Physics of Materials
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Lecture No. # 31
Brillouin Zones, Diffraction and Allowed Energy Levels

Hello, welcome to the 31 class in our course, the physics of materials. In the last few classes, we have looked at the reciprocals space, we have a looked at how rear space and reciprocal space at related, we looked at what is the reciprocal lattice, how you would create a reciprocal lattice for a given real lattice. So, and then we recognized that you know in we can think of certain types of a structures that we called the Wigner Seitz cell, which basically was defined as the regional space, which is closes to lattice point than to any other lattice point. It is a regional space that is closes to a single lattice point than to any other lattice point.

So, for a cubic array of lattice points, the Wigner Seitz cell actually turns out to be a cube. And then we defined in what is called Bragg plane, which we said is apartment particular bisector of any vector connects the origin to valid reciprocal lattice point. Then we a looked t the reciprocal lattice, and we a found that the a Wigner Seitz cell about the reciprocal lattice point. Simply consist of series of planes are about at lattice point, which are all Bragg planes. And this was then defined as the Brillouin zone be first Brillouin zone. So, we said the first Brillouin zone is the region in space in reciprocal space that can be reached from the origin by not crossing even a single Bragg place. And then the second Brillouin zone would be reached by crossing one Bragg plane, but not more than one Bragg plane. And third would be reached by crossing two Bragg plane and not more than two Bragg plane.

So, in that context we made some diagrams on the board, we will a start by simply repeating the two-dimensional version of this discussion, because that we lead as very well it to the three dimensional. Basically, we are right now discussing the Brillouin zone. We are just looking at structures trying to understand that given as structure, what is the Brillouin zone that we can, what is set of Brillouin zone that we can define or how will we defined the Brillouin zone for that is structure so that is the exercise we are currently involved. We will eventually use the information to understand the property of material that is step that we will see later in this class. So, right now, the next few slides that you are going to see are simply how you defined the Brillouin zone for a two dimensional structure and for a three dimensional structure.

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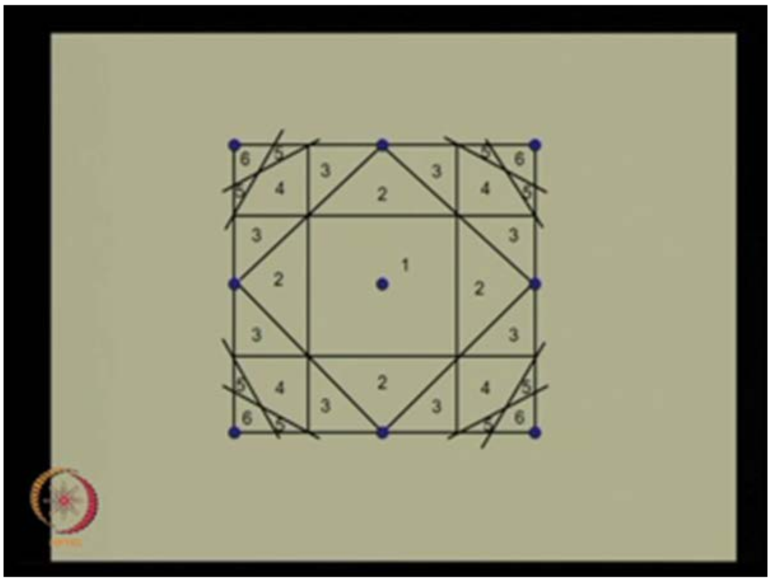

So, here we are, we will repeat the exercise that we did on the board with an array points on the slide. So, we have here three by three set of points three pointsthere, three point here and then three points here. So, we start by we will assume that the central point here as the origin, and these are all the then neighbors for those for the central point. And of course, this is the very large lattice; we have simply taken very small region in the lattice. So, this is satisfy we want to have three points by three points. In principle we would have much more than three points, we will point some either side of them extending in all directions right.

So, in this situation if you now identify the nearest neighbors, nearest neighbors are these 1, 2, 3 and 4. So, with respect to these nearest neighbors, we can draw the perpendicular by; we can draw vectors two those nearest neighbors and then drop of perpendicular bisector to those vectors. So, perpendicular bisector would appear here, would appear there, appear there and appear here. So, that is basically what you will see. So, these are lines that perpendicularly bisect the vector joining this origin to all it is immediately near neighboring lattice points so that is one set of the bisectors.

We will continue the exercise, we will get other another set of bisectors based on lines that connect this point to its next nearest set of neighbors which are here. So, this is what we would do. Then we; third set of nearest neighbors would actually be points along this line, but further away in fact, the next lattice point. Therefore, line going through these lattice points would then constitutive the line the perpendicularly by steps that vector. So, the next set of perpendicular bisectors would appear here.

And continuing that exercise if you actually look at the points that we have we will have one more point here one for lattice point here. So, we can think of line joining that lattice points and the origin and therefore, we would; we can except the there will be a perpendicular bisectors somewhere here. Similarly, there is the, another lattice point further down here. And therefore, again we can draw vector to the origin from that lattice point and naturally we can expect the perpendicular bisector vector to that somewhere here drawn by here. So, taking the next set of neighbors together, we have another set of perpendicular bisector we will do this all around that origin so, in all four directions around the origin we get it and so, we find lines vectors. So, having got this array of perpendicular bisectors to a lines joining the origin to all this nearing all the neighbors around the central lattice point. We can now, identify Brillouin zone based on the definition we have given Brillouin zones, which is basically that the first Brillouin zone is the regional space around this point which can be reach from this points without processing a single Bragg plane and therefore, that will be the region that is identified here. So, this region around this point is therefore, the first Brillouin zone. If you cross one Bragg place, but you do not cross the second Bragg plane then that region is a second Brillouin zone.

We find around this points several location where this is true so, this is one region where this is true, you have crossed one Bragg plane to get in to the region, but you not cross further Bragg planes. And all this perpendicular bisectors are the Bragg plane, by the definition that we have given this. So, we crossed one Bragg plane within cross second Bragg plane so, this is belongs to the second Brillouin zone. But there is in other region here which also belongs to the second Brillouin zone for exactly the same definition because it is the fixed the same definition, this is the another search region and this is the another search region. So, taken together we have four locations where we identify the second Brillouin zone so those are the second Brillouin zone.

Similarly, you cross one more Bragg plane, you; that means, you now, cross two Bragg planes and you do not cross the third Bragg plane that you put you in this region that would done be the third Brillouin zone and there are several such location where you would effectively be access the same method Brillouin zone. So, these are all the third Brillouin zone. So, continue the exercise further in exactly the same manner we can identify the forth Brillouin zone as those four location; are it is those location that you see that. And then you again you continue this process you at least within the context for the figure we have drawn, this is then the fifth Brillouin zone and this is find the sixth Brillouin zone.

So, for a simple two dimensional array of a square array of points, where we only taken the just three points on are screen, three by three metrics of points. So, we only have nine points on screen we will be nine able to identify for this lattice all the Bragg planes and therefore, all the Brillouin zones. And please keep in mind always the Brillouin zones are defined with respect to reciprocal lattice. So, originally, we would have some material that would have some real as; that would have a lattice and real space using the standard convention for how do you would get the reciprocal, corresponding reciprocal lattice we would generate the corresponding reciprocal lattice.

In that reciprocal lattice we would identify the Bragg planes similar to what we have just done. Once we have identify the Bragg plane using the convention of using the definition of what is sub Brillouin zone, what is the n Brillouin zone, we will identify the n th Brillouin zone. So, the n th Brillouin zone requires you to cross n minus 1 Bragg planes, but restrict you and prevents you from crossing the n th Bragg plane so, between the n minus 1 and the n th Bragg plane you have the n th Brillouin zone. So, this is something that we have seen it two dimensions.

We will now extend this in two couple of structures in three dimensions is especially is structures that we most commonly encounter in material science. The two structures that we look at are the face centered cubic and the body centered cubic structure. So, first we what will do is we simply defined what is the wingers size cell for a body centered cubic structure and what is the wingers size cell for a face centered cubic structure. So, this is the this is we will we will discuss it only as the Wigner Seitz cell at this point, which means there is no real reference to reciprocal lattice at this point. So, we do this exercise and then we will consider what the consequences are with respect to identifying a Brillouin zone.

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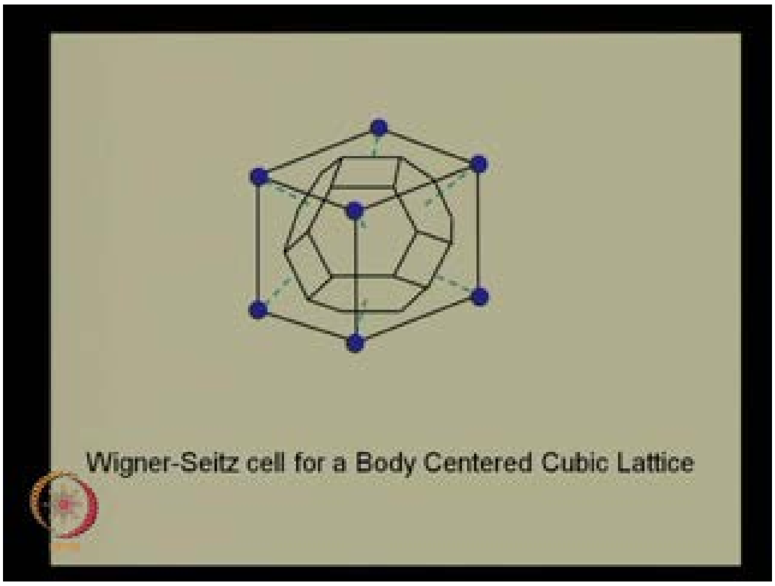

So, if you look at a body centered cubic lattice which is sort of what is which is basically what is shown here. Please, ignore the figure in the middle for the moment. So, what we have here is we have four atoms of the corners or four lattice points you going to talk about lattice points. So, four lattice points of the corners and there are four more at the in the at the base there is one hidden behind the structure which we are not looking at and there is one lattice point, right in the middle of this cubic structure, that is what defined the body centered cubic structure. So, now, the given this body centered cubic lattice, the process of identifying a Wigner Seitz cell is really straight forward. It (( )) the definition that we use we simply extended to three dimension. So, we take the central atom which is not being shown here and we connected to all its neighbors.

So, for example, using this dotted green lines, dashed green lines, we have connected this central atom to this all the atoms are a rounded, having done the we draw the perpendicular bisectors to those lines. So, those are vectors the joined the as origin to the points that are arrange around the origin or around the body center and then we simply take perpendicular bisector to those points. What we will; what happens is since is the three dimensional structure that we are looking at the perpendicular bisectors are planes so there is the large plane that is perpendicularly bisecting this region. And so for example, this plane here the hexagon that you see here, bisect the line that joins this particular atom to the atom at the center. It is the actually, have plane which is in which has which is in insensible has in infinite dimension; I mean it is infinitely long in both in both the directions. But the part of it that belongs to the that identify the Brillouin zone where is if it comes where intersect the plane the that bisect the line joining this atom to the center.

So, we can take, we can draw several such planes, for every two atoms that every, I am sorry, every two lattice point that you can identify in this structure, you can identify a plane which bisect the line connecting those two lattice point, especially, with respect to the same origin. So, you will treat the central atom as the origin, will keep connecting to as many (( )) atoms surrounded it has possible. And in each case we will simply take a perpendicular bisector. And when you do that the structure that you see here is what remains has the center most region close to this point, which is which now identifies the region that is closes to the central point than to any other lattice point.

For example, this structure that you see here, this it is part of a plane that bisects the line joining the body center of this single cube that you are seeing here and the neighboring body center. So, if you add continued this lattice, if you are drawn the next set of lattice points herel you would one second found one other body center. So, you connect the body center of this particular single lattice that is your seeing here, unit cell that you are seeing here, to the next cell. And when you connect this unit cell to the body centers of those two unit cells the perpendicular bisector of, will actually be this plane. Because simply because, the body centers are exactly half way into the structure unit cell.

So, you go half way into this structure you will get to this body center, you go half way in to the next unit cell, you get the next body center, Therefore, this plane here bisect the line joining those two body center of which this small section here becomes part of; becomes the surface of the brills of the Wigner Seitz with respect to this lattice point that is in the middle. So, therefore, this shape that you see here is the Wigner Seitz cell for a body centered cubic lattice. So, that is as straight forward as that you are able to imagine what the body center is because it is the right in the middle there. You are able to see the atoms here lattice points here, you are able to see the line joining them that planes that perpendicular bisect those lines and therefore, and the structure that emerges when all those planes intersect to the each other. So, that is the structure that is setting the middle.

This structure encloses all the points that of closes to that central lattice point then to any of the other lattice points available in this structure. So, this is all there is and so going by the definition of a Wigner Seitz cell this is the Wigner Seitz cell for a body centered cubic lattice.

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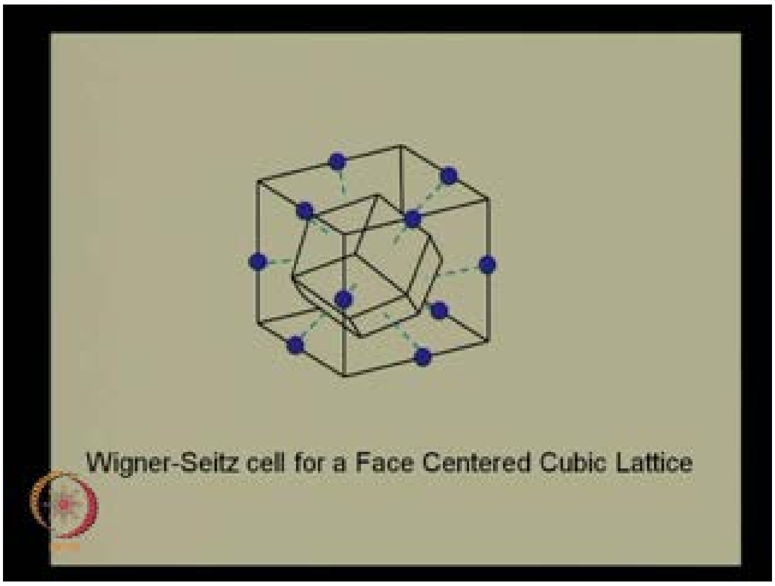

We will now, look at the Wigner Seitz cell for a face centered cubic lattice. Again this is still, it just a lattice. So, we are not really specifying anything on whether or not this is in real space or the reciprocal space, will assume in real space. Here, first thing I want to you pay attention to his although I have described here as face centered cubic lattice, this is not normally how you draw of a centered cubic lattice, the set of points that you see here is not normally how you would draw face center cubic lattice. So, for a moment let first make sure that we are that satisfy for ourselves what we have drawn here is In fact, of a centered cubic lattice so that is the exercise you do immediately and then we will go head an use this. What I just tell you, what I have done here, we will; I show it you on the board and then we will get back to this drawing here what I have actually done is I have taken of face centered cubic unit cell of face centered cubic lattice and taken only half of it what you see here as the top of his top of a face centered cubic lattice and what is seen at the bottom is the bottom half of another is the half of another unit cell.

So, the lower part of this diagram is the top half of one unit cell and the upper part of the diagram is the bottom half of another unit cell which is about this picture. So, taking those to half together to be having got this unit cell so I just show that to you on the board before we comeback to this diagram.

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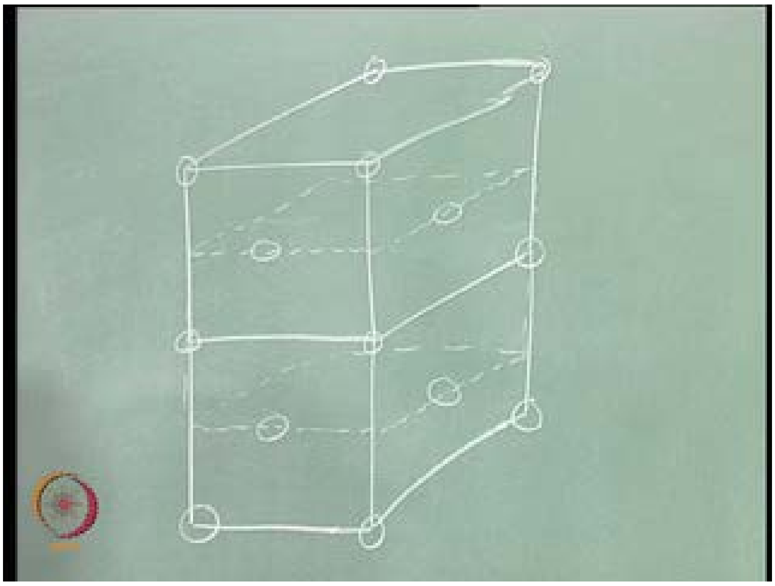

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So, what we are drawing here as are two unit cells of the f c structure. So, we will have atoms, I am sorry lattice points at this location and this will be the face center. So, we can always imagine as diagram where we basically take this line here (No audio from 15:39 to 15:50) and then look at the unit cell that way. The reason we would like to do this because this plane which is between this two unit cell write in the middle of it there is one lattice point. That is the face center of this base cell plane of this unit cell on the top plane of the other unit cell. So, write in the middle there is an atom lattice point which is somewhere there that is the center of this plane that is between these two unit cells.

So, with that the reason; so that becomes convenient for us because we now have a lattice point right at the middle. And for our purposes we are looking to; we are looking for symmetry so that we can look at the lattice point and build thing is I mean look at the space surrounded with respect to it is entire neighbor. So, this becomes convenient rather than any of the other points as the origin so that is the reason we have choose in this. So, therefore, you will see if you do this, you will have lattice points in the middle of the diagram on top and are the bottom and that the corners in the middle of the diagram so that is basically, what you will see in diagram here. At the corners we have lattice point here and in the middle we have lattice point here. And that lines that I have drawn here, the straight lines are drawn here, they all go to the middle of this structure which is the plane half way through this unit cell that we showing you here. And therefore, that is the face centered, in fact, of the of both this unit cell.

So, effectively that is the face center of one half of unit cell that is up here and that is also the face center of one half of another unit cell which is down here. So, therefore, the diagram I am showing you here, even though it does not immediately appear as the face centered cubic lattice diagram. In fact, it is simply a different I will just shifted the diagram by half a unit lattice vector basis so that is all I have done I moved on half. So, I will get half of one unit cell and half of another unit cell, still it total sub to one complete unit cell.

So, this is the; and what we have done? We have done exactly the same procedure; we draw vectors which connect the central point to all this neighbors, all these neighboring points and we drop of perpendicular bisectors to those vectors. Those perpendicular bisectors are planes and they themselves pump in to each other along these lines. And as the result, you end up with some structure that this visible here. So, this structure that you see in the middle here is therefore, the Wigner Seitz cell for a face centered cubic lattice. So, it is quietly here we are now already defined the Wigner Seitz cell for a body centered cubic lattice and we are now defined the Wigner Seitz cell for a face centered cubic lattice.

What we are also seen in our discussion is that when you look at the relationship between lattice in real space, and lattice in reciprocal space, we find that if you have face centered cubic lattice in real space it gets represented as a body centered cubic lattice in reciprocal space. This is an exercise that we did couple of classes ago and we are able to see how the vectors would then defined a body centered cubic lattice in reciprocal space. In other words you start with the face centered; if you have you have a material that has the face centered cubic structure, when you represent this materials in reciprocal lattice notation, it to the represented by a set of points that have the symmetry of a body centered cubic lattice.

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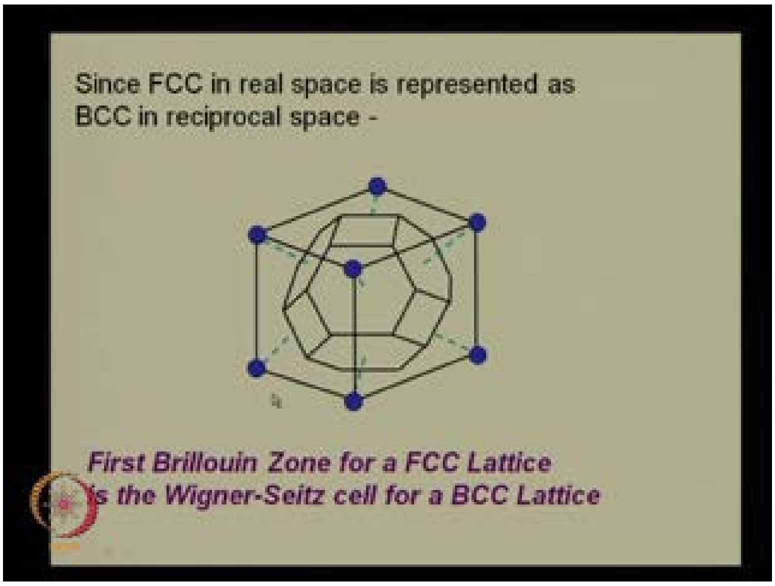

So, therefore, if you have a material in real space that is face centered cubic, it is going to be represented as body centered cubic in reciprocal space and we have also defined that the Brillouin zone, the first Brillouin zone of a structure is simply the Wigner Seitz cell about a reciprocal lattice point. So, you will find that the therefore, we find that the first Brillouin zone for a face centered cubic lattice in real space is the Wigner Seitz cell for a body centered cubic lattice in reciprocal space. So, this occurs because of the inversion.

So, you are talking of a face centered cubic lattice which happens to be real space and since it is represented as the body centered cubic lattice in reciprocal space it is Wigner Seitz at the Wigner Seitz cell of the body centered cubic lattice is therefore, defined as the first Brillouin zone for a face centered cubic lattice material. So, this is slightly tricky first time encounter it, I suggest that you look at this little put slowly and carefully so that you understand what we have done here.

What we are doing is definitions talks of reciprocal space is talks of reciprocal lattice, the Brillouin zone definition. So, therefore, we can only defined Brillouin zone, the first Brillouin zone and subsequence Brillouin zone can all be only defined with respect to whatever is the reciprocal lattice. So, whatever happens to be real lattice, in some way shape and form it is going to be represented in the reciprocal space as a reciprocal lattice. And what you get there as the Brillouin zone is then link to the real space material is simply stated as that we real space lattice has the following Brillouin zone.

So, FCC becomes BCC and therefore, BCC is Brillouin zone is the FCC is; BCC is Wigner Seitz cell is the FCC Brillouin zone. So, therefore; so that is what we are depicting here.

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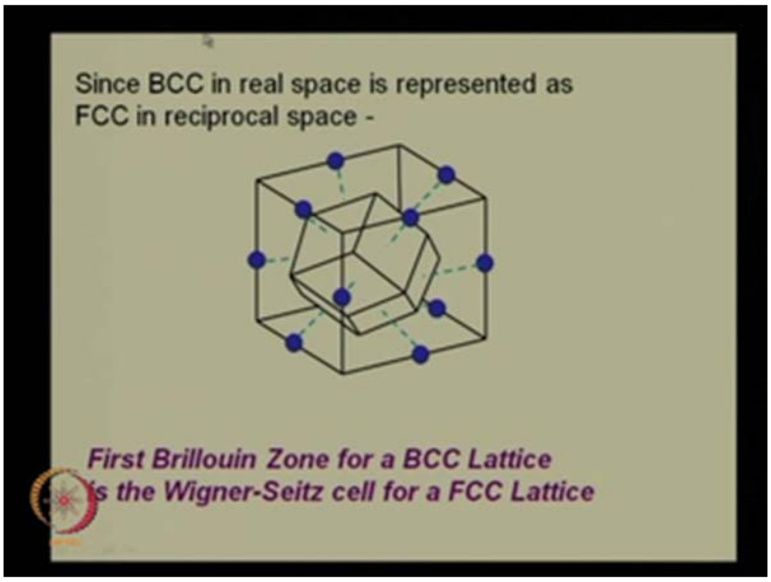

Again the inverse is true when you start with the material that is BCC in real space and so; something that is BCC real space is represented as FCC in reciprocal space. And therefore, the first Brillouin zone for a BCC lattice, where the lattice we are talking of is and real space is the Wigner Seitz cell for a FCC lattice. So, this is something I would like you to I would appreciate I mean I would suggest that you actually exam in this little careful. So, you understand what is happening as the go from one space to the other space and you also understand what is the scope of the each definition and where is said that we are applying the definition. So, if you just follow this things carefully, you should in you will not have a conclusion, you will be able to identify the Wigner Seitz cell correctly, you will also be able to identify the Brillouin zone correctly.

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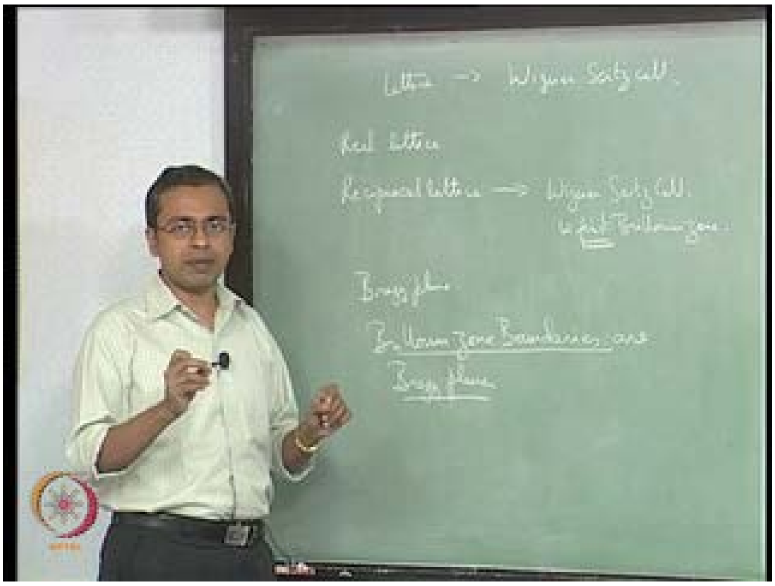

So, this is what we have done. We will now continue or discussion by looking at some other diagrams. So, basically, we have a looked at few things, we have looked at real space real, lattice, we have looked at reciprocal lattice, we have defined; we can say that you know with respect to any lattice, we can defined Wigner Seitz cell.

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Is the, first Brillouin zone. So, Wigner Seitz cell in reciprocal for a reciprocal lattice is the Brillouin zone. So, subsequence Brillouin zones we were able to depict in are two dimensional case. In three dimensions, the concept is exactly the same, the approach we take is exactly the same, the processing we do is exactly the same simply, because it is three dimensions. Instead talking of lines we have planes, and all those plane intersect along lines and show the shape that we identify start beginning to do complicated.

So, I have been able to show you the first Brillouin zone rather clearly. If you look at the second and third Brillouin zone in 3D, it looks rather complicated, but the process is exactly the same. You simply keep looking at identifying planes that bisect the reciprocal lattice vectors to further and further neighbor sort of further and further way. And then you keep identifying, the structures where you cross only one Bragg plane and (( )) further Bragg planes and we have defined what is the Bragg plane. So, based on what we have done so far, we realize that Brillouin zone boundaries (No audio from 24:02 to 24:12) are Bragg planes.

So, we originally defined Bragg plane independently, then we used it and then and that is how defined the Brillouin zones. But now, having defined it, we understand that in any structure when I identify the Brillouin zones effectively all the boundaries of Brillouin zones are Bragg planes. And if it is the n th Brillouin zone, then the boundaries are we have cross n minus 1 Bragg plane, we have not cross the n th Bragg plane so that is all the Brillouin zone is so effectively the Brillouin zone boundaries are Bragg plane. So, this is the very important in information that you should keep in mind.

So, Brillouin zone boundaries are Bragg planes and therefore, we will we will now look at what is the significance of Bragg plane and that therefore, implies the same significance for the Brillouin zone boundary. So, now, as so far we actually you learn all this independently today we are going to a start pulling them together. So, we have already defined what is the Bragg plane, it is a the plane that bisect the vector joining the origin of reciprocal lattice to any reciprocal lattice point so that is the Bragg plane. Once you do all that you have able to identify Brillouin zone and therefore, we identify that we realize now that any Brillouin zone that you look at the boundaries of that Brillouin zone are Bragg planes.

So, if something is happening at the Bragg plane, if I am able to show you that you know if you arrival the Bragg plane certain phenomenon will occur. If I am able to show you that it is simply means that whenever you arrival the boundary of a Brillouin zone that phenomenon will occur because the boundary is the brills Bragg plane so that is the thing you would like to keep in mind. So, now, let us go back to something that we discussed the few classes before where we will and we will begin to see what is the use of a Bragg plane, what is the use of the definition we have got in looked at now and all the discussion we have had so far. So, we looked at the manner in which diffraction occurs in reciprocal space and how it is depicted in reciprocal space. We looked at and we said that you know we use a and evolves spheres construction which in two dimension look like a circle.

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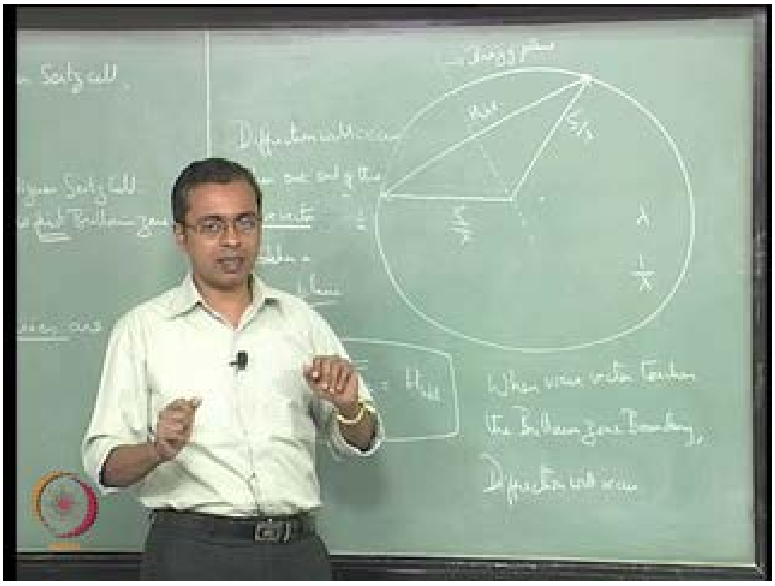

So, basically, we said that you have an origin and you have reciprocal lattice points. And then you can draw on the same; so, this is at some scale, right. So, this is are some scale all this diagrams are made to some scale. On the same scale we will look at a whatever is are radiation we are interested in are wave they are at lamda. So, we will look at 1 by lamba for example, it will it not actually be 1 by lamda, but it is of that it will just to avoid conclusion will assume that this is 1by a and that is 1 by lamda. If you assume that is the case then so, now, we are they drawn to the same scale and they are the same units so, have to speak then we can draw then incident being vector such that it ends at the origin and then we draw sphere or a circle.

And what we said is any time; so, this is s naught by lamda and we said this is s by lamda and we said that the condition for diffraction. We realize, we recognize that the condition for diffraction simply that s by lamda minus s naught by lamda should equal HHKL. So, we immediately see suddenly we have a I mean we already saw this we have reciprocal lattice vector here, a validate reciprocal lattice vector. So, we are saying that for example, if this is the validate point here, this is the validate reciprocal lattice point, this is HHKL. So, this is the discussion we have done if few classes go you can re visited there, but this is basically what construction we had this is the equation we had and that is the plot of that equation that is how it would show upon the figure.

Now, let us look at something we will to relate thus to what we have discussing just immediately; if you look at the figure carefully, what do we have here? The wave length lamda is fixed so that is why we have a circle, circle or sphere. In this case, let us assume the wave length fixed are for a given wavelength we are discussing this, for that wavelength the circle is fixed. Therefore, if it is the circle by definition if you draw any line that intersect the circle at two point the perpendicular bisector to the line will pass through the origin. So, any line that again draw like this if I take the perpendicular bisector of that line it will passing through the origin. So, we will just draw the perpendicular bisector like this.

So, if you draw the perpendicular bisector of any line that connects to any two points within this circle it will pass through the origin. So, what have we got here? This perpendicular bisector here is actually the perpendicular bisector of a validate reciprocal lattice vector the origin is this so the origin is fixed. This is some valid reciprocal lattice vector HKL, I have just drawn the perpendicular bisector to the valid reciprocal lattice vector. And therefore, by our definition this perpendicular bisector is the Bragg plane. So, this is the Bragg plane in two dimension it showing of a line, but it is the plane if you look at a fear it is the it is the plane. So, we already see that definition that we did for some other purpose where we were only looking at the structure is suddenly showing up here where we are talking of diffraction.

So, we see that perpendicular bisector to reciprocal lattice vector passes through the though this point so that is the origin of this circle. But it is not the origin of reciprocal space origin of reciprocal space is sitting here right. So, this is the origin of reciprocal space this is the origin of the circle that circle basically is the defined by the ends of the wave vectors. So, In fact, for this to be true, regardless of how you move this always that bisector would have to go through this particular point, only then going to have diffraction.

So, diffraction another way of saying this is simply that diffraction will occur when one end of the wave vector such the Bragg plane. So, I have just restated definition or rather described in a different way, because we find that this is true. We find that whenever you draw this diagram, whenever this equation a satisfy, which will which then always represent diffraction condition is whenever this equation is satisfied, we find that diagram shows as that if you draw the perpendicular bisector of HKL it will show of going through that point. So, since that is very clearly visible here and no matter how you any lattice point, you take any lattice point, you take which as where this getting satisfied if you draw the client joining the origin to the lattice point that is the validate HHKL you draw the perpendicular bisector it will go through that point. So, therefore, one end of this reciprocal one end of this way vector will always such that Bragg plane.

So, therefore, whenever diffraction occurs one end of the way vector will (( )) Bragg plane. So, we find certainly that you know definition that we only made with respect to the reciprocal lattice. We were not that point we were not in any way associating the definition with any radiation arriving that on the sample, any wave that are in the sample nothing, it was simply a structure in that we put in place in reciprocal space. We just said that you draw vectors you take perpendicular bisector that is it. And that help does come up with Wigner Seitz cell the help (( )) in reciprocal lattice we identified them a Brillouin zones. So, we find that when diffraction occurs when one end of the way vector touches a Bragg plane. Therefore, diffraction occurs whenever the way vector touches the Brillouin zone boundary.

Because we defined that Brillouin zone boundaries are Bragg plane, this definition we; so this are all independently done, independently we have there is no contour verse on this now. We independently know that this is the definition and independently we find that whenever the wave vector touches the Bragg plane diffraction occurs. Therefore, whenever the wave vector touches the Brillouin zone diffraction occurs.

So, we have now in linked up couple of different features here. The way vector here is something that has got to do with the waves that are arriving at the sample or are in the sample for we will regard as where they arrived from. So, they are they could be electron beam related waves x ray anything, they are waves electromagnetic waves that are in that are now interacting with that sample. So, there are there could be any number of reason which affect the wave length of that radiation or wave length of those waves so that is an independent process. What is the wave length of those wave is something that is an independent process and independent phenomenon. Given that those that you have a certain set of waves, we find the defect the Bragg plane and Brillouin zone and such ask specific to that lattice.

So, these are two separate thing Bragg plane is something that has got to do with the material, the Bragg plane and the Brillouin zone and such are aspect of associated with the material so that is an independent aspect. So, you have a sample, it has a lattice, it has the reciprocal lattice, it has a Brillouin zone. So, those that is the relationship there so that is one piece of information. Another piece of information is waves that are arriving at the sample or are in the sample. So, there are wave vectors with respect to that wave. So, this is something associated with the wave, this is something associated the sample, this is what you have what you have return here is the interaction of that wave with that sample and we find that whenever that wave vector such as Bragg plane or therefore, whenever the wave vector such as Brillouin zone diffraction occur.

So, this is the principle idea that we have actually narrow down to. So, this is the principle concept that we have narrow down to we will learn several different thing we needed to learn a several different thing to come here but in the process we have been able to narrow down to this. So, this is the very useful information. So, we will now take this one single line of a information with us, which is that when the wave vector such as the Brillouin zone boundary diffraction will occur. So, when wave vector.

(No audio from 35:19 to 35:47)

So, this is something that we have done. Now, what we will do? So, this is the single line information that we are concluding from all the discussion that we have had, we will keep this mind. We need to now look we already understand the sample has some structure associated with it.

We also looked at the realistic wave of them indicating the potential of that exist in the sample as you remove across the sample or a that is experience by an electron it moves across the sample. What we would like to do is given that we understand this now this idea, that we accept this idea. We would like to see, what are the waves that could be in the sample and therefore, what is the interaction that could occur. So, we know this can this interaction will occur. So, we just have to understand what are the waves in the sample are and given that the sample has the certain crystal structure we can then understand the interaction. So, to do that we will take a step back and then look at simply what are the waves an also lets understand the scale of thing that we are talking on because that is that is how that is diagram will get understood.

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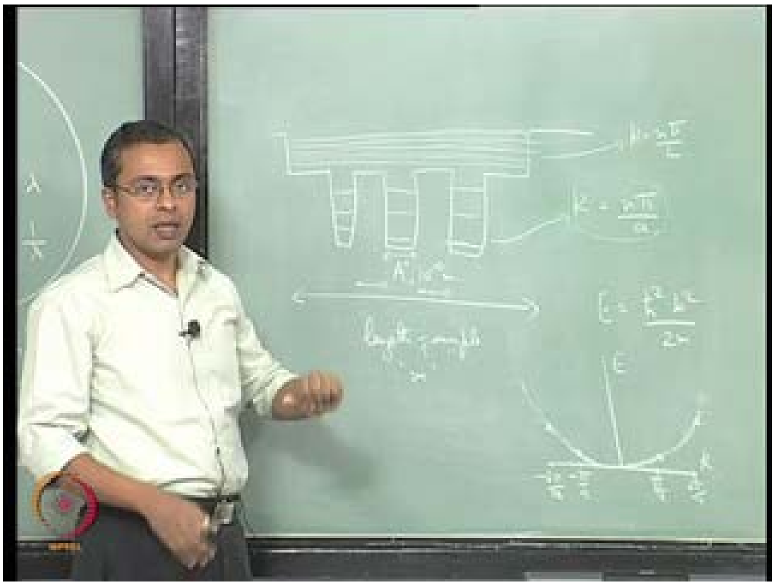

So, we found that when you have actually some dimension a, within which an electron is confine then allowed values of k or n pi by a because of the confinement, this is something that we found. That k allowed values of k are n pi by a. Now, we also noted that you know in this sample that we are dealing with there is two levels of confinement. We have this is the length of the sample, let just say one dimension, so we talk of length length of sample could be of the order of meters, this is the width of that ionic core, this is of the order of Armstrong or 10 power minus 10 meters.

Now, information in reciprocal lattice, reciprocal lattice layout is something that is in Armstrong inverse. So, it is; so, the scale is like that. So, we will just say. So, we also said that you know you can have electrons that are confine here or you can have electron that are confine here. Right in both cases, it is n pi the wave vectors allowed are n pi by the at the length are the dimension associated the length as the extend of length of that in that particular direction. So, in this case, it is k is n pi by a, in this case it is case n pi by L. Now, clearly L is very very large relative to a, there is the factor of 10 power 10. So, clearly there is the big difference between L and a. L is of the order of a meters, this is 10 powers minus 10 meters. So, when you look at the same scale so, in the same scale this is 10 power, this is the very small number, n is the very small number. So, therefore, 1 by a is the very large number so, this k vectors here r is when you go is the step of k vectors here are large.

So, this is n times large number. So, n plus one times are large number would be again large number. So, the spacing between the k vectors allowed k vectors. In this case is large the spacing between the allowed k vector is small so that is why even in this figure you can see this is the last spacing. I mean of course, this only as a indicate on I have indicator, I have show when you in principle the several several orders of magnitude difference between the a spacing of the allowed energy levels here, relative to the allowed energy levels here.

Now, we also said that energy is the h bar square k square by 2 m. And I said that you know for a free electron all possible values of k are allowed therefore, you get a parabola so, e verses k becomes the parabola for a truly free electron. For a electron that is confined based on it is confinement you will actually have only allowed values of k. The relationship would still hold, but only are specific values you can have a allowed value of energy. So, suddenly only these particular values of energy are allowed. So, this is whatever pi by a, this is 2 pi by a and so on, minus pi by this would represent the direction minus 2 pi by a. So, now, only allowed values of energy are allowed are permitted therefore, these values are not allowed. But the form is still going to be parabolic if you connect the point it looks parabolic. So, therefore, what is the parabola for a free electron?

From that parabola only specific values remain which are now allowed once you confine that electron to some location. The point you have to understand is the difference between these two levels of confinement. Now, this is n pi by a so, n pi by a source of here I said that is L is the very large number. So, the phenomenon still true one you once you confine it two distance L. In principle, exactly, the something is hole going to hole two that is what is the continuous parabola we is no longer going to be permitted, instead you are going to have only specific point along the parabola that are allowed. Only difference is since L is very large those specific points are actually very very close. On this scale when drawn to this scale when drawn to this scale pi by L is the extremely tiny number. So, you will have several points of n pi by L permitted before you arrival pi by a.

That is all saying, that you going to have several points of pi by L if you draw it is to this scale so that is go, that is what is going to happen. So, in other words if both this information are shown the same plot you will find that n pi by L or x huge number of tiny points which appear between this point and this point. In fact, they are going to go they are going to be. So, close that on this scale it will look like a straight line, it look like a continuous line, not a straight line, continuous curve; it look like a continuous curve. It will not appear like discrete set of points.

But it is only; that is only a impression that is their it is simply because that is the scale of the diagram. So, our reason by we are saying doing this is that the crystal structure is defined by the location of this ionic course. So, therefore, the crystal structure is all also of that order of spacing. So, the reciprocal lattice is defined by this spacing. We want to know the impact of this spacing are this periodic arrangement on the wave like behavior of the electrons that of confined by the length of the sample. These are the nearly free, they are the electron that running across the sample, they are the electrons that helpers understand the electrical behavior of material or obvious or the; or several property of the material or in fact directly by this nearly free electron which are running across the length of the sample.

The issue that we have not accounted for so far was we never bother about the structure when we simply said the number of free electrons for unit volume. We treated these nearly free electrons as though they were not affected by the presence of this periodic structure. What we now recognizes there is the wave vector associated with this nearly free electron. Those wave vectors are given by allowed wave vectors are given by allowed wave vectors are given by this information here. Those allowed wave vectors can and will interact with the periodic structure that is the defined by these location. So, in other words this is this location. So, what really need is we need are reciprocal lattice depiction of this structure. In that reciprocal lattice depiction of the structure, we will plot the allowed wave vector of this electron. And from what we have understood so far, what we have looked at so far, what will find is when the wave vector of these electrons such as the Brillouin zone of the structure defined by this spacing here diffraction will occur so that is the key idea.

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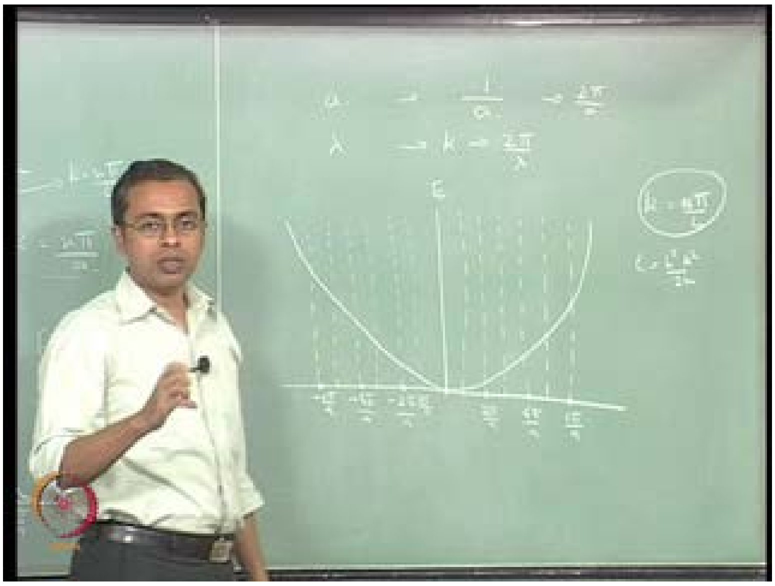

So, for example, we will we will just say that we have a real lattice of spacing a, linear single one dimensional lattice of spacing a, and therefore, we can represent it as a reciprocal lattice of spacing one by a. Only thing will do now is one small additional thing we will do here just to keep us in the same scale. Remember, we have to draw things to the same scale only then we can actually we look at the phenomena. If they are want to two different scale, we cannot look at them, look at a phenomenon phenomena on the diagram.

Normally, when something is lamda wave vector wave length is lamda, we have been representing it as k which is two pi by lamda. So, we have got a multiplicate and factor there is simply a constant, the constant is simply a scaling factor. So, therefore, it is not something that is affecting the us phenomenon any significant by it simply a scaling factor 2 pi by lambda. So, therefore, something that is lamda in real space is being represented as 2 pi by lamda in k space. So, therefore, in the same way what is a? Should not simply represented as 1 by a, it should actually represented as 2 pi by a, only then we can actually, compare the information we are looking.

So, if you keep that mind and now will draw the diagram we have a look some origin here, and we have the distance marked around here. So, therefore, we can we can say that you know we will have two pi by a as the reciprocal lattice vector 2 pi by a minus 2 pi by a then we have 4 pi by a 6 pi by a and so on.

(No audio from 47:00 to 47:11) So, notice carefully what we have done? We have taken a real lattice a, it is represents; it is being represented in reciprocal space as 1 by a. We are actually trying to represent all this information not just in the reciprocal space, but in case space. Case space as a scaling factor of 2 pi so, we have multiplied with 2 pie. So, instead of representing the lattice points at one by a we are representing the lattice point in 2 pi by a, unit of multiples of 2 pi by a. So, we have now got on this board here, the reciprocal lattice representation of the lattice linear lattice of spacing a.

Now, for this reciprocal lattice, where are the Bragg plane, what is the Brillouin zone? The Bragg planes are simply the perpendicular bisector of the vector joining the origin to this points so, they are simply at all these location. You have a Bragg plane at minus pi by a, because that will bisect this point. Another Bragg plane at 2 pi by a because at bisect the four pi by a point and so on. So, for at every n pi by a, you will have a Bragg plane, because at every 2 n pi by a, you do have a lattice vector, valid reciprocal lattice vector. So, we will have Bragg planes at every end pi by a, because at every 2 n pi by a we have valid reciprocal lattice vectors. So, these are all Bragg plane, therefore, these are all Brillouin zones.

So, we have a the first Brillouin zone view cross you do not cross any Bragg plane you are within this region this is the first Brillouin zone between here and here and here and here is the second Brillouin zone between here and here and here and here is the third Brillouin zone and so on. Now, on this plot we can make a plot of the allowed values of wave vector that the electron is sorted to have. So, the electron is allowed to have 2 pi by; actually, the wave vectors allowed for the electron are n pi by L.

So, drawn to this scale because a is very large, you will have several values of n pi by L between 0 and pi by a, because L is a very large number, a is the very small number we discuss that therefore, pi by a is the very large number which what is here or up to here and pi by L is the very small number. So, you will have several points between the symbols. So, on this scale, when you when you plot, when you have this rule that k the allowed values of k are this is energy allowed values of k are n pi by L and e equals h bar square k square by 2 m. What you get is? You will get a parabola, it look like a parabola like that. Now, these are all; this is the plot of h bar square k square by 2 m where the only allowed valued of k or n pi by L except that these are very closely space values.

So, it is actually not a continuous parabola this is the series of points, except there are 1000 of; I mean not just 1000, the several orders of magnitude of point between this two locations. So, for in our scale, it looks like a continuous plot, looks like a continuous curve and therefore, this is how it look. So, we have no got all the information here of our system, we have got the reciprocal lattice spacing of it, we have got the in represented in case space, we have got the Brillouin zone of that sample identify and we have plotted all the allowed values of the energy values that are currently allowed in the system simply because that is how the energies allowed associated with the k vector.

So, will conclude by saying that what is going to happen is we have already seen that when the k vector such as the Brillouin zone boundary diffraction occurs. Because diffraction occurs what; So, therefore, diffraction is occurring at all of these locations. At all of these location, we have got, we have put all the information together that all of the location the k vector is touching the boundary of a Brillouin zone. So, therefore, at all of these location diffraction is occurring. And wherever diffraction occurs it turns out that certain level of a energy values are for become forbidden.

So, therefore, at Brillouin zone boundaries this e verses k relationship begins to distort. And this, it is the result of this distortion that result in the bans structure of the material. Right now, I am saying that in the general sense what we will do in our next classes. We will examine this interaction little; we will start with this diagram will examine in the interaction little more carefully. And we will see that the interaction results in gaps in energy which are now forbidden for the system and therefore, that results that translate to the ban gap that we are more familiar with. And we will analyze that in a greater detail and understand how that happen and what is the extend of that interaction, what is the extend of the gap. And that would complete that would significantly improve our sense and feel for the material and it is properties and would incorporate most of the features of the material in to that feature. With that we halt for today. Thank you.