Introduction to Reciprocal Space

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Lecture -05
Wigner Seitz Cell and Brillouin Zones

In the last class, we looked at the reciprocal space, we looked at diffraction as it is described in the reciprocal space. We had already described it in real space, we looked at its description in reciprocal space. And we also looked at, what is actually happening as you convert something from real space to the reciprocal space okay. So, this is a process that we looked at. In particular I emphasize the fact that ultimately, we just have materials which are in real life objects that we are able to handle and see and they have crystal structures and lattices which are in real space, the space that we are accustomed to.

It is only because that there is some convenience in terms of analysis. That we start looking at other ways of representing this information, and the reciprocal lattice manner of representing this information is extremely useful in that context because with respect to diffraction, there are several specific details that are better described in the context of the reciprocal space okay. So, that is the context in which we have discussed it, that is the context in which the subject exists so to speak okay.

In also in this context, I showed you that you know you may have a real space material that may consist, that we have a simple cubic lattice or you may have something that is FCC or BCC body centered cubic in real space. If you represent this same information in reciprocal space, in some cases the structure will change, in reciprocal space. The material structure is not changing; it is only its representation in reciprocal space that is different from what it is in real space.

If it is a simple cubic material the representation in reciprocal space also happens to be simple cubic okay. Only the dimension of the side of the tube is different. It is 1 by the dimension of the 1 by the length of the cube in real space. But what is laid out as a simple cube in real space continues to be laid out in a cubicle in a cube kind of a layout in the reciprocal space. So, there is no change in that sense.

If you take something that is face centered cubic and you represent it in reciprocal space. Its representation in reciprocal space has the same layout as that of a body centered cubic structure okay. So, something that is, so a material that is in real space having a face centered cubic structure will end up, being represented in reciprocal space with the layout of points that look exactly like a body centered cubic structure.

And the inverse is also true if we start with a body centered cubic structure, you which, in real space and you represent it in reciprocal space the layout of the same of the points will now look like a face centered cubic structure. So, this is representation and it is important to understand that there is, that there can be some changes when you make this representation because we will use the reciprocal space notation.

So, we should keep in mind that some changes occurred in its representation or the very fact that we are representing in reciprocal space has created some changes in the way the information might look. So, when we interpret it we should keep that in mind, we should always keep that in mind and appropriately use this interpretation okay. So, this is just some information regarding what we have discussed.

As we proceed forward, I also think it is important that we should step back for a moment and understand the purpose of what we are doing right now okay. Our ultimate purpose is to understand the interaction of electrons with the periodic structure of the material because that is a detail that we have not looked, incorporated into our model so far.

So, that is the primary purpose of our discussion, whatever we have built up until now in the last two three classes where we looked at reciprocal space, the creation of reciprocal space, the properties of reciprocal space, how materials can be represented in reciprocal space, how diffraction can be represented in reciprocal space. All of these are tools that will enable us to serve this one purpose which is to understand the interaction of electrons with the periodic structure okay.

So, we are headed only in that direction these are all tools that we are building because we will need all these tools to understand that interaction. And continuing in that same context in today's class we will look at some specific terms and specific construction so to speak. Which are all again tools that we, that are necessary for us to understand the interaction and then in a in a class also we will start looking at the interaction. So that is the direction in which we head off.

So please keep that in mind when you look at some of the topics that we are discussing because taken by themselves they may look like a bit independent topics which are disconnected but they are not. They are all going to add up to something that we are going to discuss okay, so that is what it is. So we looked at this now, today we will introduce a concept, we will introduce a few concepts, a couple of different concepts and two or three terms we will look at. The first is something called a Wigner Seitz cell, Wigner a Wigner Seitz cell okay.

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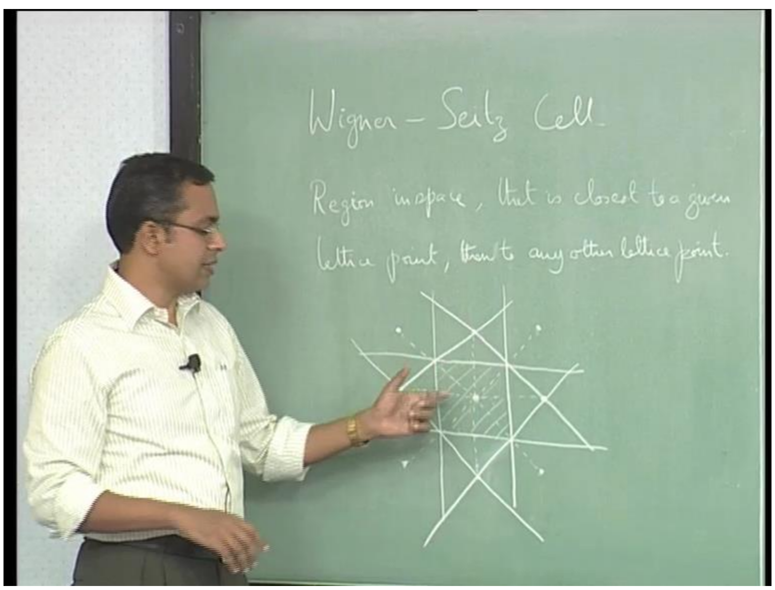

It is defined as follows, it is the region in space that is closest to a given lattice point than to any other lattice point. So, this is the definition, it is simply says, so this is again something to do with the structure okay. So, this is something associated with the structure of the material as you can see. It says, it is the region in space that is closest to a given lattice point than to any other lattice point. So, this is just the definition, so what does this mean?

We can actually do this in one dimensions, two dimensions or three dimensions. Is a real solid object would be in three dimensions, for our representation we will start off with 1D and 2D representations. Later we will look at structures, in our next class we will look at 3D structures okay. So basically, what it says is okay, you have a set of lattice points. I will just arbitrarily draw some lattice points here.

So, set of nine lattice points three by three, I have put laid them out. Intention is to lay it out in a square fashion, so it is just when, we will assume that these are all exactly the same distance in every direction in in those lattice directions. So, we have this two-dimensional lattice okay, so it is in 2D this plane and this plain basically. So, this direction and this direction is what is incorporated. So now we will look at the central point just for an example, the same will hold true for any of the other points. So, this is for the central point, we would like to identify the region in space in this case it is two-dimensional space okay.

So, it is a two-dimensional space, we would like to identify this the region in this two-dimensional space, that is closest to this point, than it is to any of these other points. So that is the, that is what the definition says, if you identify that region that region is called the Wigner Seitz cell about this lattice point okay. So that is the definition, how do we do this, there is a very straightforward way of doing this.

What we will do is, we will take this lattice point, we will connect it to all its neighbours all right, just and we have some guideline connecting it some dotted lines connecting it to all its nearest neighbours. So, let us just do that, all its neighbours, we will just do that. So, I have used dotted lines and connected the central point here, to all of these points around it. This is to just help us identify the region. So, we are just started with this step.

Now let me take it is nearest neighbour one of its nearest neighbours. We will take this point here it is one of its nearest neighbours. What is the region in space that is closer to this point, than it is to this point? That is the first question we will ask; how do we find out that region? We will just take this line; we will draw a perpendicular bisector to this line okay, if you draw a perpendicular bisector to this line.

Whatever is on this side of that line is closer to this point than it is to this point, it is a straightforward is that. So, we just draw that we will do that you will take the midpoint of it whatever is the midpoint and draw a perpendicular bisector okay. So, if you draw a perpendicular bisector to the line joining this point, the point that we are interested in to its nearest neighbour.

We find that any anything to the, from our perspective to our right of this line is closer to this point than to this point and anything to the left of this line from our perspective is closer to this point than it is that point okay. So, with respect to this point we have already identified the region that is closer to this lattice point than it is to this lattice point, simply by drawing the perpendicular bisector.

Now we can do the same exercise for each of these points around it okay. So now we will take the point that is up here, the perpendicular bisector is somewhere there, it has to go through that point. So, it look like that, something like that, similarly a perpendicular bisector will be somewhere there. So, it will pass through that location, it will look like that and again between, so we have, I have not drawn the perpendicular bisector for the line joining these two points and I have drawn the perpendicular bisector for the line joining these two points.

So, then I can draw one more for the line joining these two points. If you have drawn it nice and square, if you do this properly nice and square this is sort of what you will see. So, with respect to its immediate for closest neighbours right, the four closest neighbours that we have there, we have already seen that this line indicates the region below this line is closer to this point than it is to that point. The region on this side of this line is closer to this point than it is to this point, region above this line is closer to this point than it is to this point and similarly the region on the left of this line is closer to this point than it is that point.

So, this region defined by the square is now closer to this central point than it is to its immediate four neighbours, close four closest neighbours okay. We can extend that argument, we can even looked at its next nearest neighbours just to see if anything else is happening. If you have drawn it nice and square what you will find is the perpendicular bisector of the line joining the central point to this point, will look something like this.

And if you continue that exercise for this, this and this you will get lines that look like this okay. So, you will find that in fact those lines which are perpendicular bisectors to the points to the lines joining these points which are diagonally positioned here will also in fact just pass through those vertices. So, they do not remove any region from what we have just identified, in this particular case, if you have drawn it as a nice straight square, that which like what is shown here.

Therefore, this region that we see here, this region consists of, in this two-dimensional sense consists of all the points in space that are closest to this point than they are to any of the other points. In so, in terms of lattice points closest to this lattice point than they are to any other lattice point, so therefore this is now the Wigner Seitz cell about this lattice point okay.

So, this is so, that is all there is to, it is a straightforward the definition is now fairly straightforward. Now we understand what the definition is, with respect to the definition this is the diagram. This is the Wigner Seitz cell about this point. Clearly if you extend this to three dimensions, you will now have a point just the way you had this neighbour here, you will have a point at similar distance in front of the plane, plane of the board. And you will have a point at similar distance behind the plane of the board okay.

And the please understand this is a two-dimensional representation here, so this looks like lines. If this were a three-dimensional representation these would-be planes. This would be a perpendicularly bisecting plane, so this would be a perpendicular bisector a plane that would be perpendicular to this board. Similarly, this would be a perpendicular bisector a plane that is perpendicular to this board. This would all be planes that are perpendicular to this board.

Now the lattice point in front will be sitting in front here and a perpendicular bisector will go like that all right. Similarly, a perpendicular bisector will exist which will bisect the line joining this point and the lattice point directly behind it okay, into the plane of the board. And so you will have now a plane, behind the plane of the board, a plane in front of the plane of the board and these planes here. And since they are all squarely laid out the dimensions should be the same, what you will get is a cube. What you are seeing as a square in two dimensions will become a cube in three dimensions okay.

So, in a in a if you have a square lattice or a cubic cube lattice the Wigner Seitz cell will be a cube okay. So, this is the basic definition of a Wigner Seitz cell. I must also point out that in general see a square lattice is a very particular case, if it is a square it is a very particular case, if it is a rectangle, it is a little less particular but still we are putting a some restriction.

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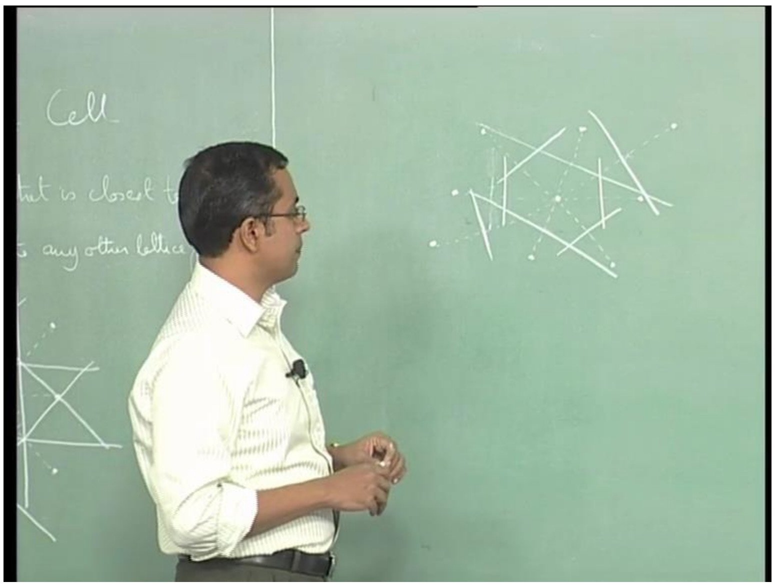

In general, you can have a set of points which are arranged like this. So, if you now have this set of points and you look at the perpendicular bisectors. Again, we will do the same exercise, now that you understand the concept we can do it relatively quickly, we join the central point to all its immediate neighbours right. And we draw the perpendicular bisectors of each.

So, perpendicular bisector of this would look something like that okay, perpendicular bisector of this would look something like that, perpendicular bisector of this would look something like that. It is not exactly in middle, would look like that perpendicular bisector of this line would look something like that, perpendicular bisector of this like that and similarly perpendicular bisector of this is somewhere here and would look something like that okay.

So, by looking at the immediate neighbours and you will find the other ones do not really impact you, this is kind of far away. So, it is line would be somewhere there, perpendicular bisector would be somewhere there, which is not really of immediate use for us. Similarly, this perpendicular bisector is somewhere here.

If you look at it or if you draw it to scale you may find some variations but the point is you will find region bounded by six sides okay. So, in general when you are not really looking at either a rectangular lattice or a square lattice, the Wigner Seitz cell about that point is going to be a six-sided figure in two dimensions, when you plot it in two dimensions okay.

So, in for a two dimension, two-dimensional lattice the most general case is a six-sided figure as the Wigner Seitz cell about any lattice point. Now this is, whatever we say about this lattice point same is going to be true for the other lattice point's okay. So, in a sense the boundary of the Wigner Seitz cell will become the boundary for the Wigner Seitz cell of the next cell okay, so for this part of the next lattice point.

So, this is going to be true for all the lattice points because of symmetry and so in general it is going to be a six-sided figure. If it is a rectangle it will become a four-sided figure which will look rectangular. And if it is a square it will square lattice, it will become a four-sided figure which is a square, so those are special cases okay. So, in general this is what a Wigner Seitz cell is.

Now so I have already introduced, so we have now understood, so this is just a definition okay, so, this is just a definition, you understand what the definition means. And you also understand how you can create this cell or how you can identify the cell because it is simply a region in space right. You only have to identify what is this region and this is the rules based on which you will identify that region.

You simply connect the point you are interested in with all its neighbours, draw perpendicular bisectors to it and then whatever shows up as the innermost region from all this perpendicular bisectors. The innermost region, is the is now the region that is closest to that point than to any other point and that then becomes the Wigner Seitz cell of that particular lattice okay. So that is all there is we have done in 2D so that it is easier to see.

Same thing is true in 3D except the perpendicular bisector should be lines in will be planes instead of line that is all it is. So, if you have the right kind of software you can take any lattice and you can do this perpendicular bisectors you can create and you can see it and you can rotate it around okay. So even see something on 3D a little later, but for now this is in 2D two-dimensional description. So, we have seen this first description called Wigner Seitz cell.

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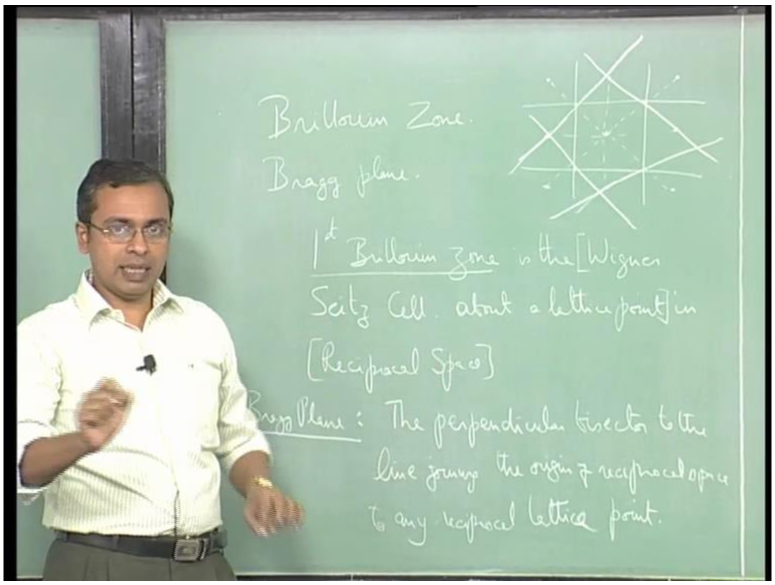

Now we will define another term which is called a Brillouin zone okay. A Brillouin zone is we will define two terms actually a Brillouin zone and we will define something called a Bragg plane okay. So first we will define something called the first Brillouin zone, the Brillouin zone actually can be called as, we will find that you know whatever it is, we once we describe what the Brillouin zone is.

We can we, will find that it can be, there are further qualifications to it we can call it the first Brillouin zone, second Brillouin zone, third Brillouin zone and so on. So, we are, there is further qualification we can provide to the Brillouin zone. So right now, I will describe what is the first Brillouin zone only. After understanding what is the first Brillouin zone, we will define what is a Bragg plane and we will then use that definition to help us define second Brillouin zone, third Brillouin zone and so on okay, so that is what we will do.

The first Brillouin zone is the Wigner Seitz cell about a lattice point in reciprocal space. So right now, in this definition itself we are pulling together some of the concepts we have discussed in the last class and we are currently discussing. So, this is a new term we have introduced Brillouin zone, we are going to look at what it means. And we have, we are defining the first Brillouin zone as the Wigner Seitz cell, which we just now discussed what a Wigner Seitz cell is.

This is going to be a Wigner Seitz cell about a lattice point, so that part Wigner Seitz cell about the lattice point is something that you are now clear about, because we just discussed it. So, this part of the definition you are already clear about okay. Wigner Seitz cell about a lattice point, any lattice I give you, understand the concept of how you can come up with a Wigner Seitz cell about that lattice point that is very straightforward process right.

So, the first Brillouin zone is the Wigner Seitz cell about a lattice point, so that part is clear. Except that the further qualification we are adding is that, it is a lattice point in reciprocal space okay. So now this is a concept we learnt yesterday independently, yesterday in the last two classes, rather in the last two classes we have learned this concept independently reciprocal space.

We understood how real space relates to reciprocal space and such, so reciprocal space we independently defined and we understood, so reciprocal space consists of reciprocal lattice point’s right. So, we can fill reciprocal space with reciprocal lattice points. For a given reciprocal lattice point you can find the Wigner Seitz cell as a second activity so this independently you know how to get to reciprocal space.

You know that in real space, if you have a1, a2 and a3 you know how you can go from a1, a2, a3 in real space to b1, b2 and b3 in reciprocal space. So, given a material in real space which is what your real life is about, a material in real space, you know its crystal structure therefore you know the lattice it is based on. So, for that lattice you know how to independently create the reciprocal lattice of it.

Because we know the relationship between a1, a2, a3 and b1, b2, b3, we already did that for simple cubic, FCC and BCC. Same procedure you follow regardless of the lattice and you come up with the reciprocal lattice. So, given a real lattice you know how to get where reciprocal lattice. So therefore, you know this step and regardless of the lattice you know how to construct a Wigner Seitz cell okay.

So, if you do a Wigner Seitz cell about a reciprocal lattice point that a structure that you obtain or the structure that you identify, the region that you identify is called the first Brillouin zone all right. So, we just did diagrams for a layout of a square layout of points okay. So, we did a diagram here for a square layout of point’s right. So, we just did this diagram, now if this set of lattice points per lattice points in reciprocal space okay.

When I drew this lattice points I did not say anything about, we did not have any restriction that it has to be a real space set of lattice points or a reciprocal set of space set of lattice points. That restriction we had not placed on the system. Supposing this were a set of lattice points in reciprocal space then this region that we have identified which is the Wigner Seitz cell about the lattice point in reciprocal space.

Would then now become the Brillouin zone the first Brillouin zone okay. So therefore, you see that you know a diagram that we have drawn is simply if we have called this reciprocal lattice points this is Brillouin zone that is all it is okay. So, the Brillouin zone term is, if since you may be encountering these two terms for the very first time a Wigner Seitz cell and a Brillouin zone. It is not something that we typically discuss in high school physics.

But this is all they mean, they are constructs or structures that we can imagine in space which we can which we associate with real space for reciprocal space and based on what we are doing we would call it either just a Wigner Seitz it or if it were specific to reciprocal space and reciprocal lattice it would get called the first Brillouin zone okay. So, this is all the definitions.

So now we understand a few of the concepts and how they are connecting, reciprocal lattice Wigner Seitz cell and Brillouin zone. In fact, real lattice, reciprocal lattice, Wigner Seitz cell and Brillouin zone these are four concepts, we have now linked them up okay, so this is what we have done. Now we will come back here, so this is the first Brillouin zone based on what we just did we have already been able to understand what is the first Brillouin zone.

We will now add one more definition called a Bragg plane, once we add the definition we can find out what are the other Brillouin zones that we have available to us okay. So, a Bragg plane is the perpendicular bisector to the line joining the origin of reciprocal space to any reciprocal lattice point okay. So, the Bragg plane is, now is again a definition, we are defining it as the perpendicular bisector to the line joining the origin of reciprocal space to any reciprocal lattice point okay.

So, this is a definition, so let us understand what this means. When we, when you define a reciprocal lattice for sake of convenience we will designate one point as the origin of reciprocal space okay. So that is a by convenience we just defined one point, since it is since all of these lattices are all based on symmetry. If you define a particular point as the origin it is not going to make a big difference.

You can choose and one of the adjacent points in principle the symmetry would still remain the same. So, we can select it by our convenience, we select a point as the origin by our convenience. We can connect that origin to any other lattice point right, I mean it is just an imaginary connection when I say connect where we can we can always draw straight lines between that lattice point and any other lattice point that is available in reciprocal space okay.

So that we can always do, so any such line that we draw we can also imagine a perpendicular bisector to that line right. So, there is nothing these are just two imaginary things, you have two points you can always draw a line connecting those two points you can always draw a perpendicular bisector to that line connecting the two points okay. The fact that it is in real space or reciprocal space is irrelevant you can always do this.

In this particular case, we happen to be doing it in reciprocal space that is all. In reciprocal space, you look at all the lattice points, you take the origin and you keep connecting it to any lattice point that you wish and you draw a perpendicular bisector to that line. That perpendicular bisector is referred to as a Bragg plane okay. This is a bit confusing because in diffraction we talk of planes and we talk of Bragg's law of diffraction and so on.

So, Bragg equation and such and so the term Bragg plane can slightly be confusing the first time you encounter it but this is all it is. If you look at this definition and you implement this definition safely it is a straightforward definition I mean it helps you straight forwardly identify what are the Bragg planes right. So now we understand what is a Bragg plane.

So, we can immediately see you are probably already able to see now how this relates to the Brillouin zone and Wigner Seitz cell okay. Wigner Seitz cell was simply something that we did in any space we did not really specify that it was real space for reciprocal space for any such thing. In the reciprocal space, we were able to say that we have we have designated the Brillouin zone as the Wigner Seitz.

The first Brillouin zone as the Wigner Seitz cell about a lattice point in reciprocal space, so that is how we have defined it. Now think about it carefully what do we have, if you have you know a set of points, so we did this three by three okay. Three by three set of points and we found that you know if we just draw the perpendicular bisectors you will end up getting this square region which is then your Brillouin zone.

The first Brillouin zone, we will assume that this is now these are now reciprocal lattice points. What have we done, we have drawn perpendicular bisectors to the lines joining this point to its neighbours. If you designate this point as the origin of reciprocal space and that is as I said your convenience, you can always designate this as the origin of your reciprocal lattice reciprocal space right.

If you designate this as the origin of your reciprocal space then these lines which are perpendicularly bisecting the lines joining this origin to its neighbours right, if you draw it correctly it will all go through those points that we would not have this region there okay. So, these are lines that that originally when we defined a Wigner Seitz cell we simply said this is a line that perpendicularly bisects the line joining a point and its immediate neighbour okay.

This is not drawn exactly to scale, if you draw it to scale you would get it much better than what I have drawn here. Now we have said that if you do this in reciprocal space this line which is the perpendicular bisector of the line joining the origin to this lattice point is called a Bragg plane okay, so that is all it is. The perpendicular bisector to the line joining the origin of reciprocal space to any reciprocal lattice point right.

So, this line here the solid line here is a Bragg plane, this solid line here is a Bragg plane, this solid, this Bragg plane bisects the line joining this point this the origin and this reciprocal lattice point. This Bragg plane bisects the line joining this origin and this reciprocal lattice point. This Bragg plane bisects the line joining the origin to this reciprocal lattice line and so on.

So, we have a 1 Bragg plane here, 2 Bragg planes, 3 Bragg planes, 4 Bragg planes this is a Bragg plane, this is a Bragg plane, this is a Bragg plane, this is a Bragg plane okay. So, they are all simply lines and in fact these are lines in two dimensions and we I also always said that you know if you draw this in three dimensions this will be a plane. So that is where the name Bragg plane comes okay.

So of course, the Bragg, the name Bragg being incorporated here suggests that somewhere intuitively suggests to us that you know this person has been linked to diffraction, so possibly there is some link to diffraction in this. There is a link we will get to that in a little while, a possibly in our next class. In fact, we will get to it right now let us not worry about the link to diffraction. We simply say that these are Bragg planes okay. So, these are all black Bragg planes by the definition of what a Bragg plane is.

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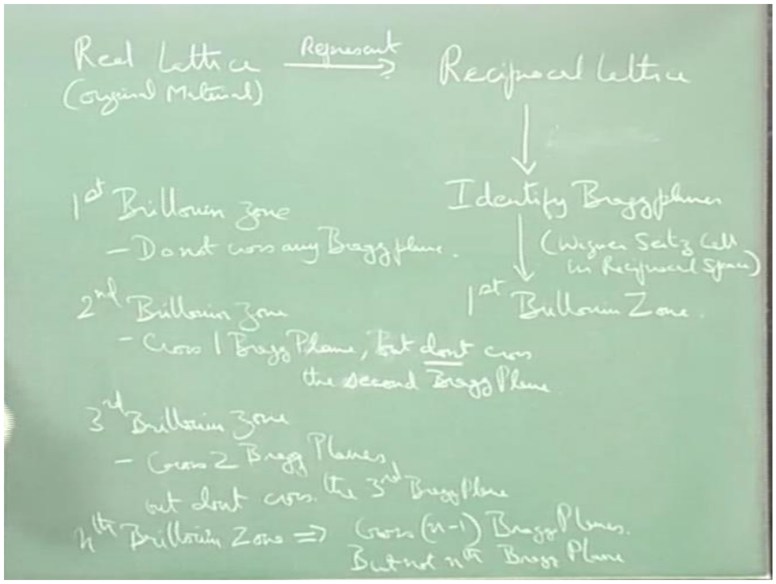

So, we now see how, much more elaborate link, we have real space, real lattice, we can convert it or represented in reciprocal space. So, it will become reciprocal lattice. So, this is your original material right, original material. So, it will have a real lattice, we can represent it in reciprocal space as a reciprocal lattice. If you represent it in reciprocal space you can draw Wigner Seitz cell okay.

We will say we can use Bragg planes, identify Bragg planes, we can identify Bragg planes. If you identify those Bragg planes, the region that you will identify is the first Brillouin zone okay. And this is now Wigner Seitz cell in reciprocal space okay. So, this is how the concepts that we have discussed today tie up to each other okay.

So, we have real lattice that can be represented in as a reciprocal lattice. In the reciprocal lattice, we can identify Bragg planes which are perpendicular bisectors of lines joining the origin of the reciprocal space to any of those lattice points. If you do that the innermost region that you will find is the Wigner Seitz cell about that reciprocal lattice point. And that Wigner Seitz cell about that reciprocal lattice point is called the first Brillouin zone okay.

So, this is the definition this is how they all connect up, later we will see the link to diffraction. Now we have just done it for we have no idea we simply identified the first Brillouin zone. But this concept is a little more general, what is general about it is that if you start at the origin of reciprocal space which you have designated by your choice. If you go away from the origin at some point you will you will touch the first Bragg plane.

The nearest Bragg plane to that origin right, as long as you do not cross that Bragg plane in any direction, the region that you identify is called the first Brillouin zone, I am merely restating what we have done okay. So, what have we done here, we come here we look at the center, this is the center, this is the origin of the reciprocal space. If you move away from this origin as long as you do not cross this Bragg plane.

As long as you do not cross any Bragg plane right, as long as you are within this region. When you are within this region no matter where you go you will not cross a Bragg plane. These are all the Bragg planes right, these are all Bragg plane surrounded as long as you stay within a region where you do not cross even a single Bragg plane. That region is now called the first Brillouin zone.

So, we are simply restating the definition of the Brillouin zone in a slightly different way. So, the first Brillouin zone is the region in space that you can reach from the origin of the reciprocal space without crossing a single Bragg plane okay. So that is simply the definition of the first Brillouin zone. So, you can therefore now guess what might be the definition of the second Brillouin zone.

The second Brillouin zone is the region in space that you will reach by crossing only one Bragg plane and no more okay. So, you start from here, you if you continue forward you will cross one Bragg plane. Then you get into the second Brillouin zone, but you should not cross the second Bragg plane, see this is another Bragg plane that is here.

These are all Bragg planes, so therefore this region here, this region here, this region here and this region here are all regions belonging to the second Brillouin zone right. So now you see how we are generalizing the definition. The definition for the Brillouin zone started off by saying that it is simply the Wigner Seitz cell about the reciprocal lattice point. Then we said look the Wigner Seitz cell the boundaries of the Wigner Seitz cell are Bragg planes okay.

And therefore, you can have several Bragg planes that we can identify. And now is therefore we have to restate the definition for a Brillouin zone because we can identify additional regions which have which are in concept similar but have something different about them. And now so we rechanged, I mean we restated the definition by saying the Brillouin zone is that region which you can.

The first Brillouin zone is the region that you can access from the central lattice point, the origin of reciprocal space without crossing a single Bragg plane. The second Brillouin zone is the region that you will access after you have crossed the first Bragg plane, but you do not cross the second Bragg plane right, so that is how you go.

So, first Brillouin zone, so the second Brillouin zone you access the second Brillouin zone, you do not cross, you cross one Bragg plane but you make sure that you do not cross the second Bragg plane. Similarly, we will continue so I just put on one more and then we will generalize. Third Brillouin zone it is the region in the reciprocal space that you can access by making sure that you cross two Bragg planes, but do not cross the third Bragg plane okay.

In a given direction, we will actually make a two-dimensional representation it will become very clear to you. So therefore, in the most general sense your nth Brillouin zone will imply that you have crossed n-1 Bragg planes right. For the first one 0 Bragg planes, second one, 1 Bragg plane, third one 2 Bragg planes and so on, you will cross n-1 Bragg planes, but no more okay.

Not more than that but not the nth, in other words it is the region between the n-1th Bragg plane and nth Bragg plane right. Except that you can do this in all directions okay, so you can start from the origin and just head off in any direction that you wish. In that direction, you cross n-1 planes but you do not cross the nth plane. You just cross keep crossing planes; you keep counting them as you cross them.

You do not cross the n-, you cross the n-1 plane but you do not cross the nth plane. That region between the n-1 plane and the nth plane in that direction belongs to the nth Brillouin zone. We will find that you know we will going to draw that in a moment for a for a two-dimensional structure. We will find that you know the progressively the Brillouin zones will consist of smaller and smaller pieces of space which are distributed around okay.

So initially we are able to identify square which is fully connected. The entire square that we draw, with that we drew was fully connected, all the regions were connected to each other. Subsequently we will find that they are smaller and smaller pieces which are spread out across space but because of symmetry in fact if you pull, if you add all those regions together the total area that you will get will be the same as the square, the original square.

So, the second Brillouin zone also if you pull all the regions that you identify is the second Brillouin zone. You pull them together you will get you will get a shape that is the same as the square. If you do the third one you will again get a square, fourth one you get a square and so on. But they will become more and more smaller and smaller pieces you just have to assemble them together you get back the square. So that in that sense the symmetry will remain the same. We will now look at a very general case and that will convey all this definition to you very clearly.

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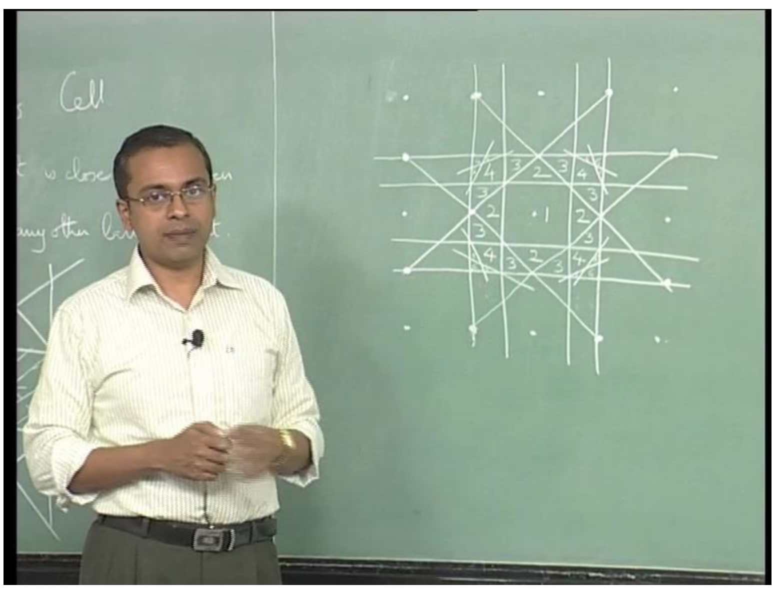

Now we will extend our understanding of how we indicate Bragg planes and Brillouin one zones in a two-dimensional system okay. So, to do this what we will do is, we will look at a set of points which will be a 5 by 5 matrix of points. Which would be points which are laid out in a square fashion okay. And in those points with respect to those points we will see if we can identify all the Bragg planes

And also, the Brillouin zones, so to do that let us put down this 5 by 5 points. So, you can follow this exercise with me and so as we do it you can you can yourself see for how this kind of a diagram comes about okay. So, we will go about it and step by step, so that you will be in a position to see how it happens.

So, first thing we have to do is, we will take the central point this central point here. And with respect to that central point, let us first see if we have a good understanding of what are its nearest neighbours okay. So, this is your central point, so with respect to this the first nearest neighbours are these four points 1, 2, 3 and 4 okay. So, there are these four points here are the first nearest neighbours.

So, I suggest you pull down this grid on a piece of paper, so you can also see how this is happening. So, the first four neighbours are here, these are the nearest neighbours. So, this is the first set of neighbours, if you want to look for the second set of neighbours, you look out here you will find the second set of neighbours.

These are the neighbours that are not the closest but the next closest set of neighbours. So, 1, 2, 3 and 4. So these four then become the next set of neighbours. The third closest neighbours will be these points okay. So, these will be the points that are the third closest neighbours with relative to the central point okay. So, if you chose another point in the air in the lattice, you can again identifies similarly the neighbours.

And then the fourth point should be all of these fourth closest points would be these, with respect to this okay. So, with respect to this these would be the fourth closest points. So, if I just looked at in this direction, this is the closest neighbour, second closest neighbour, third closest neighbour, fourth closest neighbour, that is how it is okay.

So, if you just see here closest neighbour, second closest neighbour, third closest neighbour, fourth closest neighbour, so that is how it is. So, with respect to each of these neighbours we will we will draw the lines that are that perpendicularly bisect the line joining the center point to those neighbours all right so that is what we will do and we will do this for this entire figure.

So, we will start with this point closest neighbours as I said are these four, so perpendicular bisectors should be lines that run like that okay, so we put those lines stop. So, we have now got the lines that perpendicularly bisect the lines that would the imaginary lines that would join this central point to its immediate four neighbours. So first set of neighbours have been taken care of now let us look at the second set of neighbours which are these.

So first is here, this is the second closest neighbour, so that line joining the central point to the second closest neighbour is here and it is perpendicular bisector will be something like this. And because this is a square grid of points, the perpendicular bisector actually goes through these points. If it were not a square grid you may you may not necessarily have it going through those points. But since it is a square grid we are able to do this okay.

So, let us just draw these perpendicular bisectors, they look like this okay. So, at each of these points there is a lattice point, a valid lattice point is out here available there okay. So, this is what we have got, so we took care of the first neighbour or rather we have attended to the identification of the Bragg plane with respect to the first neighbour. We had done that with respect to the second closest neighbour.

Third closest neighbour as I said is here, so this is the third closest neighbour with respect to the central point. So, this is actually two lattice spacing’s away so therefore the perpendicular bisector of the line joining them will actually go through the first lattice spacing the closest lattice spacing which is here right. So those lines would look like this and the same thing we will draw in all four directions so it will look like this.

So there, we have now taken care of the first, first the second and the third nearest neighbours, so that so they are all been attended to. So, let us now identify the fourth nearest neighbour which we already did. But on this figure, now that we have drawn some lines, let us just highlight the fourth nearest neighbour again. So, this would be one, this is another one, this is the third one. So, I have now highlighted all the lattice points.

Which are the fourth nearest neighbour neighbours to this particular lattice point okay? We have already done that before, so I have just highlighted it here. So, if you see the line joining this point the central point to the fourth nearest neighbour would sort of go through this point here. And the perpendicular bisector will sort of look like this right. This is the line, imaginary line that would connect these two points going down this way.

And the perpendicular bisector would be something like this, so this is how the perpendicular bisector looks, to the line joining the central point and this point here right. And similarly, between here and here, you will have a line which sort of looks like this and its perpendicular bisector would look like this. So, this is how you will get these perpendicular bisectors right. So, we will do the same thing now in all four directions.

If the, by symmetry look essentially exactly the same, so this would be one perpendicular bisector and this will be another perpendicular bisector. Similarly, this will be a perpendicular bisector and this will be a perpendicular bisector. And we will have one more here and one more here right. So now we have done the perpendicular bisectors.

So, we have eight perpendicular bisectors here with respect to these eight points which are the fourth nearest neighbours to the center point. So, we have done this process, so now having come this far, we have so essentially what have we done we have put down a set of points which are lattice points and let us say that this is in reciprocal space so these are reciprocal lattice points.

With and with respect to a central point we located all its nearest neighbours a one after the other and do the perpendicular bisectors to those lines joining the central point to those points. So those lines are now Bragg plane, so you know everything that we have drawn here is a Bragg plane, all these lines here is our Bragg planes right. Now with respect to our definition for a Brillouin zone.

If you start from the central point and you do not cross any Bragg plane you are in the first Brillouin zone. If you cross one Bragg plane and you do not cross anymore, you are the second Brillouin zone. If you cross two Bragg planes and not anymore then you are in the third Bragg Brillouin zone right, so that is what we have. So, if you do not cross any Bragg plane, you are in this region so this is the first Brillouin zone.

If you cross one Bragg plane but you do not cross the second one, so this is the second one here if you do not cross it, so you cross one Bragg plane you do not cross the second one you stay within this region this is the second Brillouin zone. So similarly, you will find locations around here which are all, which all meet that criteria or criterion. So, these are all second Brillouin zones.

The third Brillouin zone is reached by crossing two Bragg planes but you should not cross the third Bragg plane, so you should, that will put you in a region like this, so this is the third Brillouin zone. Similarly, this is also well if this also qualifies as the third Brillouin zone, third Brillouin zone. So, you see several regions now qualify as the third Brillouin zone.

So, the point you have to keep in mind is that therefore when you build make this kind of a diagram. The Brillouin zone of the same order, so this third Brillouin zone for example does not have to be a continuous it does not have to be at one single location. It is now spread out it is sort of fragmented and spread out across the diagram right.

In fact, as you get to higher and higher Brillouin zones they get more and more fragmented typically and get spread out more into the diagram. So that is how you will see it. So, if you cross now three Bragg planes one, two and three. But you do not cross the fourth Bragg plane that will put you in the fourth Brillouin zone. So, these are all fourth Brillouin zone regions 4, 4, 4 and 4 okay.

Please note there are other regions which would also qualify as fourth Brillouin zone, I have not marked this as the fourth one because I have not done it all over the diagram. I have just left it unmarked but in within the context of our diagram only the first, second and third Brillouin zones are completely present within this diagram okay.

So, they are not the rest of them are not completely present within this diagram. The rest of them you would have to draw much more of this diagram. We will draw this across several points to locate, all the regions that qualify as the fourth zone, all the regions that qualifies the fifth zone and all the regions that qualifies the sixth zone.

Within this context of this diagram we can still find out what are the regions that are the 4^{th}, 5th and 6th zones. So forth I have identified, 5th would be these small regions here because you would have crossed four Bragg planes but not the fifth one. So, these are all five, is a very small region, so you just have to note down that they are the fifth region.

And if you cross five Bragg planes and you do not cross the sixth Bragg plane that would put you here, this is the sixth Brillouin zone, six Brillouin zone and the sixth Brillouin zone. So you see even within the context of this figure we have been able to identify in, this is a simple figure a simple lattice so to speak, square lattice for which the reciprocal lattice was also a square lattice and just simply using our definition and incorporating our definitions into this diagram.

We have been able to identify the first, second, third, fourth and fifth and sixth Brillouin zones and except as I mentioned the fourth, fifth and sixth are not complete. You have to look for more of them, more pieces of them. If you were to extend this to three dimensions, the as you can imagine this figure will start getting more and more complicated okay. So, but the concept is exactly the same.

You locate the central point, you connect it to all its neighbours, identify perpendicular bisectors and perpendicular bisectors here are lines. In three dimensions, they would be planes and once you do that you will find some region in the middle which is which you can access without crossing any plane that would be the first Brillouin zone.

Then you would cross one plane and not the second plane that would be the second Brillouin zone and so on. So that is how we build up this Brillouin zones okay. So, in today's class we have actually seen what is a Wigner Seitz cell? we defined it, we drew it. We looked at what are Bragg planes and we also looked at what a Brillouin zones.

And we have seen how Brillouin zones can be put together, how you can identify the first Brillouin zone, the second Brillouin zone, third Brillouin zone and so on. So, we realize that you know that are set of there are range of Brillouin zones that we need to be able to identify the system. In our subsequent classes we will see what, this is for a three-dimensional structure we will look at it for the three-dimensional structure.

So that you can understand how it looks for a three-dimensional structure then we will also see what this means with respect to diffraction because that is something that we have learnt independently. We will connect it to, what we have drawn here. And finally, we will try and understand, if you take this all this information together what does it mean with respect to the energy values that are allowed for electrons in the system.

And the energy values that are forbidden for the electrons in the system that information comes when you pull all of these together, the Brillouin zones which come from the periodic structure of the material. And the wave information which comes from the electrons that are available in that material.

All of these have to be put together then you get this information on bands, allowed bands and band gaps okay. So, all of that we will see in our upcoming classes. With this we will halt for today, Thank you.