Introduction to Reciprocal Space

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Lecture -7
Brillouin Zones, Diffraction and allowed energy levels

In the last few classes we have looked at the reciprocal space. We have looked at how real space and reciprocal space are related. We looked at what is a reciprocal lattice, how you would create a reciprocal lattice for a given real lattice. So, and then we recognize that you know, in we can think of certain types of structures that we called the Wigner Seitz cell which basically was defined as the region in space which is closest to a lattice point. Than to any other lattice point okay.

So, it is a region in space that is closest 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 define what is called a Bragg plane which we said this a perpendicular bisector of any vector that connects the origin to valid reciprocal lattice point.

Then we looked at the reciprocal lattice and we found that the Wigner Seitz cell about a reciprocal lattice point simply consists of a series of planes are about that lattice point which are all Bragg planes. And this was then defined as the Brillouin zone, the 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 plane okay.

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 planes and not more than two Bragg planes. So, in that context we made some diagrams on the board, we will start by simply repeating the two-dimensional version of this discussion because that will lead us very well into the three dimensions.

Basically, we are right now discussing the Brillouin zones, we are just looking at structures trying to understand that given a structure, what is the Brillouin zone? That we can, what are the set of Brillouin zones? that we can define or How will we define the Brillouin zones for that structure? So that is the exercise we are currently involved in, we will eventually use this information to understand the property of a material that is a step.

That we will see later in this class okay. So right now, the next few slides that you are going to see are simply how you would define a Brillouin zone for a two-dimensional structure and for the three-dimensional structure.

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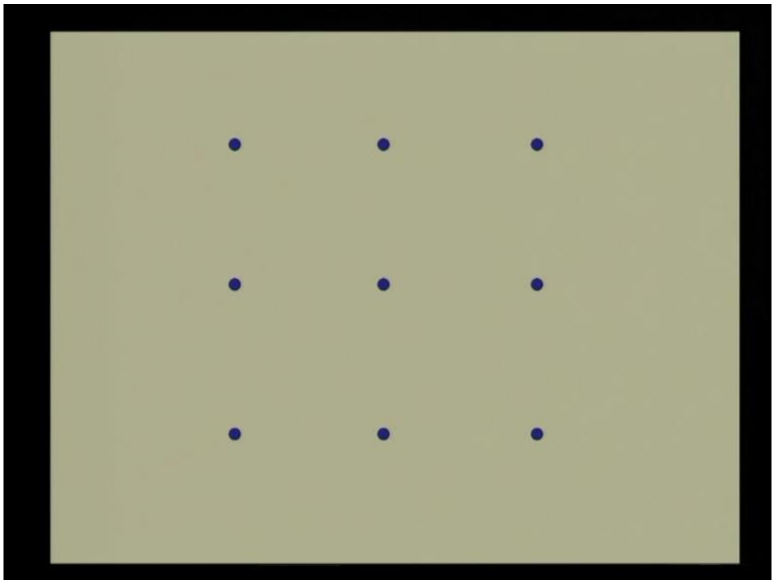

So here we are we will repeat the exercise that we did on the board with an array of points on the slide. So, we have here a 3 by 3 set of point’s, three points there, three points here and then three points here. So, we start here, we will assume that the central point here is the origin and these are all the their neighbours for those, for the central point and of course this is a very large lattice.

We have simply taken a very small region in that lattice, so this is, that is why we only have three points by three points. In principle, we would have much more than three points, we will have points on either side of them extending in all directions right, so in this situation if you now identify the nearest neighbours.

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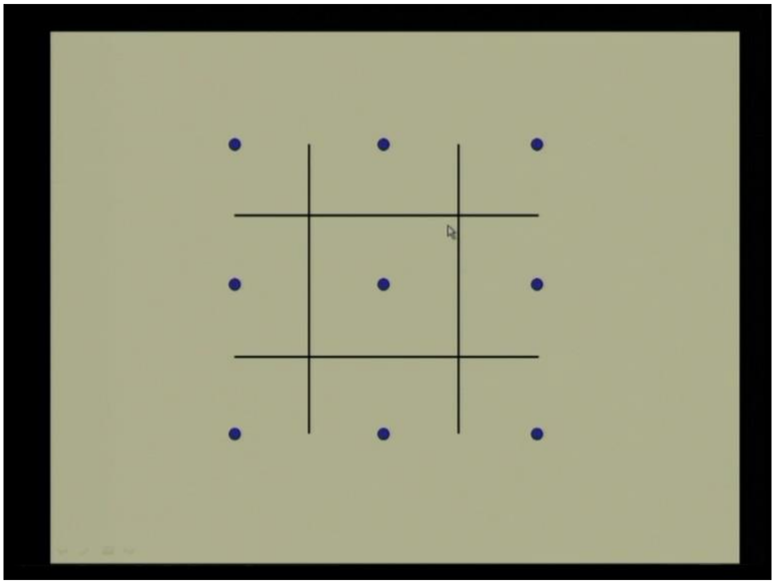

Nearest neighbours are these one two three and four, so with respect to these nearest neighbours we can draw the perpendicular, we can draw vectors to those nearest neighbours and then draw perpendicular bisectors to those vectors. So, a perpendicular bisector would appear here, would appear there, appear there and appear here okay.

So that is basically what you will see. So, these are lines that perpendicularly bisect the vectors joining this origin to all its immediately near neighbouring lattice points okay. So that is one set of such a bisectors we will continue the exercise, we will get another set of bisectors based on lines that connect this point to its next near a set of neighbours which are here right.

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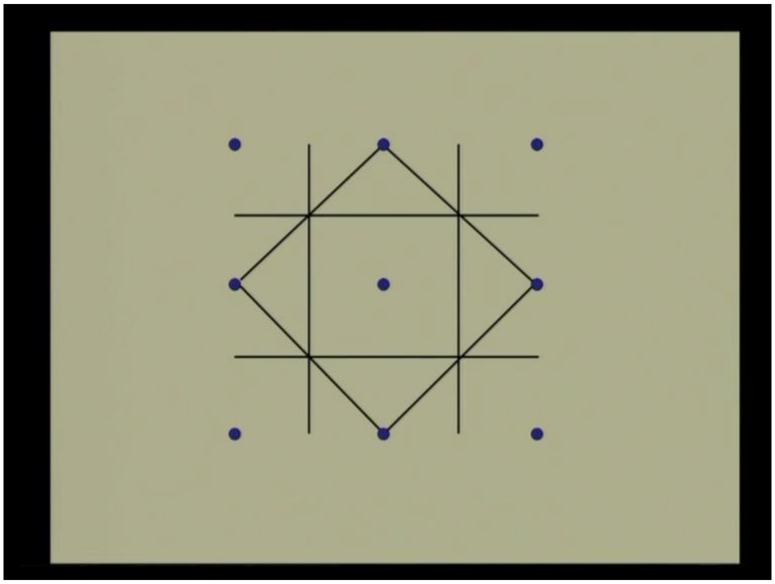

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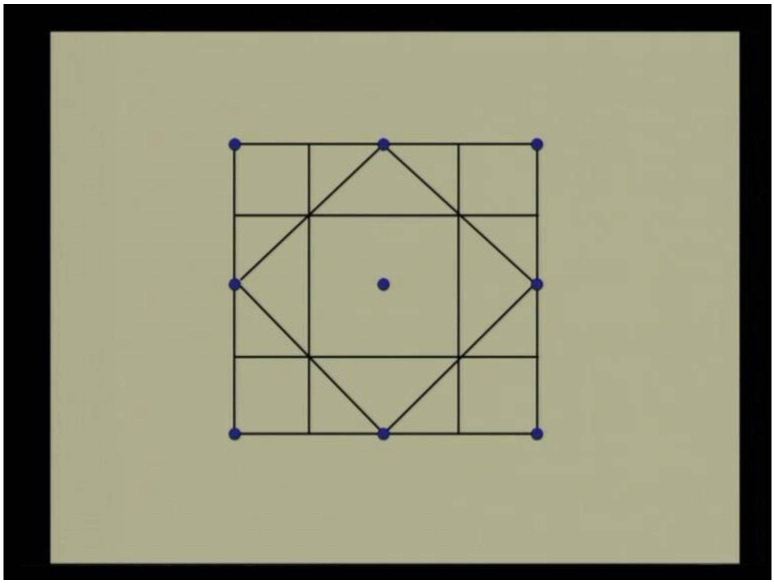

So, this is what we would do then the third set of nearest neighbours would actually be points along this line but further away in fact the next lattice point. Therefore, a line going through these lattice points would then constitute the line that perpendicularly bisects that vector. So, the next set of perpendicular bisectors will appear here and continuing that exercise if you actually look at the points that we have we would have one more point here, one more lattice point here.

So, we can think of a line joining that lattice point and the origin and therefore we would we can expect that there would be a perpendicular bisector somewhere here. Similarly, there is another lattice point further down here and therefore again we can draw a vector to the origin from that lattice point and naturally we can expect the perpendicular bisector to that somewhere there drawn like that okay.

So, taking the next set of neighbours together we have another set of perpendicular bisectors we would do this all around that origin. So, in all four directions around the origin we get it and so we find lines like this, so having got this array of perpendicular bisectors to lines joining the origin to all its nearing, all the neighbours around the central lattice point.

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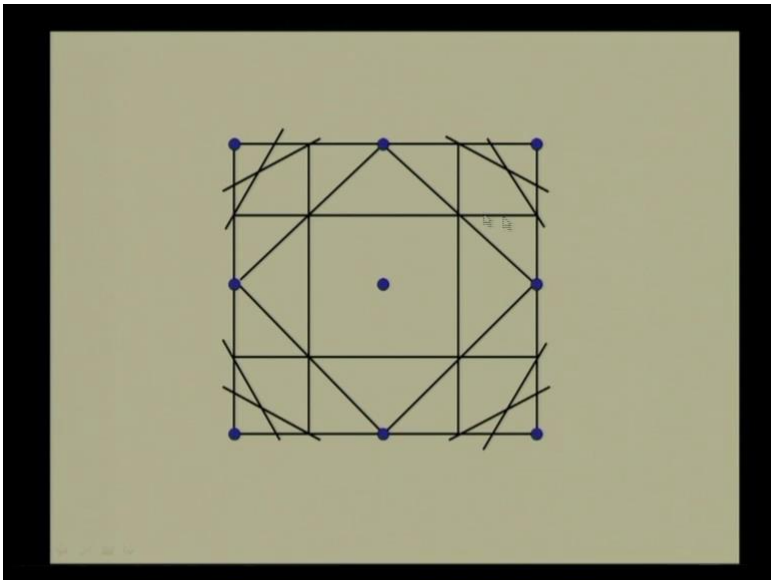

We can now identify Brillouin zones based on the definition we have given for Brillouin zones. Which is basically that the first Brillouin zone is the region in space around this point which can be reached from this point without crossing a single Bragg plane and therefore that would be the region that is identified here okay. So, this region around this point is therefore the first Brillouin zone.

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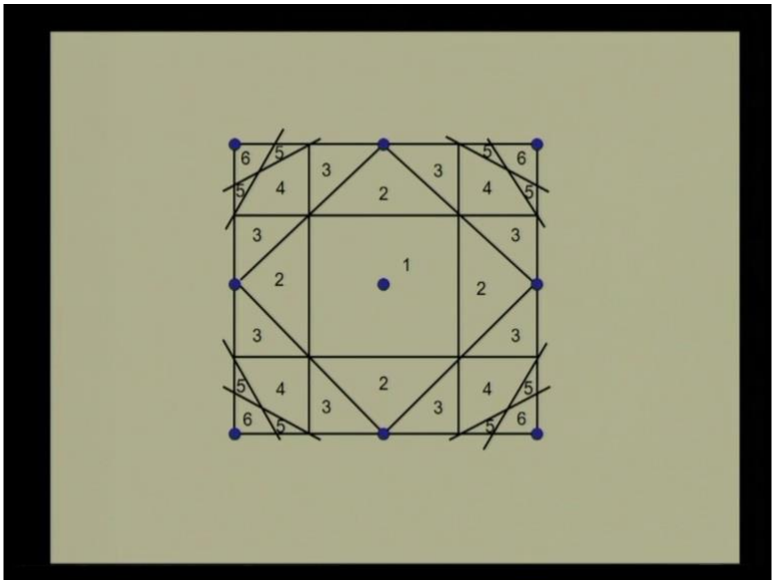

If you cross one Bragg plane but you do not cross a second Bragg plane then that region is a second Brillouin zone. We find around this point several locations where this is true. So, this is one region where this is true, you have crossed one Bragg plane to get into this region but you have not crossed further Bragg planes right.

And all these perpendicular bisectors are the Bragg planes by the definition that we have given them. So, we crossed one Bragg plane, we did not cross the second Bragg plane, so this is the this belongs to the second Brillouin zone. But there is another region here which also belongs to the second Brillouin zone for exactly the same definition because it fits the same definition.

This is another such region and this is another such 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 have now cross two Bragg planes and you do not cross the third Bragg plane that would put you in this region that would then be the third Brillouin zone.

And there are several such locations where you would effectively be accessing the third Brillouin zone. So, these are all the third Brillouin zone. If you continue the exercise further in exactly the same manner we can identify the fourth Brillouin as those four locations or at least those locations that you see there.

And then you again you continue this process you at least within the context of the figure we have drawn this is then the fifth Brillouin zone and this is finally the sixth Brillouin zone okay. So, for a simple two-dimensional array of square array of points where we only taken just three points on our screen a 3 by 3 matrix of points, so we only have nine points on screen.

We have been I able to identify for this lattice, all the Bragg planes and therefore all the Brillouin zones okay. 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 that would have a lattice in real space using the standard conventions for how 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 identified the Bragg planes. Using the convention of, using the definition of what is a Brillouin zone of what is the nth Brillouin zone, we will identify the nth Brillouin zone.

So, the nth Brillouin zone requires you to cross n -1 Bragg planes but restricts you and prevents you from crossing the nth Bragg plane. So, between the n - 1 and the nth Bragg plane, you have the Brillouin zone okay.

So, this is something that we have seen in two dimensions, we will now extend this into a couple of structures in three dimensions, especially, structures that we most commonly encounter in material science. The two structures that we will look at are the face centered cubic and the body centered cubic structures okay.

So first we what we will do is, we will simply define what is a Wigner Seitz cell for a body centered cubic structure? And what is the Wigner Seitz cell for a face centered cubic structure? So, this is; we will discuss it only as a Wigner Seitz cell at this point, which means there is no real reference to reciprocal lattice at this point. So, we will do this exercise and then we will consider what the consequences are with respect to identifying a Brillouin zone.

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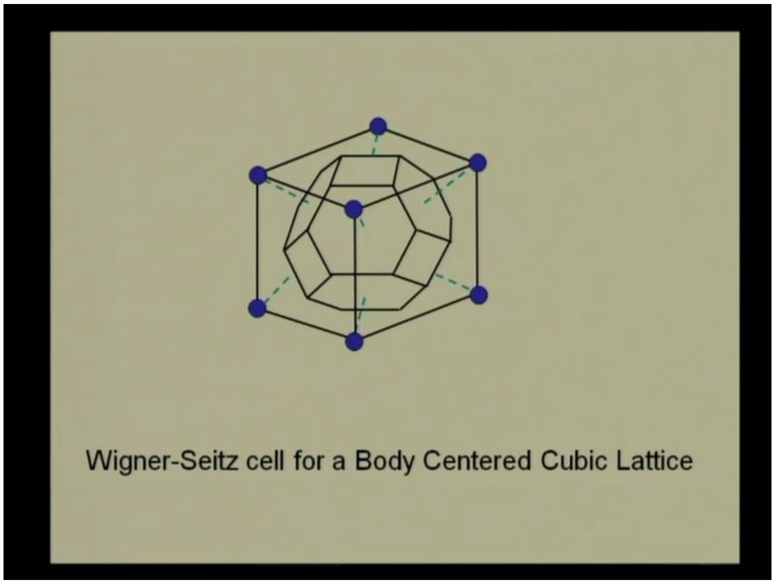

So, if you look at a body centered cubic lattice which is sort of what is, which is basically, what is shown here please ignore the figure in the middle for the moment. So, what we have here is we have four atoms of the corners or four lattice points, we will only talk of lattice points. So, four lattice points at the corners and there are four more 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 defines the body centered cubic structure right. So now the given this body centered cubic lattice the process of identifying a Wigner Seitz cell is really straight forward. The definition that we used we simply extended to three dimensions. So, we take the central atom which is not being shown here and we connect it to all its neighbours okay.

So, for example using these dotted green lines, dashed green lines we have connected the central atom to these all the atoms that are around it. Having done that we draw the perpendicular bisectors to those lines. So those are vectors that join the origin to the points that are arranged around at origin or around the body center and then we simply take perpendicular bisector to those points.

What we will, what happens is since it is a three-dimensional structure that we are looking at, the perpendicular bisectors are planes okay. So, there is a large plane that is perpendicularly bisecting this region. And so, for example this plane here this hexagon that you see here bisects the line that joins this particular atom to the atom at the center okay. It is actually a plane which is, in which as, which is in principle has infinite dimensions.

I mean it is infinitely long in both in both the directions, but the part of it that belongs to the that identifies the Brillouin zone is where it, if it comes in, where it intersects the plane that bisects the line joining this atom to the center right. So, we can take, we can draw several such planes for every two atoms that every two I am sorry two lattice points that you can identify in the structure.

You can identify a plane which bisects the line connecting those two lattice points, especially with respect to the same origin. So, you will treat the central atom as the origin we keep connecting it to as many atoms around it as 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 as the center most region close to this point.

Which is, which now identifies the region that is closest to the central point than to any other lattice point right. 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 neighbouring body center. So, if you had to continue with this lattice, if you have drawn the next set of lattice points here.

You would have once again found one other body center, so you can connect the body center of this particular single lattice that you are seeing here; unit cell that you are seeing here to the next unit cell. And when you connect this unit cell to the body centers of those two unit cells, the perpendicular bisector of it, will actually be this plane right. Because simply because the body centers are exactly half way into the structure units cell.

So, you go half way into this structure you get to this body center, you go halfway into the next unit cell you get the next body center. Therefore this plane here bisects the line joining those two body centers of which this small section here becomes part of, becomes the surface of the Wigner Seitz cell with respect to this lattice point that is in the middle okay.

So therefore, the shape that you see here is the Wigner Seitz cell for a body centered cubic lattice right. So that is as straight forward as that you are able to imagine what the body center is because it is right in the middle there. You are able to see the atoms here, lattice points here we are able to see the lines joining them, the planes that perpendicularly bisects those lines and therefore and the structure that emerges when all those planes intersect with each other.

So that is the structure that is sitting in the middle. This structure encloses all the points that are closest to that central lattice point than to any of the other lattice points available in this structure okay. 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. We will now look at the Wigner Seitz cell for a face centered cubic lattice.

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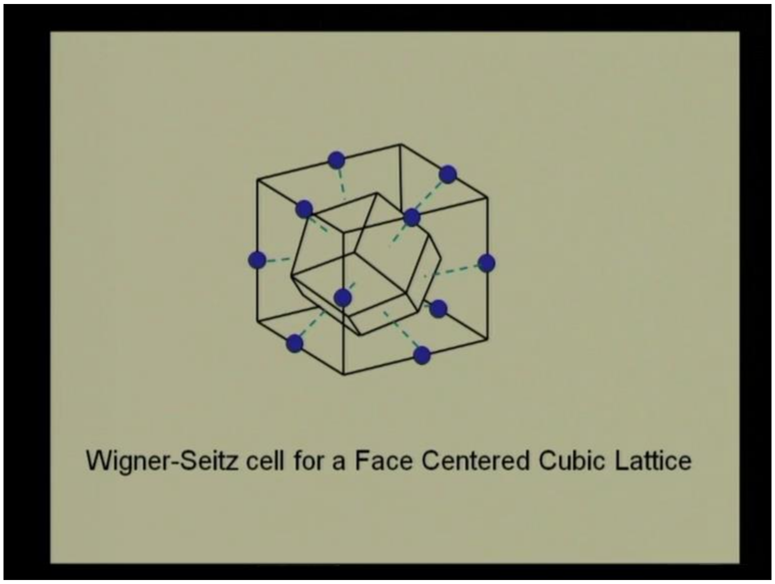

Again, this is still it is just a lattice we are not really specifying anything on whether or not this is in real space or reciprocal space, we will assume it is in real space. And here first thing I want you to pay attention to, is although I have described it here as face centered cubic lattice this is not normally how you would draw a face centered cubic lattice. The set of points that you see here is not normally how you would draw a face centered cubic lattice.

So, for a moment let us first make sure that we are, let us satisfy for ourselves that what we have drawn here is in fact a face centered cubic lattice okay. So that is the exercise we will do immediately and then we will go ahead and use this. What I just tell you what I have done here we will, I will show it to you on the board and then we will get back to this drawing here. What I have actually done is I have taken a face centered cubic.

A unit cell of a face centered cubic lattice and taken only half of it what you see here as the top half is, top half of a face centered cubic lattice and what you see at the bottom is the bottom half of another face is the half of another unit cell okay. So, the lower part of this diagram is the top half of one unit cell and the upper part of this diagram is the bottom half of another unit cell which is above this picture. So, taking those two halves together we have got this unit cell, so I just show that to you on the board before we come back to this diagram.

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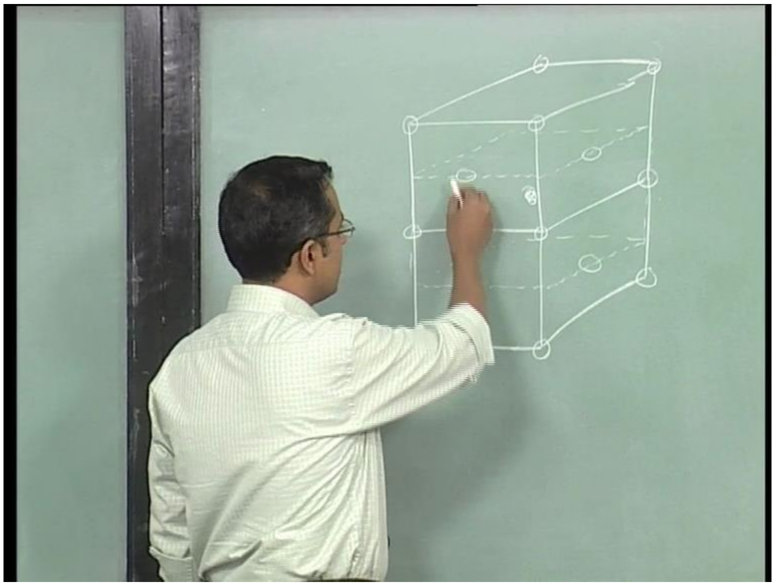

So, what we are drawing here is our two unit cells of the FCC structure, so we will have atoms I am sorry, lattice points at these locations. And these would be the face centers all right. So, we can always imagine as a diagram where we basically take this line here and then look at the unit cell that way.

The reason we would like to do this is because this plane which is between these two unit cells right in the middle of it there is one lattice point that is the face center of this basal plane of this unit cell or the top plane of this other unit cell. So right in the middle there is an atom a 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 things, I mean look at the space around it with respect to all its neighbours. So, this becomes convenient rather than any of the other points as the origin.

So that is the reason why we have chosen this, so therefore you will see, if you do this you will have lattice points in the middle of the diagram on top and at the bottom and at the corners in the middle of the diagram right. So that is basically what you will see in our diagram here at the corners we have lattice points here and in the middle, we have lattice points here.

And the lines that I have drawn here, the straight lines I have drawn here they all go to the middle of this structure which is a plane halfway through this unit cell that we are showing you here. And therefore, that is the face center in fact of the of both these unit cells. So effectively that is the face center of one half of a 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 a face centered cubic lattice diagram. In fact, it is, it is simply a different, which is shifted the diagram by half a unit lattice vector spacing right. So that is all I have done, I have moved down half, so I am getting half of one unit cell and half of another unit cell. Still it totals up to one complete unit cell right.

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 these neighbours, all these neighbouring points and we draw perpendicular bisectors to those vectors. Those perpendicular bisectors are planes and they themselves bump into each other along these lines right. And in the as a result you end up with some structure that is visible here.

So, this structure that you see in the middle here is therefore the Wigner Seitz cell for a face centered cubic lattice okay. So, it is quite clear 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 have also seen in our discussion, is that when you look at the relationship between a lattice in real space and a lattice in reciprocal space. We find that if you have a 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 a couple of classes ago and we were able to see how the vectors would then define a body centered cubic lattice in reciprocal space.

In other words, you start with the face centered, if you have a material that has a face centered cubic structure. When you represent this material in reciprocal lattice notation, it will be represented by a set of points that have the symmetry of a body centered cubic lattice okay.

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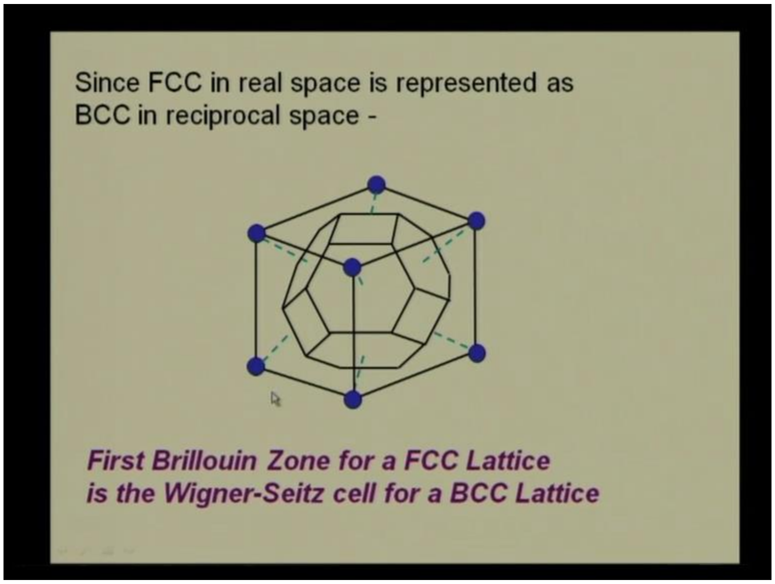

So therefore, if you have a material in real space that is face centered cubic, it is going to be represented as body centered cubic in reciprocal space and we have also defined that the

Brillouin zone, the first Brillouin zone of a structure is simply the Wigner Seitz cell about a reciprocal lattice point okay.

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 okay. So, this occurs because of this inversion. So, you are talking of a face centered cubic lattice which happens to be in real space and since it is represented as a body centered cubic lattice in reciprocal space it is Wigner Seitz cell.

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 okay. So, this is, so this is slightly tricky the first time you encounter it, I suggest that you look at this little bit slowly and carefully. So that you understand what we have done here okay. What we are doing is our definition talks of reciprocal space its talks of reciprocal lattice the Brillouin zone definition.

So therefore, we can only define Brillouin zones, the first Brillouin zone and subsequent Brillouin zones can all be only defined with respect to whatever is the reciprocal lattice. So, whatever happens to be your real lattice in some way shape and form it is going to be represented in reciprocal space as the reciprocal lattice and what you get there as the Brillouin zone is then linked to the real space material.

Is simply stated as that real space lattice has the following Brillouin zone, so FCC becomes BCC and therefore the BCC is Brillouin zone is the FCC's a BCC Wigner Seitz cell is the FCC is Brillouin zone. So therefore, so that is what we are depicting here, again the inverse is true when you start with the material that is BCC in real space and so something that is BCC in 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 in real space is the Wigner Seitz cell for a FCC lattice okay. So, this is something I would like you to, I would appreciate, I mean, I would suggest that you actually examine this little carefully. So, you understand what is happening as you go from one space to the other space.

And you also understand what is the scope of each definition and where is it that we are applying the definition okay. So, if you just follow these things carefully you should not, you will not have a confusion, you will be able to identify the Wigner Seitz cell correctly. You will also be able to identify the Brillouin zones correctly right. So, this is what we have done. We will now continue our discussion by looking at some other diagrams.

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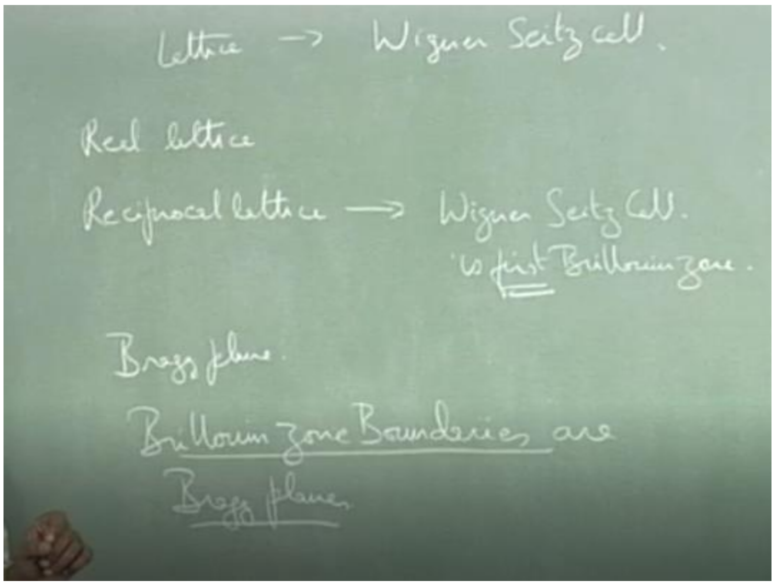

So basically, we have looked at a few things, we have looked at real space real lattice, we have looked at reciprocal lattice, we have defined, we can say that you know, with respect to any lattice we can define Wigner Seitz cell is the first Brillouin zone. The Wigner Seitz cell in reciprocal, for a reciprocal lattice is the first Brillouin zone.

So subsequent Brillouin zones we were able to depict in our 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 of talking of lines we have planes and all those planes intersect along lines and so the shapes that we identify start beginning to look complicated okay.

So, I have been able to show you the first Brillouin zone rather clearly, if you look at the second and third Brillouin zones 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 neighbours that are further and further away.

And then you keep identifying the structures where you cross only one Bragg plane and moves further Bragg planes. And we have defined what is a Bragg plane? So, based on what we have done so far, we realize that Brillouin zone boundaries are Bragg planes okay. So, we originally define Bragg plane independently then we used it and then and that is how we defined a Brillouin zone.

But now having to find it we understand that in any structure when I identify the Brillouin zones, effectively all the boundaries of those Brillouin zones are Bragg planes. And if it is the nth Brillouin zone then the boundaries are we have crossed n -1 Bragg planes, we have not cross the nth Bragg plane, so that is how the Brillouin zone is. So effectively the Brillouin zone boundaries are Bragg planes.

So, this is a very important information that you should keep in mind okay. So, Brillouin zone boundaries are Bragg planes and therefore we will now look at what is the significance of a Bragg plane and that therefore implies the same significance for the Brillouin zone boundary okay. So now as so far, we have actually learned all these things independently today we are going to start pulling them together.

So, we have already defined what is a Bragg plane? It is the plane that bisects the vector joining the origin of reciprocal lattice to any reciprocal lattice point okay. So that is the Bragg plane, once you do all that you are able to identify Brillouin zones 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 if I am able to show you that you know if you arrive at the Bragg plane, certain phenomenon will occur, if I am able to show you that, it simply means that whenever you arrive at the boundary of a Brillouin zone, that phenomenon will occur because the boundary is the Bragg plane right. So that is the thing we would like to keep in mind.

So now let us go back to something that we discussed a 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 definitions we have got in, had looked at now and all the discussion we have had so far right. So, we looked at the manner in which a diffraction occurs in reciprocal space and how it is depicted in reciprocal space.

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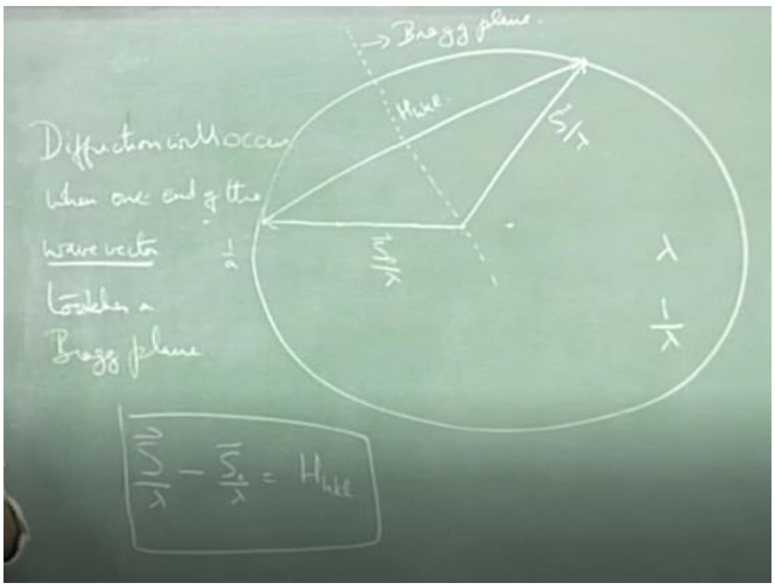

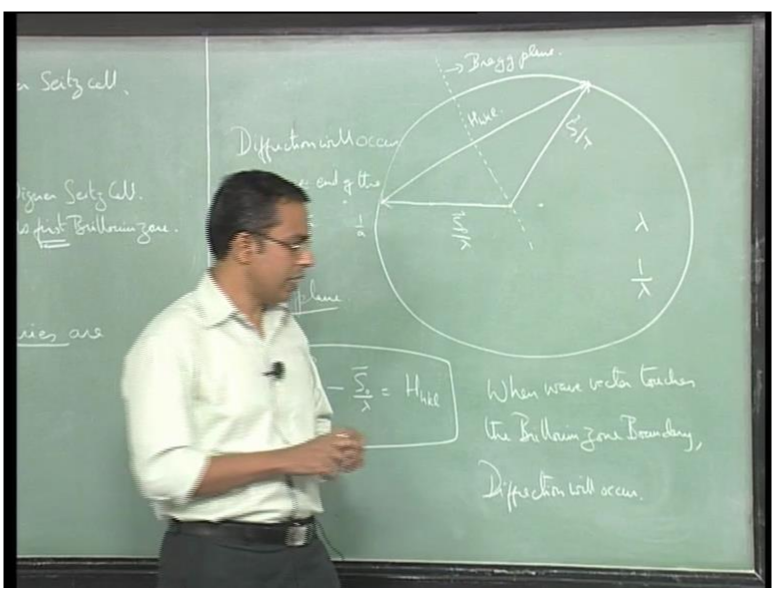

We looked at and we said that you know we use an Ewald sphere construction which in two dimensions looks like a circle. So basically, we said that you have an origin and you have reciprocal lattice points and then you can draw on the same, so this is a, to some scale right. So, this is at some scale, all these diagrams are made to some scale. On the same scale, we will look at whatever is our radiation we are interested in or waves they are at lambda.

So, we will look at 1 by lambda for example it will not actually be 1 by lambda but it is of that to, just to avoid confusion we will assume that this is one by a and that is 1 by lambda. If you assume that is the case, then so now we are, they are drawn to the same scale and they are the same units so to speak. Then we can draw the incident beam vector such that it ends at the origin and then we draw a sphere or a circle right.

And what we said is anytime, so this is S 0 by lambda and we said this is S by lambda and we said that the condition for the diffraction, we realized we recognize that the condition for diffraction is simply that S by lambda - S 0 by lambda should equal Hhkl okay. So, if we immediately see, suddenly we have a, I mean we already saw this, we have a reciprocal lattice vector here, a valid reciprocal lattice vector all right.

So, we are saying that for example, if this is a valid point here this is a valid reciprocal lattice point this is Hhkl right. So, this is a discussion we have done a few classes ago, you can revisit it 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 up on the figure. Now let us look at something we will relate this to what we have discussed in just immediately.

If you look at this figure carefully, what do we have here, the wavelength lambda is fixed right. So that is why we have a circle okay, circle or a sphere, in this case, let us let us assume the wavelength is fixed or for a given wavelength we are discussing this, for that wavelength the circle is fixed right. Therefore, if it is a circle, by definition if you draw any line a line that intersects the circle at two points.

The perpendicular bisector to that line will pass through the origin right. So, any line that I can draw like this if, I take the perpendicular bisector of that line it will pass through the origin. So, you just draw the perpendicular bisector like this okay. So, if you draw the perpendicular bisector of any line that connects 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 valid reciprocal lattice vector. The origin is this, so the origin is fixed, this is some valid reciprocal lattice vector Hhkl, I have just drawn the perpendicular bisector to that valid reciprocal lattice vector right. And therefore, by our definition this perpendicular bisector is a Bragg plane alright.

So, this is a Bragg plane in two dimensions its showing up as a line but it is a plane, if you look at a sphere it is a plane right. So, we already see that a 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 right. So, we see that a perpendicular bisector to a reciprocal lattice vector passes through the, through this point okay.

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 defined by the ends of the wave vectors okay. 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 right only then you are going to have diffraction alright.

Diffraction another way of saying this is simply that diffraction will occur when one end of the wave vector touches the Bragg plane okay. So, I have just restated the definition or rather described it in a different way because we find that this is true, we find that whenever you draw this diagram, whenever this equation is satisfied which then always represents diffraction condition this is whenever this equation is satisfied.

We find that the diagram shows us that if you draw the perpendicular bisector of Hhkl it will show up going through that point right. So, since that is very clearly visible here and no matter how you, any lattice point you take, which is, where this is getting satisfied if you draw that line joining the origin to that lattice point that is a valid Hhkl, you draw the perpendicular bisector it will go through that point.

So therefore, one end of this reciprocal, I have one end of this wave vector will always touch that Bragg plane. So therefore, whenever diffraction occurs, one end of the wave vector will touch the Bragg plane all right. So, we find suddenly that you know a definition that we only made with respect to the reciprocal lattice. We were not at that point we were not in any way associating this definition with any radiation arriving at that on the sample.

Any waves 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 bisectors that is it, and that helped us come up with Wigner Seitz cell, that help her come in and in reciprocal lattice we identified them as Brillouin zones. So, we find that when diffraction occurs when one end of the wave vector touches a Bragg plane.

Therefore, diffraction occurs whenever the wave vector is a Brillouin zone boundary okay. Because we define that Brillouin zone boundaries are Bragg planes. This definition, we so these are all independently done, independently we are, we have, there is no controversy on this now. We independent we 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 linked up a couple of different features here. The wave vector here is something that has got to do with the waves that are arriving at the sample or are in the sample, for regardless of where they have arrived from okay. So, they are, they could be electron beam, related waves, x-rays anything.

They are waves electromagnetic waves that are in, that are now interacting with the sample. So, there are, there could be any number of reasons which affect the wavelength of that radiation or wavelength of those waves. So that is an independent process, what is the wavelength of those waves is something that is an independent process and independent phenomenon.

Given that you have a certain set of waves, we find the defend the Bragg planes and Brillouin zones and such are specific to that lattice okay. So, these are two separate things. The Bragg plane is something that has got to do with the material the Bragg plane and the Brillouin zone and such are aspects associated with the material okay. So that is an independent aspect.

So, you have a sample, it has a lattice, it has a 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 those waves. So, this is something associated with the wave, this is something associated to the sample.

This is, what you what we have written here is the interaction of that wave with that sample and we find that whenever the wave vector touches a Bragg plane or therefore whenever the wave vector touches the Brillouin zone diffraction occurs okay. So, this is the principal idea that we have actually narrowed down to okay. So, this is the principle concept that we have narrowed down to.

We have learnt several different things, we needed to learn a several different things to come here but in the process, we have been able to narrow down to this alright. So, this is a very useful information, so we will now take this one single line of information with us which is that, when the wave vector touches a Brillouin zone boundary diffraction will occur okay. So, when wave vector okay, so this is something that we have done.

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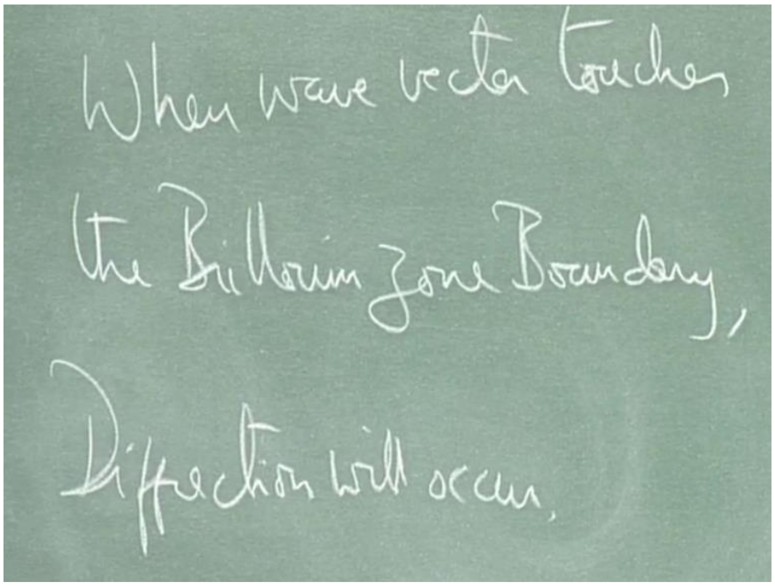

Now what we will do, so this is the single line information that we are concluding from all the discussion that we have had, we will keep this in mind. We need to now look, we already understand that the sample has some structure associated with it. We have also looked at a realistic way of them indicating the potential that exists in the sample.

As you move across the sample or that is experienced by an electron as 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 right. We would like to see what are the waves? That could be in the sample and therefore what is the interaction? That could occur okay. So, we know that this can this interaction will occur so we just have to understand what are the waves in the sample?

And given that the sample has a 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 and also let us understand the scale of things that we are talking off. Because that is how the diagram will get understood alright.

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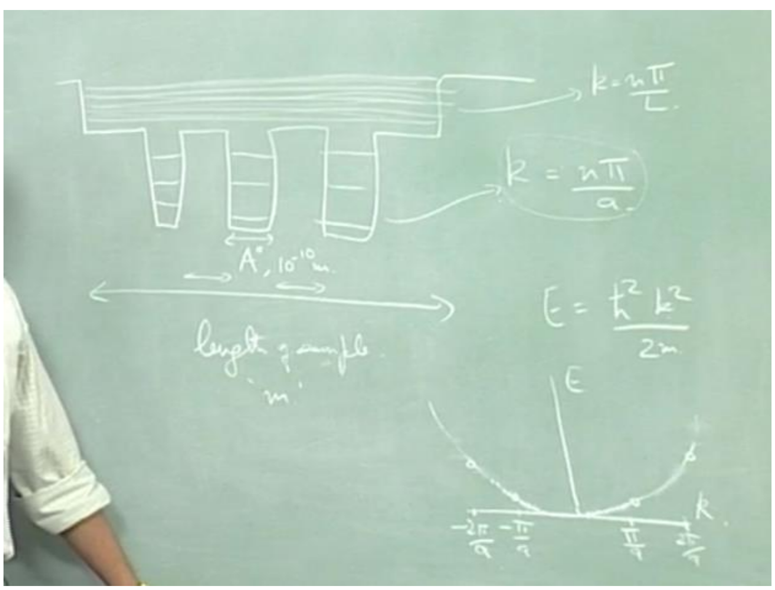

So, we found that when you have actually some dimension a within which an electron is confined then allowed values of k are n pi by a okay, because of the confinement this is something that we found, that k allowed values of k are n pi by a. Now we also noted that you know in these samples that we are dealing with there is two levels of confinement. We have, this is the length of the sample.

Let us just say it is one dimensional, 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 angstroms or 10 power -10 meters okay. Now information in reciprocal lattice, a reciprocal lattice layout is something that is in angstrom inverse okay. So, it is so the scale is like that okay.

So, we will just say, so we also said that you know you can have electrons that are confined here or you can have electrons that are confined here right. In both cases it is n pi, the wave vectors allowed are n pi by the length or the dimension associated the length, the extent of the length of that, in that particular direction right. So, in this case it is k is n pi by a, in this case it is case k is n pi by L.

Now clearly L is very, very large relative to a, there is a factor of 10 power 10. So clearly there is a big difference between L and a, L is of the order of meters, this is 10 power -10 meters. So, when you look at the same scale right, so in the same scale, this is 10 power, this is a very small number, a is a very small number, so therefore 1 by a is a very large number okay, one by a is very large number.

So, this k vectors here are when you go in the steps of k vectors here are large okay. So, this is n times a large number, so n +1 times a large number would be again a large number, so the spacing between the k vectors, allowed k vectors in this case is large. The spacing between the allowed k vectors is small.

So that is why even in this figure, you can see that this is large spacing I mean of course there is only as an indication, indicator I have shown you. In principle that there is several, several orders of magnitude difference between the spacing of the allowed energy levels here, relative to the allowed energy levels here right.

Now we also said that energy is h bar square k square by 2m alright. And I said that you know if for a free electron all possible values of k are allowed therefore you get a parabola. So, E versus k becomes a parabola for a truly free electron, for an electron that is confined based on its confinement, you will actually have only allowed values of k, the relationship would still hold but only at 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 2pi by a and so on, -pi by a, this would represent the direction -2pi 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 points it looked parabolic right. So therefore, what is a 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 shows up here, I said that this L is a very large number, so the phenomenon is still true, once you confine it to a distance in, in principle exactly the same thing is going to hold true.

That is what is a continuous parabola which is no longer going to be permitted instead you are going to have only specific points along the parabola that are allowed, only differences is since L is very large, those specific points are actually very, very close on this scale, when drawn to this scale pi by L is an extremely tiny number, so you will have several points of n pi by L permitted before you arrive at pi by a okay.

That is all we are saying that you are going to have several points of pi by L, if you draw it to this scale, so that is what is going to happen. So, in other words if both this information are shown in the same plot, you will find that n pi by L are its 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 looked like a continuous line not straight line, a continuous curve it looked like a continuous curve, it will not appear like discrete set of points but it is only that is only a impression that is there, it is simply because that is the scale of the diagram okay. So, our, the reason why we are saying doing this is that the crystal structure is defined by the location of this ionic cores okay.

So therefore, the crystal structure is also of that order of spacing. So, the reciprocal lattice is defined by this spacing. We want to know the impact of this spacing or this periodic arrangement on the wave like behaviour of the electrons that are confined by the length of the sample. These are the nearly free electrons they are the electrons that are running across the sample.

They are the electrons that help us understand the electrical behaviour of the material or the, or several properties of the material are impacted directly by these nearly free electrons which are running across the length of the sample. The issue that we had not accounted for, so far worse we never bothered about the structure, when we simply said the number of free electrons per unit volume.

We treated these nearly free electrons as though they were not affected by the presence of these, periodic structure. What we now recognize is, there is a wave vector associated with this, nearly free electrons. Those 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 defined by these locations.

So, in other words these locations, so what we really need? Is we need a reciprocal lattice depiction of this structure. In that reciprocal lattice depiction of the structure, we will plot the allowed wave vectors of this electron. And from what we have understood so far, what we have looked at so far, what we will find is, when the wave vector of these electrons touches the Brillouin zone of the structure defined by this spacing here diffraction will occur okay.

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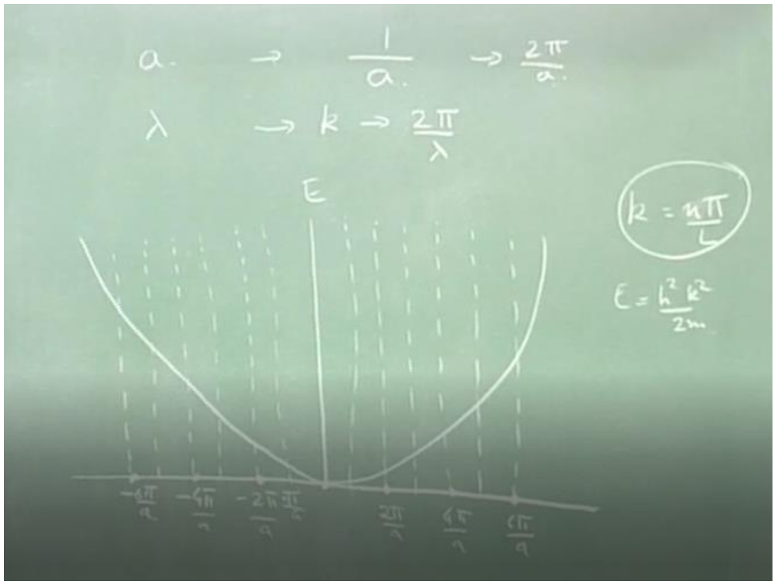

So that is the key idea. So, for example we will we will just say that we have a real lattice of spacing a, a linear single one-dimensional lattice of spacing a and therefore we can represent it as a reciprocal lattice of spacing 1 by a alright. Only thing we will do now is one small additional thing 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 look at the phenomena.

If they are drawn to two different scales, we cannot look at them look at a phenomenon, phenomena on the diagram okay. Normally when something is lambda wave vector, wavelength is lambda, we have been representing it as k which is 2pi by lambda, so we have got a multiplication factor here, it is simply a constant right a constant is simply a scaling factor.

So therefore, it is not something that is affecting the phenomenon in any significant way, it is simply a scaling factor 2pi by lambda. So therefore, something that is lambda in real space is being represented as 2pi by lambda in k space. So therefore, in the same way what is a? Should not simply be represented as 1 by a, it should actually be represented as 2 pi by a.

Only then we can actually, only then we can actually compare the information that we are looking at all right. So, if you keep that in mind and now we will draw the diagram we have a look, some origin here and we have the distance marked around here. So therefore, we can say that you know, we will have 2pi by a, as the reciprocal lattice vector 2pi by a, -2 pi by a, then we will have 4pi by a, 6pi by a and so on.

So, notice carefully what we have done, we have taken a real lattice a, it is representing being represented in reciprocal space as 1 by a. We are actually trying to represent all this information not just in reciprocal space but in k space, k space has a scaling factor of 2pi, so we have multiplied it by 2pi. So instead of representing the lattice points at 1 by a, we are representing the lattice points in 2pi by a, units of multiples of 2pi by a.

So, we have now got on this board here, the reciprocal lattice representation of the lattice, linear lattice of spacing a okay. Now for this reciprocal lattice where are the Bragg planes? What is the Brillouin zone? The Bragg planes are simply the perpendicular bisectors of the vectors joining the origin to these points, so they are simply at all these locations. You will have a Bragg plane at -pi by a because that will bisect this point.

Another Bragg plane at 2pi by a, because that will bisect this 4pi by a point and so on. So, for at every n pi by a, you will have a Bragg plane because at every 2npi by a, you do have a lattice vector a valid reciprocal lattice vector right. So, we will have Bragg planes at every n pi by a, because at every 2npi by a, we have valid reciprocal lattice vectors. So, these are all Bragg planes. Therefore, these are all Brillouin zones okay.

So, we have the first Brillouin zone, you 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 allowed to have right.

So, the electron is allowed to have 2pi by actually, the wave vectors allowed for the electron are n pi by L right. 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 small, very large number, a is a very small number. We just discuss that therefore pi by a, is a very large number which is what is here, up to here and pi by L is a very small number.

So, you have several points between this and this. So, on this scale when you plot when you have this rule that the allowed values of k are n pi by L this is energy allowed values of k are n pi by L and e =h bar square k square by 2m, what you get is, you will get a parabola it look like a parabola like that okay. Now these are all, this is a plot of h bar square k square by 2m.

We are the only valid values of k are n pi by L, except that these are very, very closely spaced values. So, it is actually not a continuous parabola this is a series of points except that there are thousands and I mean not this thousands there are several orders of magnitudes of point between these two locations. So, for in our scale it looks like a continuous plot okay. It looks like a continuous curve and therefore this is how it looks.

So, we have now got all the information here of our system. We have got the reciprocal lattice spacing of it, we have got the, in represented in k space, we have got the Brillouin zones of that sample identified 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 energy is allowed associated to the k vectors.

So, we will conclude by saying that what is going to happen is we have already seen that when the k vector touches the Brillouin zone boundary, diffraction occurs all right because diffraction occurs, what so if therefore diffraction is occurring at all of these locations. At all of these locations we have got, we have put all the information together. So, at all of these locations the k vector is touching the boundary of a Brillouin zone okay.

So therefore, at all of these locations diffraction is occurring and wherever diffraction occurs it turns out, that certain level of energy values are for become forbidden all right. So therefore, at Brillouin zone boundaries this E versus k relationship begins to distort okay. And this, it is a result of this distortion that results in the band structure of the material okay.

Right now, I am saying that in the general sense, what we will do in our next class? We will examine this interaction little, we will start with this diagram we will examine this interaction little bit 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 translates to the band gap that we are more familiar with okay.

And we will we will analyze that in a greater detail and I understand how that happens and what is the extent of that interaction? What is the extent of the gap? And that would complete, that would significantly improve our sense and feel for the material and its properties and will incorporate most of the features of the material into that picture okay. So, with that will halt for today. Thank you