rectangular Lattice.

I emphasize that I have not really discussed lattices in detail, but just take this as a given that this is a centered rectangular lattice. And you can easily see that if you choose the unit cell, you can you can easily see that you can choose this yellow shaded region has a unit cell and this unit cell will contain two points this contains two points; probably yellow is not very visible let me use a different colour to show this.

So, this cell contains two points. So, so this shaded yellow cell it contains two points per unit cell and how did we get two? Because each of these this is a two dimensional lattice. So, so each of these are they contribute to this atom you write here it contributes to four cells it is a part of four cells it is a part of this cell, this cell, this cell and this cell. So, so to this unit cell it contributes one fourth and. So, each of these contribute one fourth. So, you have a total of one atom due to this and then you have one atom which is entirely inside the cells.

So, we have two points or atoms if these were atoms per unit cell in this yellow cell. So, now, now let us construct a Wigner Seitz cell ok. So, how will we construct a Wigner Seitz cell? So, the way to construct a Wigner Seitz cell is to choose a So, we will start the first step is to choose an atom or an atom I should not use atom, I should really I should

really say choose a point because these are what we have considered here are just points and look at nearest neighbours ok. So, N stands for nearest neighbours. So, if I choose let us say I choose this point and I identify its nearest neighbours let me identify it in light blue.

So, the points nearest to this or this, this, this and this it depends I mean if it depends on whether this length is longer or this length is longer ok, but let us and that really depends on the dimensions of the rectangle ok. So, let us consider a case where these lengths of the shortest ok. Then what you do is you draw this line from here to here and so, you consider this line and you bisect it. So, you bisect it, you cut in half and draw line perpendicular to this line. So, let me draw it this way similarly I draw a line perpendicular to this line, I draw a line perpendicular to this line and finally, I draw line that is perpendicular to this line ok.

So, these are lines that are perpendicular to each of these lines that join the nearest neighbors ok. So, so the second step I should write is to draw perpendicular lines bisecting segments and what I mean when I say segments. What I mean just bisecting the segments that join the atom that join the point to its nearest neighbor point ok. Next what we do? Next you consider next to nearest neighbors and repeat ok. So, in this case let me mark the next to next to nearest neighbors I will choose a different color. So, the next to nearest neighbors are this and this, these two are the next two nearest neighbors and if I draw lines bisecting them, then I will get so, I will get something like this and I will get a line that looks like and as the procedure goes you are supposed to continue ok.

But we already see that. So, repeat and then choose common area ok. Now you can already see that if you just take the nearest and next to nearest neighbors ok. So, the common area let me mark it in green. So, this we represents the common area now the question is should you go to more cells more nearest neighbors. So, if you go to this nearest neighbor. So, for example, if you go to the third nearest neighbor, you can easily see that it would not contribute anything else ok.

So, we take this orange colour for the third nearest neighbor. So, so then third nearest neighbor as these points and you can see that the bisector comes here and that the common area of the three of the three regions is still is still this ok. So, you need to go in this case you need to go only up to the second nearest neighbor, in some cases you have

to go to more nearest neighbors to get the common intersection area ok. What I want to emphasize is that, is at this region in green, it is formed by the intersection of all these segments corresponding to the nearest neighbor two successive neighbor points ok.

So, this is the basic construction of a Wigner Seitz cell and you can do this for any lattice ok. So, what do we get at the end? You at the end you get this, this is your primitive cell and this contains exactly one point as you can see and it turns out that it has all the symmetries of the crystal ok. Its actually it looks like a regular hexagon, but it is not actually a regular hexagon, it is I mean the whether its regular or not depends on the exact dimensions of the rectangle ok, but it is not it is not meant to be a regular hexagon ok. And what is more is that it contains all the symmetries of the crystal and you can see that by translating it, you can you can form the entire crystal without any voids ok.

So,, you have to consider translation vectors ok. So, for example, if you translate along these two directions, you can you can easily generate the entire crystal without any voids ok. So, this is the idea of the Wigner Seitz cell. Now it turns out that you can do this for an FCC. You can take an FCC in three dimensions and you can do this. Now this is considerably harder to visualize because in three dimensions you will have you will not have perpendicular lines as in 2D ok. So, this perpendicular you will have a plain that is perpendicular to each segment that connects a point from its neighbor.

So, and here you have in 3D. So, I will just mention this that in 3D you have planes of intersection planes intersecting. So, instead of having lines ok. So, instead of having lines intersecting, here we have you will have planes that are intersecting ok. So, so for example, if you had if you had an FCC let us say let us say you had a ok. So, so if you had a if you had a face centered cubic lattice then if you take any point ok. So, so let us say you take you take this point in red and you look at its nearest neighbors it will actually have it will have a total of 12 nearest neighbors ok.

So, the 12 will be this, this, this, here this and then are. So, these four will be in this unit cell then there will be four more in another unit cell. So, so I can I can just show. So, so this neighbouring unit cell there will be a point here there will be a point in this the cell that comes out in this direction, there will be another point here. So, essentially if I take this out and I show it. So, I will have a point like this and I will have nearest neighbors, I will have 4 in the perpendicular direction 4 in this direction ok.

So, So, I have 4 this way and you will have four more in the in the third plain that is perpendicular to these 2 ok. So, and that will be the plain of this paper. So, we will have 4 in this direction ok. So, we will have a total of 12 nearest neighbors and you are aware that the coordination number of FCC is 12. So, so these are the remaining 4 ok. So, so there are 12 nearest neighbors, and now if you imagine if you imagine that you are dropping segments to the nearest neighbors.

Now, what is perpendicular to this will be a plain ok. So, the object that is perpendicular to this will be a plain that goes in this direction and it is perpendicular to this line. So, we will have plains intersecting and now you can see that its a its a lot of work to actually find out the Wigner Seitz cell. I mean you need to draw bigger cells and see what is the plains plain of intersection , but again this can be done with a with a lot of effort and what you will find is that the Wigner Seitz for cell for FCC is a rhombic dodecahedron the Wigner Seitz cell for BCC is a truncated octahedron ok.

So, these actually can be you can do this ok. So, this rhombic dodecahedron has exactly one lattice point per rhombic dodecahedron and it has all the symmetries of the FCC lattice ok. So, the idea of Wigner Seitz cell is very useful we would not actually be working so, much with Wigner Seitz cell, but it is very useful to know that there is something called a Wigner Seitz cell and this information that you can always find a primitive cell that contains exactly one point and that and that has all the symmetries of the crystal is very useful information ok.

However when we are dealing with unit cells for FCC. When we are dealing with unit cells for FCC or BCC we will use the conventional cell. So, the conventional cell conventional unit cell unit cell is a cube and for FCC it has four atoms four points per unit cell for BCC it has two points per unit cell ok.

So,, I will conclude this discussion on unit cells here and in the next lecture, what I would like to do is to talk about lattices more formally ok. So, we have been talking about lattices in this lecture ok, but we have been talking about it informally ok. In the next lecture I will formally introduced the lattice and what are the different kinds of lattices.

Thank you.