Metallurgy and Material Science

Prof. Dr. Prathap Haridoss
Department of Metallurgical and Materials Engineering
Indian Institute of Technology, Madras

Lecture No. # 30

Winger Seitz Cell and Introduction to Brillouin Zones

Hello welcome to the 30-th class in our course physics of materials. 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 in real space, we looked at it is description in reciprocal space, and we also looked at what is actually happening as you convert something some real space to the reciprocal space. So, this 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. So that is the context in which we have discussed it, that is the context in which the subject exists so to speak. In also in this context I showed you that know you may have a real space material that may consist, that may 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 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, only the dimension of the side of the cube is different. It is one by the dimension of the one 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 cubical 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 phase centered cubic and you represent in a reciprocal space, its representation in reciprocal space has the same layout as that of a body centered cubic structure.

So, something that is so, a material that is in real space having a phase centered cubic structure, will end up being represented in reciprocal space with a layout of points that that look exactly like a body centered cubic structure. And the inverse is also true. If you start with a body centered cubic structure you with in real space and you represent it in reciprocal space, the layout of the same of the points will now look like a phase center cubic structure. So, this is representation and it is important to understand that there is there can be some changes we you make this presentation, 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 interpreted we should keep this in mind, we should we should always keep that in mind and appropriately use this interpretation. 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. 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 incorporated into our model so far. So, that is the primary purpose of our discussion whatever we have built up and till now in the last two three classes where we have looked at reciprocal space, the creation of reciprocal space, the properties of the 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.

So, we are headed only in that direction these are tools that we are building because we will need all these tools to understand that interaction. And continuing in the same context in today 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 the some of the topics that we are discussing, because I have taken by themselves they may look like a bit independent topics which are disconnected, but they are not they are all add up to something that we are going to discuss. So, that is what it is.

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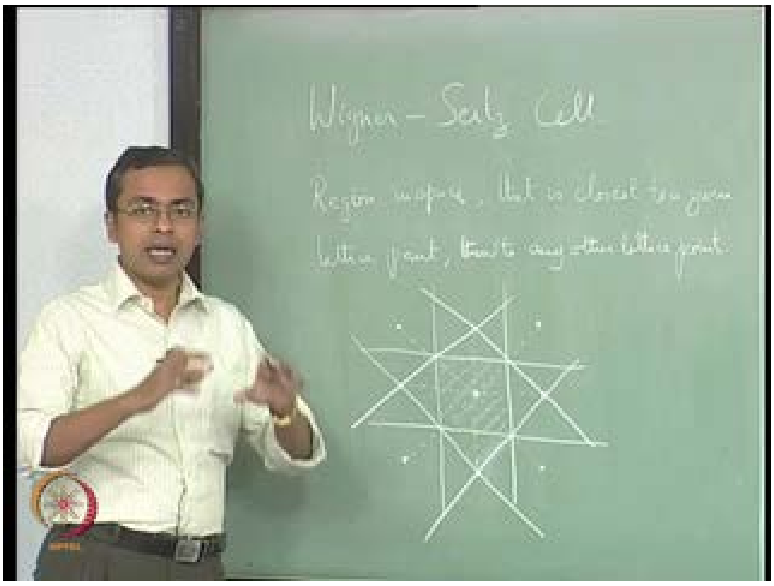

So, we looked at this now today we will introduce a concept we will introduce a few concepts couple of different concepts and two or three terms we will look at. The first is something called a Wigner Seitz cell. Wigner Seitz cell its defined as follows, it is the region in space that is closest to a given lattice point than to any other lattice point. So, this is the definition it simply says. So, this is again something to do with the structure. 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 just the definition. So, what does this mean?

We can actually do this in one dimensions in one dimension two dimensions or three dimensions. So, real solid object could to be in three dimensions for our representation we will start off with 1 d and 2 d representations, later we will look at structure in our next class we look at 3 d structures. So, basically what it says is, you have a set of lattice points I will just arbitrarily draw some lattice points. So, set of 9 lattice 3 by 3 have put laid them out our intension is to lay it out in a square fashion. So, it is just a we will assume that these are all exactly the same distance in every direction in those lattice directions. So, we have this two dimensional lattice. So, it is 2 d this plane and this plane basically. So, this direction and this direction is what is incorporated.

So, now we will look at this central point just for an example the same will hold true for any of the other points. So, this is the for the central point we would like to identify the region in space in this case its two dimensional space. So, it is a two dimension space we would like to identify this region in this two dimensional space, that is closest to this point than is to any of these other points. So, that is that is what the definition says if you identify that region that region is called the Wigner Seitz cell about this lattice point. So, that is the definition. How do we do this? There is a very straight forward way of doing this, What we will do is? we will take this lattice point we will connect it to all its neighbors, just a and we will have some guideline connecting it some dotted lines connecting it to all its nearest neighbors. So, let us just do that we will do that all its neighbors 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 have just started with this step. Now, let me take its nearest neighbor, one of its nearest neighbors we will take this point here it is it is one of its the nearest neighbors. What is the region in space that is the 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, 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 as straight forward as that. So, we will just draw that we will do that you will take the midpoint of it whatever is the midpoint and draw a perpendicular bisector.

So, if you draw a perpendicular bisector to the line joining this point the point that we are interested in to its nearest neighbor we find that anything to the ah from our perspective to our of this line is closer to this point, than to this point. And anything to the left of the line from our perspective is closer to this point than it is to that point. 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. So, now we will take the point that is up here the perpendicular bisector is somewhere it has go through that point.

So, it will 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 now 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 4 closest neighbors, the 4 closest neighbors 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 this point. The region on this side of this line closer to this point than 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 to that point. So, this region defined by the square is now closer to this central point than it is to its immediate four neighbors close four closest neighbors.

We can extend that argument we can even look at its next nearest neighbors 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 this central point will look something like this, and if you continue that exercise for this and this you will get lines that look like this. 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 we 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 a straight square that which like what it is shown here.

So, 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 other points. 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. So, this is so that is all that is to it is a straight forward the definition is now fairly straight forward now you 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 three dimensions you will now have a point, just the way you had this neighbor here, you will have a point at similar distance in front of the plane of the board and you will have a point at similar distance behind the plane of the board. And the please understand this is the 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 bisector 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 these 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. Similarly, a perpendicular bisector will exist which will bisect the line joining this point and the lattice point directly behind it in into the plane of the board and. So, you will have now a plane behind the plane of the board a plane front of the plane of the board and these planes here, and since they are all squarely laid out the dimensions will be the same what you get is a cube. What you are seeing as a square in two dimensions will become a cube in three dimensions. So, in a if you have a square lattice or a cubic cube lattice Wigner Seitz cell will be a cube. So, this is the basically definition of a Wigner Seitz cell. I must also point out that in general see a square lattice is a very particular case if you if it is square it is a very particular case if it is a rectangle its little less particular, but still we are putting a some restriction. In general you can have a set of points which are arranged like this.

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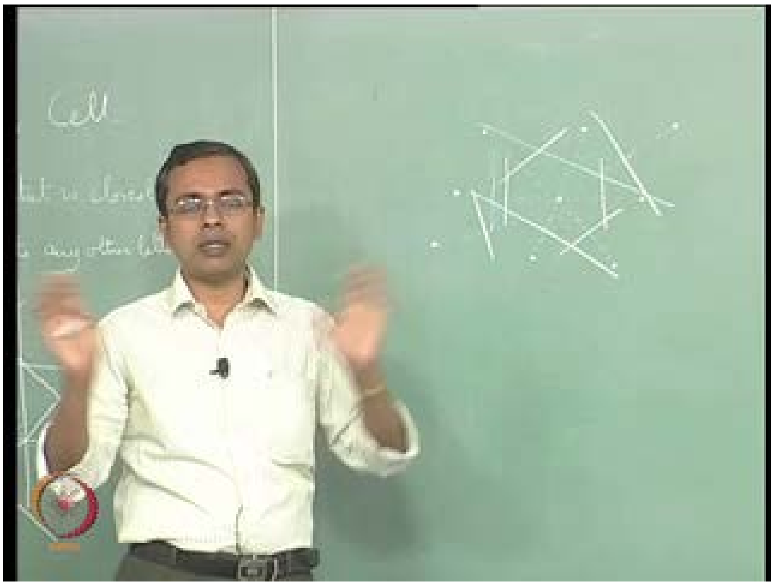

So, if you now have this set of points and you look at the perpendicular bisectors again we will do the same exercise. Now, that you understand the concept we can do it relatively quickly we join the central point to all its immediate neighbors, and we draw the perpendicular bisector of each. So, perpendicular bisector of this would look something like that, perpendicular bisector of this would look something like that, It is not exact 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 would look something like that. So, by looking at the immediate neighbors and you will the other ones do not really impact you this is kind of faraway.

So, its line will be somewhere there perpendicular bisector will 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 to scale you may find some variations, but the point is you will find a region bounded by six sides. 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. 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 points. So, in a sense the boundary of the Wigner Seitz cell will become the boundary of the Wigner Seitz cell of the next cell. So, for this for of the next lattice point. So, this is going to be true for all the lattice points because of symmetry and. So, it is in general it is going to be a six sided figure if it is a rectangle it will become a four sided figure which look rectangular and if it is a square, it will square lattice it will become a four sided which is a square.

So, those are special cases. So, in general this is what a Wigner Seitz cell is now. So, I have already. So, now we have understood. So, this is just a definition. So, this is just a definition you understand what the definition means and you also understand how you can create the cell, or how you 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 we will identify that region you simply connect the point you are interested in with all its neighbors. Draw perpendicular bisectors to it and then whatever shows up as the inner most region from all this perpendicular bisectors inner most region is the is now the region that is closest to that point than to any other and that then becomes the Wigner Seitz cell of that particular lattice.

So, that it is all there is we have done in 2 d. So, that it is easier to see same thing is true in 3 d, except the perpendicular bisectors will lines will be planes in sort of lines that is all it is. So, if you have the right kind of software you can take any lattice and you can do these perpendicular bisectors you can create and you can see it and you can rotate it around. So, we will see something on 3 d a little later, but for now this is in 2 d 2 dimensional lattice descriptions. So, now, we have seen this first description called Wigner Seitz cell.

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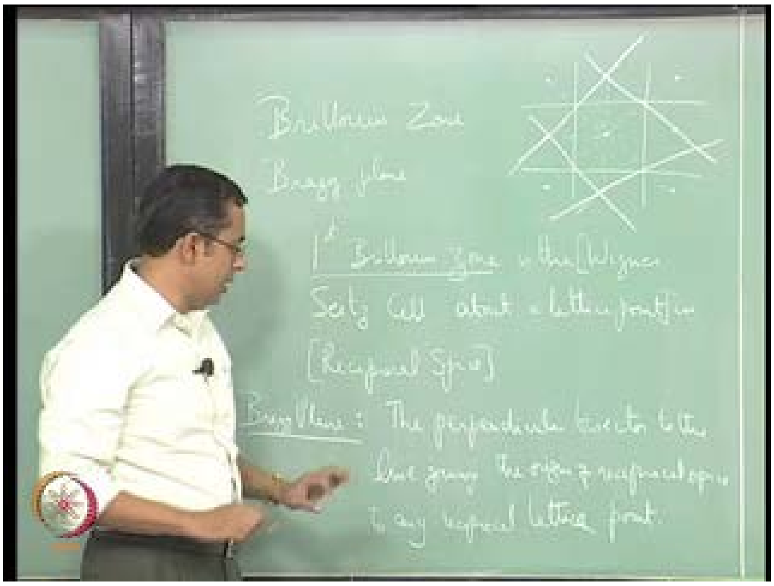

Now, we will define another term which is called a Brillouin zone a brillouin zone is we will define two terms actually a brillouin zone and we will define something called a bragg plane. So, first we will define something called the first brillouin zone the brillouin zone actually can be can be called as we will find that you know whatever it is we once we describe, what a brillouin zone is we can we will find that it can be a 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 the n the use that definition to help us define second brillouin zone third brillouin zone and so on. So, that is what we want the brillouin zone. The first brillouin zone is the Wigner Seitz cell about a lattice point in reciprocal space. So, 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 a new term we have introduced brillouin zone, we are going to look at what it what it means. And we have we are defining the first Brillouin zone as the Wigner Seitz cell which we just now 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 a Wigner Seitz cell about a lattice point is something that you are now clear about because we just discussed it. So, this part of the definition your already clear about Wigner Seitz cell about a lattice point, any lattice I give you understand the concept of how you come up with a Wigner Seitz cell about that lattice point that is a very straight right process.

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. So, now this is a concept we learnt yesterday independently yesterday in the the last two classes rather in the last two classes, we have learnt this concept independently reciprocal space. We understood how real space ah relates to reciprocal space and such. So, reciprocal space we independently defined and we have understood. So, reciprocal space consists of reciprocal lattice points. 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 we have a 1 a 2 and a 3, you know how you can go from a 1 a 2 a 3 in real space to b 1 b 2 and b 3 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 ah based on. So, for that lattice you know how to independently create the reciprocal lattice of it, because we know the relationship between a 1 a 2 a 3 and b 1 b 2 b 3 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 to a reciprocal lattice. So, therefore, you know the this step and regardless of the lattice you know how to construct a Wigner Seitz cell.

So, if 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. So, we just did diagrams for a layout of a square layout of points. So, we did a diagram here for a square layout of points. So, we just did this diagram. Now if this set of lattice points per lattice points in reciprocal space, 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 reciprocal set of space set of lattice points. That restriction we have 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 a lattice point in reciprocal space would then now become the brillouin zone the first brillouin zone.

So, therefore, you see that you know a diagram that we have drawn simply if we have called this reciprocal lattice points this is brillouin zone that is all it is. So, the brillouin zone term is if since you may be encountering these 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. I mean they are ah constructs or structures that we can imagine in space, which we can which we can associate with real space or reciprocal space. And based on what we are doing we would call it either just a Wigner Seitz cell or if it were specific to reciprocal space and reciprocal lattice it would get called the first brillouin zone.

So, this is all the definition is. So, now you understand a few of the concepts and how they are connecting lattice Wigner Seitz cell and brillouin zone. In fact, real lattice reciprocal lattice Wigner Seitz and brillouin zone these are four concepts we have now linked them up. So, 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 that definition we can find out what are the other brillouin zones that we have available to us.

So, a Bragg plane is the perpendicular bisector to the line joining the origin of reciprocal space to any reciprocal lattice point. 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. So, this is a definition. So, let us understand what this means when you define a reciprocal space for sake of convenience we will designate one point as the origin of reciprocal space. So, that is by convenience we just define one point. Since it is since all of these lattices are based on symmetry if you define a particular point as the origin it is not going make a big difference, you can chose an one of the adjacent points in principle the symmetry would still remain the same.

So, we can select it by our convenience we select the point as the origin by our convenience we can connect that origin to any other lattice point. I mean it is just an I mean imaginary connection when I say connect we can we can always draw straight lines between that lattice point and any other lattice point that is available and reciprocal space. 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 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.

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 the 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. This is a bit confusing because in diffraction we talk of a planes and we talk of Bragg law of diffraction and so on. So, Bragg equation and such and. So, the term Bragg plane can slightly to be confusing the first time you ah encounter it, but this is all it is if you look at this definition and you implement this definition. So, it’s a straight forward definition I mean it helps you straight forwardly identify what are the Bragg planes.

So, now, we understand what a Bragg plane is. So, we can immediately see you are probably already able to see now how this relates to the brillouin zone and Wigner Seitz cell. Wigner Seitz cell was simply something that we did in any space we did not really specify that it was real space or reciprocal space or any such thing. In the reciprocal space we were able to say that 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 3 by 3, 3 by 3 set of points and we found that you know if you just draw the perpendicular bisectors we will end up getting this square region which is then your brillouin zone. The first brillouin zone we will assume this now these are now reciprocal lattice points, what have we done? We have drawn perpendicular bisectors to the lines joining this point to its neighbors.

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, 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 neighbors. If you draw it correctly it will all go through those points there you would not have this region there. So, these are lines that that originally when we define a Wigner Seitz cell we simply said that this is a line that perpendicularly bisects the line joining a point and its immediate neighbor, this is not drawn exactly to scale if you draw it the scale you will 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. So, that is all it is the perpendicular bisector to the line joining the origin of reciprocal space to any reciprocal lattice point. So, this line here this 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. So, they are all simply lines and. In fact, these are lines in two dimensions and we I all say always said that that you know if you draw this in three dimension this will be a plane. So, that is where the name Bragg plane comes. So, of course, the Bragg the name the name Bragg being incorporated here suggest that somewhere intuitively suggest to us that you know this person has being 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 possible in our next class. In fact, we will get to it. Now lets us not worry about the link to diffraction we simply say that these are Bragg planes. So, these are all Bragg planes by the definition of what a Bragg plane is.

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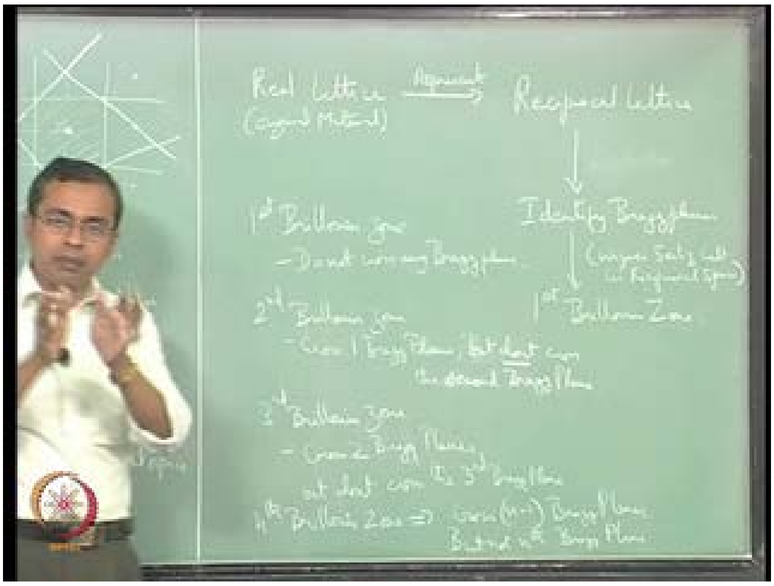

So, now we see much more elaborately, we have real space, real lattice we can convert it or represent it in reciprocal space. So, it will become reciprocal lattice. So, this is your original material. So, it will have a real lattice we can represent it in reciprocal space as a reciprocal lattice, if you represent it in reciprocal space you can draw Wigner Seitz cell. 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. And this is now Wigner Seitz cell in reciprocal space. So, this is how the concepts that we have discussed today tie up to each other.

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 inner most 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. So, this is the definition this is how they all connect up latter we will see the link to diffraction. Now, we have just done it for we have now I 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 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. 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, as long as your within this region. When your within this region no matter where you go you will not cross a Bragg plane these are all the Bragg plane. These are all Bragg planes around it 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. 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 no more. 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 and this region here are all regions belonging to the second brillouin zone. 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 Wigner Seitz cell the boundaries of the Wigner Seitz cell are Bragg planes. And therefore, you can have several Bragg planes that we can identify. And Now, therefore, we have to restate the definition for a brillouin zone because we can identify additional regions which have which have which are in concept similar, but have something some different about them.

And now we rechanged I mean we restated the definition by saying the brillouin zone is that region which you can the first brillouin is the region that you can access from the center 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 second Bragg plane, but you do not cross the second Bragg plane. So, that is how you go. So, first brillouin zone. So, second brillouin zone you to 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 have just put down a 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 third Bragg plane in 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 minus one Bragg planes, for the first one 0 Bragg planes second 1 Bragg plane third one two Bragg planes and so on. You will cross n minus one Bragg planes, but no more not more than that but not the nth.

In other words it is a region between the n minus one th Bragg plane and the nth Bragg plane right except that you can do this in all directions. So, you can start from the origin and just head off in any direction that you wish in that direction you cross n minus one 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 minus you cross the n minus one th plane, but you do not across the nth plane that region between the n minus one th plane and the nth plane in that direction belongs to the nth brillouin zone.

We will find that we are going to draw that in a moment for a for a two dimensional structure we will find the you know the progressively the brillouin zones will consist of smaller and smaller pieces of space which are distributed around. So, initially we are able to identify a 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 as a square the origin of square.

So, the second brillouin zone also if you pull all the regions that you identify as a second brillouin zone you put them together you will you will get the 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 will back the square. So, the 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.

Now, we will extend our understanding of how we indicate Bragg plane and brillouin zone in a two dimensional system. 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 will be a point which are laid out in a square fashion. So, and those points with respect to those points we will see if we can identify all the Bragg planes and also the brillouin zones.

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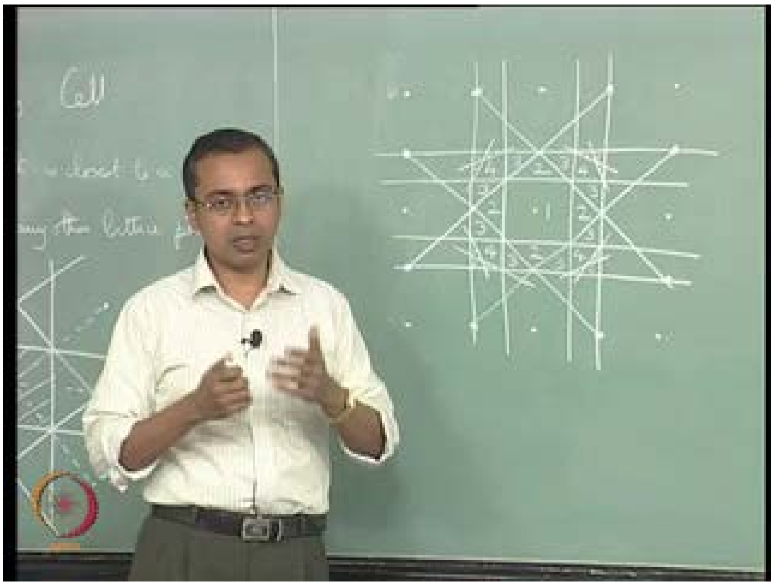

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So, to do that lets put down this 5 by 5 points see you can follow this exercise with me and. So, as we do it you can you can yourself see for how this kind of a diagram comes about. So, we will go about it step by step. So, that you will be in a position to see how it happens. So, first thing we have to do is we will take this central point this central point here and with respect to that central point lets first see if we have a good understanding of what are its nearest neighbors. So, this is your central point. So, with respect to this the first nearest neighbors are these 4.123 and 4. So, they are these four points here are the first nearest neighbors. So, I suggest you put down this grid on a piece of paper. So, you can also see how this is happening. So, the first four neighbors are here these are the nearest neighbors.

So, this is the first set of neighbor if you want to look for the second set of neighbors, you look out here you will find the second set of neighbors these are the neighbors that are not the closest, but the next closest set of neighbors. So, 1 2 3 and 4. So, these four then become the next set of neighbors the third closest neighbors will be these points. So, these will be the points that are the third closest neighbors with relative to the central point. So, if you choose another point in the lattice you would again identify similarly the neighbor and then the fourth points would be all of these fourth closest points would be these with respect to this. So, with respect to this these would be the fourth closest points.

So, if I just look at this in this direction this is the closest neighbor second closest neighbor third closest neighbor fourth closest neighbor that is how it is. So, if you just see here closest neighbor second closest neighbor third closest neighbor fourth closest neighbor. So, that is how it is. So, with respect to each of these neighbors we will we will draw the lines that are that perpendicularly bisect the line joining the center point to those neighbors alright. So, that is what we will do and we will do this for this entire figure. So, we will start with this point closest neighbors as I said are these four. So, perpendicular bisectors will be lines that run like that. So, we will put those lines now.

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 neighbors. So, first set of neighbors have been taken care off now let us look at the second set of neighbors which are these. So, first is here this is the second closest neighbor. So, the line joining the central point to the second closest neighbor is here and its 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 having going through those point, but since it is a square grid we are able to do this.

So, let us just draw these perpendicular bisectors they look like this. So, at each of these points there is a lattice point a valid lattice point is out here available there. So, this is what we have got. So, we took care of the first neighbor or rather we have attended to the identification of the Bragg plane with respect to the first neighbor we have done that with respect to the second closest neighbor third closest neighbor as I said is here. So, this the third closest neighbor with respect to the central point. So, this is actually two lattices spacing 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.

So, those lines w ill look like this and the same thing we will draw in all four directions. So, it will look like this. So, there we have taken now taken care of the first the second and the third nearest neighbors. So, that is a they have all been attended to. So, let us now identify the fourth nearest neighbor which we already did, but now on this figure now that we have drawn some lines let us just highlight the fourth nearest neighbor again. So, this would be one this is another one this is the third one. So, now I have now highlighted all the lattice points which are the fourth nearest neighbor neighbors to this particular lattice point 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 neighbor 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 this central point and this point here.

And similarly between here and here you will have a line which sort of looks like this and its perpendicular bisector would 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 it 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 you will have one more here and one more here.

So, now we have done the perpendicular bisector. So, we have eight perpendicular bisectors here with respect to these eight points which are the fourth nearest neighbors to this 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 the 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 neighbors 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, in everything that we drawn here is a Bragg plane all these lines here is are Bragg plane 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 in the second brillouin zone if you cross two Bragg planes and not anymore then you are the third brillouin zone. 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 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, the third brillouin zone for example, does not have to be a continuous does not have to be at one single location it is now spread out its sort of fragmented and spread out across the diagram. In fact, as you get to higher and higher brillouin zones they get more and more fragmented typically and gets spread out more into that diagram.

So, that is how you will see. 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 four and four 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 unmark, but in within the context of our diagram only the first second and third brillouin zone are completely present within this diagram.

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 of this diagram you have to draw this across several points to locate all the regions that qualify as the fourth zone all the regions that qualify as the fifth zone and all the regions that qualify as the sixth zone within this context of this diagram we can still find out what are the regions that are the fourth fifth and sixth region. So, fourth I have identified fifth 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 regions. So, you just have to note down that they are the region and if you cross 5 Bragg planes and you do not cross the 6 Bragg plane that would put you here this is the sixth brillouin zone sixth brillouin zone and the sixth brillouin zone. So, you see even within the context of this figure we have been able to identify 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 zone 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. So, but the concept is exactly the same you locate the central point you connect it to all its neighbors identify perpendicular bisectors and the 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. So, in today's class we have actually seen what is Wigner Seitz cell we defined it we drew it we looked at what are Bragg planes and we also looked at what are brillouin zone and we have seen how brillouin zones are put together how you can identify the first brillouin zone the second brillouin zone third brillouin zone and so on. So, ww realize that you know that there 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 structures. 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 the material all of these have to be put together. Then you get this information on bands allowed bands and band caps. So, all of that we will see in our upcoming classes with this we will halt for today. Thank You.