Optoelectronic Materials and Devices

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Module - 01
Lecture - 05
Reciprocal Lattice I I Brillouin Zone and Bragg's Diffraction Condition

So welcome to lecture number 5. Now, let us go back to first lecture, we were working on reciprocal lattice, I will repeat what we said yesterday one more time in the beginning.

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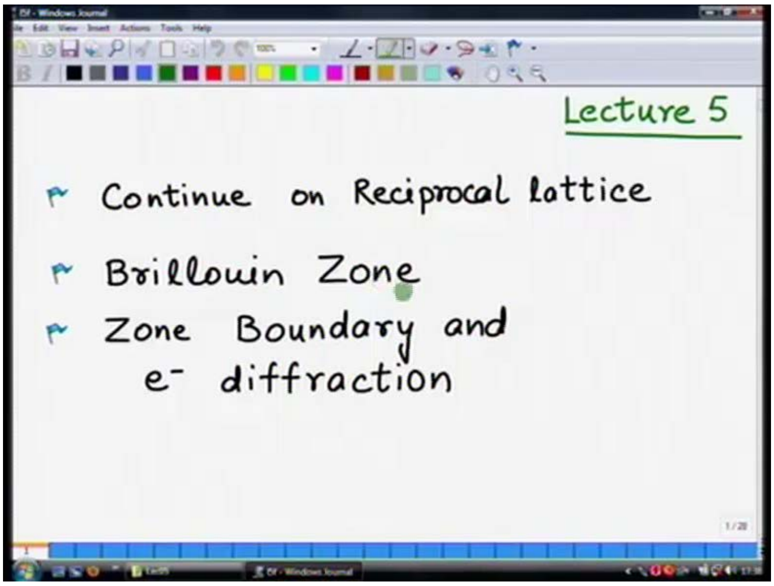

So, today's topics are first thing we will cover, is continue on this reciprocal lattice business and finish it off, I will show you reciprocal lattice is for simple cubic body centered cubic and face centered cubic. Following that, I am going to then come to the main thing which I will, which I was making this reciprocal lattice which is I will show you the Brillouin zones or the first Brillouin zone at least I will show you.

This Brillouin zone construction is something very similar I mentioned that in a while doing crystal structure crystal lattices. I mentioned that this Wigners itself though not use often in a direct lattices. But, it has a great utility in reciprocal lattices and that is really what that construction will be in brillouin zone. So, that we will do today and then why we are doing Brillouin zone something very interesting will happen on the zone boundaries on the zone boundary Brillouin zone. Something will happen and that is related to electron diffraction and therefore, in electron or wave which conducts because which conduction happens therefore, something will happen to that. So, those are three things topics which will be covered today.

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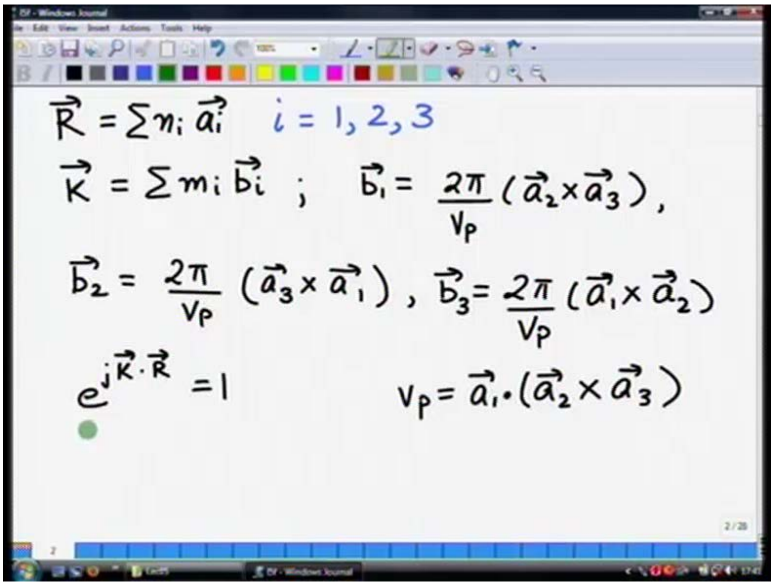

So, let us recall what we did in lecture number four, we said that if a 1 a 2 and a 3 are if a 1 is 1 comma 2 comma 3; that means, if I have three primitive lattice vectors a 1 a 2 and a 3 then any lattice point any lattice point direct lattice can be generated by this vector r. This can be used by the integer values of n 1 n 2 and n 3 multiplied by this lattice primitive lattice vectors. So, we can locate any lattice point on any with this vector r. So, R represents the lattice points if that is. So, then we defined another vector this way initially we just defined it that consider there is vector like this then we decide decided then we will call b 1 define b 1 like this b 2 like this expression.

Here, b 3 like this here and where V p was the volume of the primitive cell in direct lattice. The real lattice where the lattice points are ranged, so those in that lattice and I will use that word direct lattice for it as a reciprocal lattice I will. So, that is the volume, so that volume can if I have 3 vectors a 1 a 2 a 3 defining the primitive cell then the volume of that primitive cell can simply be taken as a scalar product this scalar product here. So, that is the volume of the primitive cell, now we said that the way I have chosen this K is that I want that it part j capital K dot R should become equal to 1 and you can notice that if you substitute this K and R.

Then, what will you get if you substitute in their K and R you can prove that this indeed is equal to 1 for this particular values of k. So, these values of k will substituted in will give you this 1 and this is what we had done an admonition that this then gives you in reciprocal space. This allows you for you can do a for your analysis of any electron wave a, if there is a periodicity in direct lattice, then these are good for your analysis, but that is not what we want do really.

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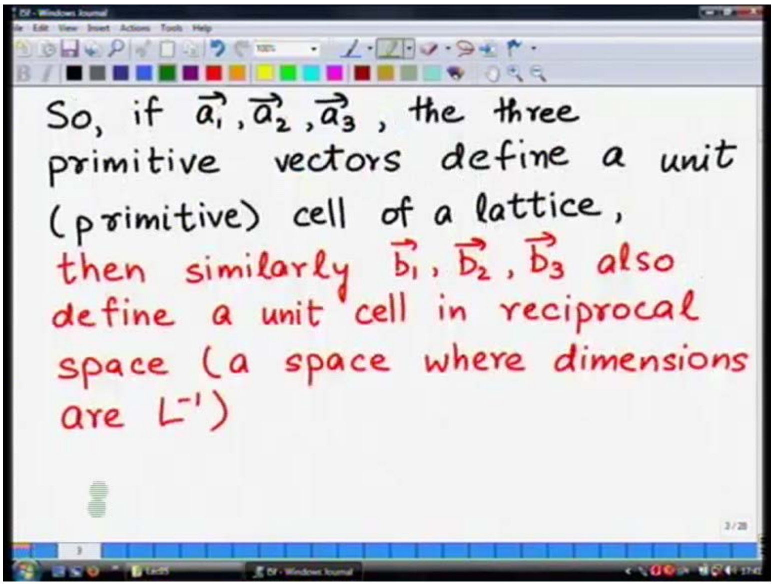

What we want do is this though. So, if a 1 a 2 a 3 are the three primitive vectors which define a unit cell, a primitive unit cell, primitive unit cell meaning one lattice point per cell per cell. Then, if this is really what is defining the primitive cell in the direct lattice then if I generate b 1 b 2 b 3 like this.

Similarly, I can think of b 1 b 2 b 3 also as a three vectors which define unit cell. Now, this time in reciprocal space what is the meaning of reciprocal space simply means a space where dimension are inverse of length which you can see that that this has a dimension l square. Then V p of course, is volume, so then l cube. So, then L square divided by L cube by L. So, b has a dimension of per unit length all b's have dimension of per unit length.

So, therefore this space we are calling as a special reciprocal space that is the reason we started calling it as reciprocal space, but if b 1 just like a 1 a 2 a 3, three vectors defined a volume and a volume which could be repeated and generated the lattice points. Similarly, we can think of b 1 b 2 b 3 generating a volume which then can be repeated and it can generate a lattice. That we will call reciprocal lattice which obviously belongs to reciprocal space, so that was the general idea. So, once I have defined that, so now I am going to do is I am going to apply this to various conditions of simple cubic body centered cubic and face centered cubic. So, let us begin with that.

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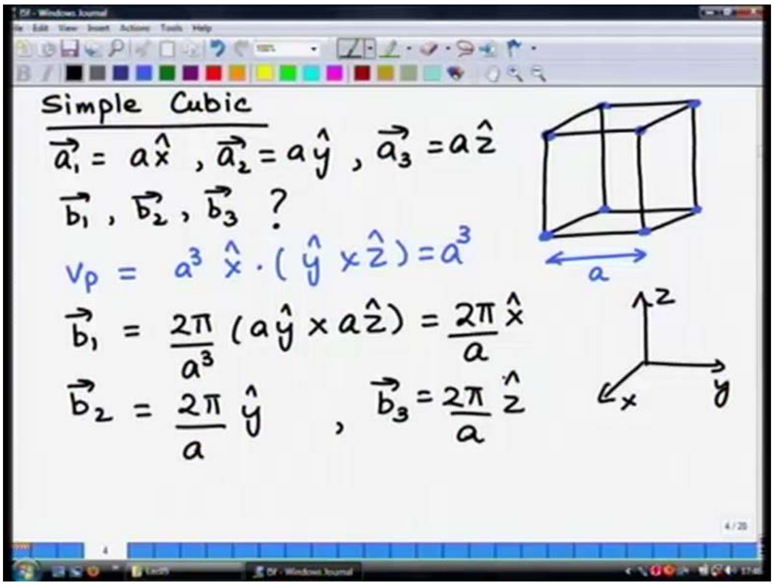

So, let us start with therefore, simple cubic system just to understand this what are the lattice vectors. So, primitive lattice as you know that simple cubic is simply like this with lattice points being here, here, here, here, here, here at the corners of the unit cell are the lattice points. If the lattice parameter is a, this distance is of the cube is a, then it is simple enough to write these lattice vectors, primitive lattice vectors as being equal to a times x hat a 2 equal to a times y hat unit vector in y direction a 3 as a times z hat.

Here, you can think of you if you wish this is x this is y and this is z, if you wish. So, these are the of course, primitive cell, there is only one lattice point per unit cell because lattice positions are the only at the corner of the unit cell. So, that is a simple cubic. So, corresponding to that if you apply formula for generating b 1, our question is what is b 1 b 2 and b 3. So, that really is the question we are trying to ask what are these values? But, then you already know the formulas right here are the formulas for you can given a a vectors, you can figure out this with these formulas you can figure out what b 1 b 2 and b 3 is.

Now, what V p of course in this case that simply will be simply will be a cube times x hat dot y hat cross which of course is just a cube. So, which you expected that with the volume of primitive cell which should just a cube if you use the black pen, so now we can determine b 1 if you determine b 1 then b 1 is what. Let us see 2 pi by V p 2 pi by V p a 2 cross a 3. So, let us use that 2 pi by V p, V p is a cube a 2 cross a 3, a 2 cross a 3 is a y hat cross a z hat.

So, what does that mean? That off course means 2 pi by a x hat that is all, so b 1 is just this quantity. Similarly, you can generate b 2, b 2 will be 2 pi by a cube y hat and b 3 will be equal to 2 pi by a. So, I make a mistake here, so I will fix this, so this will be since this a square I should have that is fine. This is a cube, this should be only a. So, let us write, so now 2 pi by a red hat and clearly this is dimension of inverse of length s.

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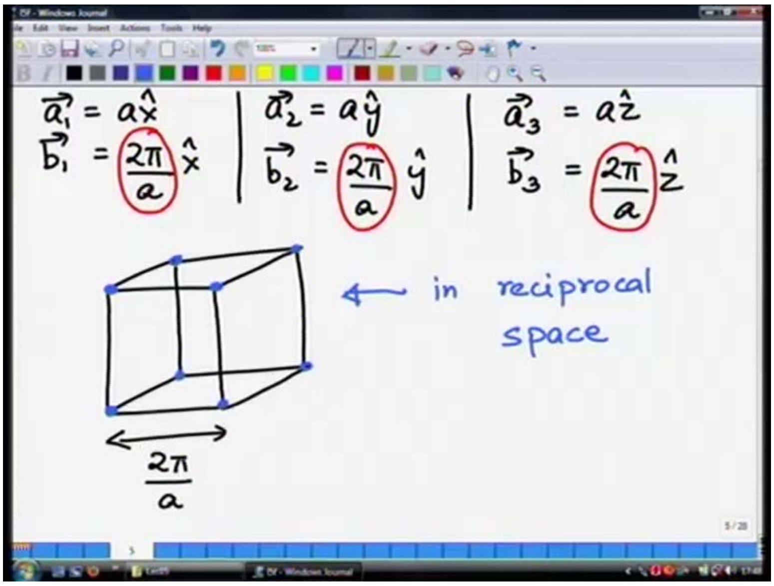

Now, notice now make a comparison a 1 was a x hat and what is b 1, b 1 is 2 pi by a x hat what was a 2, a 2 was a y hat and what is b 2, b 2 is 2 pi a y hat. Similarly, look at a 3 that was a by z hat, a multiplied by z hat and b 3 is equal to 2 pi by a z hat. So, now you can see by analogy what kind of lattice it represents in reciprocal space. Look a 1 a 2 a 3 just like a 1 a 2 a 3 b 1 b 2 b 3 are three vectors and they have same form they have same form as a 1 a 2 a 3 except instead of a. Now, in the front we have 2 pi by a we have 2 pi by a instead of a what does that mean?

That means, I can draw therefore, a reciprocal in reciprocal space also I generate a lattice which looks like a cube, but this time in reciprocal space and that will be simple cube. So, in the in reciprocal space in the reciprocal space lattice point also be in just like by analogy this must also be, therefore simple cubic. So, at the corners only and the length of this now should be 2 pi by a. So, lattice parameter in reciprocal space in reciprocal space.

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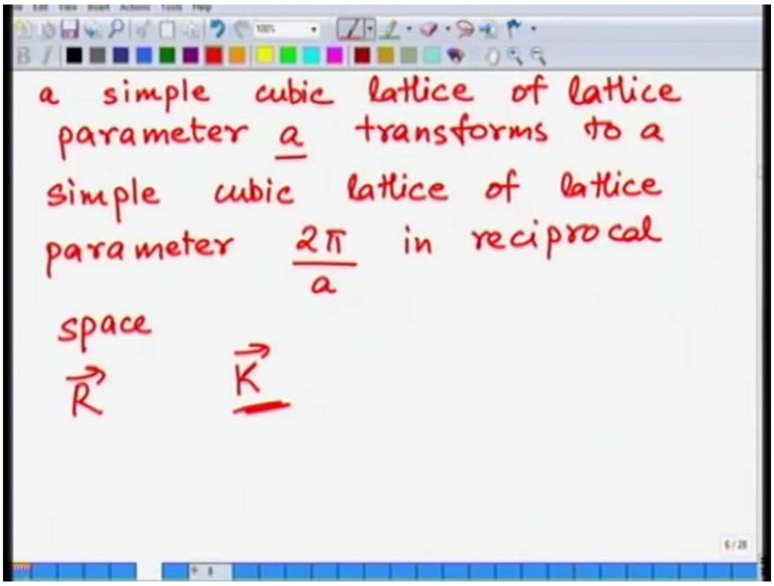

So, the statement I make is that simple cubic lattices of lattice parameter a transforms to a simple cubic lattice of lattice parameter 2 pi by a in reciprocal space. So, that is what it is that is simple cubic leads to a lattice a lattice reciprocal space which is also a simple cubic and the lattice parameter off course is 2 pi by a, so that is the transformation. So, that is what in a reverse, I can generate another lattice in reciprocal space which looks like by this repeating this volume, this unit cell.

I can keep repeating it and then I will generate a. So, this I will generate various lattice points and those lattice points were defined will be defined by this vector K if R defines the lattice points in direct lattice, then K defines the lattice points in reciprocal lattice. So, with this let us do this, let us move on, now we will move on to body centered cubic.

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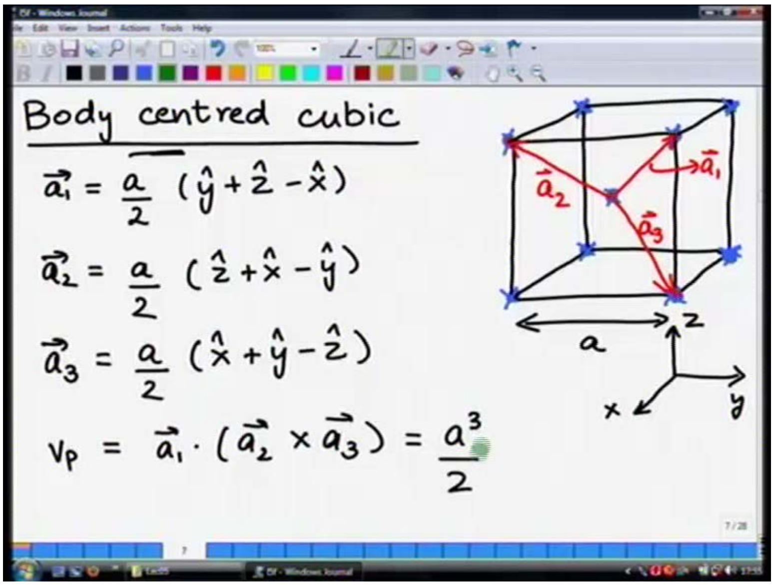

Now, this body centered cubic we are going to do now and I since in yesterday when was doing last lecture when I was doing direct lattice in body centered cubic the primitive vectors for not looking very nice, so I am going to draw that again. So, let us first write down our primitive vectors in direct lattice which is a 1. We have taken this as a by 2 y hat plus z hat minus x hat and a 2 was equal to a by 2 z hat plus x hat minus y hat and a 3 was a by 2 x hat plus y hat minus z hat. So, let us draw this lattice vectors first draw this lattice vectors.

So, you know what I am showing you here in this case is, so what I have done is shown you a shown you a cube which I am going to show you a body centered cube. So, you know that the lattice points are located. In fact, let me put crosses in there to show you the lattice points with the blue. I will put crosses like this, like this, like this, like this, like this, like this, like this, like this, and like this. If the body centered lattice points as you know these are the place where the body centered lattice points.

Now, let us do this in order to this primitive lattice vectors what we are going to do is let us take let us take a center at the origin right at the center. At this point use this lattice points as as a origin and with respect to this origin let us draw all these lattice vectors. So, all these lattice vectors remain within the cube itself and the orientation off course I am using is x in this direction. In this direction x in this direction y and in this direction z what I am using, so let us look at a, let us look at a 1, this a 1 we are going to move a by

2 distance in y direction a by 2 distance in z direction and a by 2 distance in the minus x direction.

So, let us do that. So, from this point let us move on to in y direction let us move to a by two in z direction let us move to a, a by two and then in x direction. Let us move to a, a by 2, now I will generate the lattice point. So, here is the lattice point right here, so let us generate that. So, right here is a lattice vector I am going to draw this from here to here and this is a 1 this is a 1 lattice vector and similarly, let us do a 2 a two we move half in z direction right here.

So, we move up to z direction and half and then we move in x direction half and then we move in minus y direction right here. Then we move and then locate this a 2 point. So, this must be a 2 vector this must be a 2 vector, similarly a 3 vector a 3 vector x direction. So, let us move half, so in this plane we move half in y direction we move half and in z direction, we move half write here and then this is therefore, this is the a 3 vector right here. So, this is the a 3 vector, using these a 3 vectors, we can imagine we can construct a volume and we can construct a primitive cell.

Now, in this primitive cell clearly if I take the volume with the primitive cell, then you can carry out this exercise a 1 dot a 2 cross a 3, you can calculate this and this clearly will come out as you try this out this will come out as a cube by 2. That should be obvious because if this lattice parameter was a of that is a body centered cube. Then whole volume should have been a cube.

And since, there are two lattice points in such a, in this whole picture which have drawn with black lines there are two lattice points. So, if you draw a primitive cell which are the only one lattice point per unit cell then the volume of that primitive cell should be half of the whole cell. So, that is a cube by two therefore. So, that is will be the primitive cell with this now let me write.

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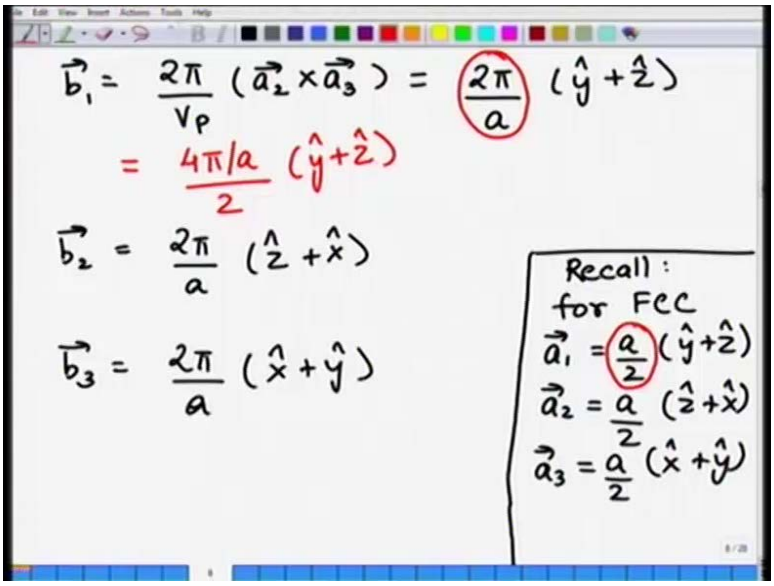

Let me write the b 1 b 2 and b 3. So, b 1 b 2 and b 3 are the three things you are going to write down again. So, the again we use our same formula 2 pi by 2 pi by V p a 2 cross a 3. So, due to this 2 pi by V p a 2 cross a three. So, you go ahead do this calculation and will find that that b one will come out as 2 pi by a and b 2 will come out as 2 pi by a and b 3 will come out as 2 pi by a or z plus x. Actually we should write and let me write it down as z plus x b 3 as this vector does this look familiar to you does it not look like it F C C.

So, let us do the recall here let us make a block here recall for F C C not B C C for F C C face centered cubic we had a 1 primitive unit vectors as a 1 a by two y plus z a 2. We had as a by 2 z plus x and we had a 3 as a by 2 x plus y these were the primitive vectors of face centered cubic now compare b 1 b 2 b 3 do not they look the same. Except that, remember here I have a by 2 in front and here I have 2 pi by a. So, if I write this quantity as something as 4 pi by a divided by 2 y plus z then you can think that. So, the clearly then a body centered cubic these vectors. Therefore this a 1, a 2, a 3 body centered cubic when we look at the reciprocal vectors then reciprocal vectors have a form of face centered cubic.

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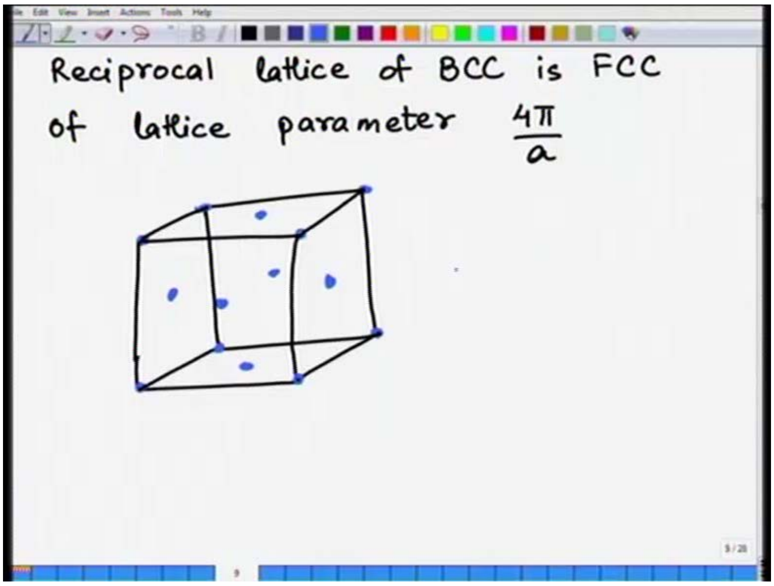

That means, in reciprocal space the reciprocal lattice of a B C C is F C C of body centered cubic is face centered cubic of lattice parameter 4 pi by a by comparing this form by comparing this form. So, there I have a 4 pi a here and I have a here just a here 1 here I have a is in here. So, therefore, I am comparing these a s and 4 pi by a if in F C C. The lattice parameter was a then here in this case n the lattice parameter will be 4 pi by a which I have written here. So, that is what this would look like.

So, if I transform this and I make F C C, then let me draw it then, then it should be this primitive a F C C should generate a F C C something like this on the corners. Then, on the face center here on the top, on the bottom on the back side on the front on the left side on the right side. So, these should be the lattice points all these lattice points should get generated by these lattice vectors. So, in other words B C C will look like F C C in reciprocal space very good. So, primitive cell will look off course different.

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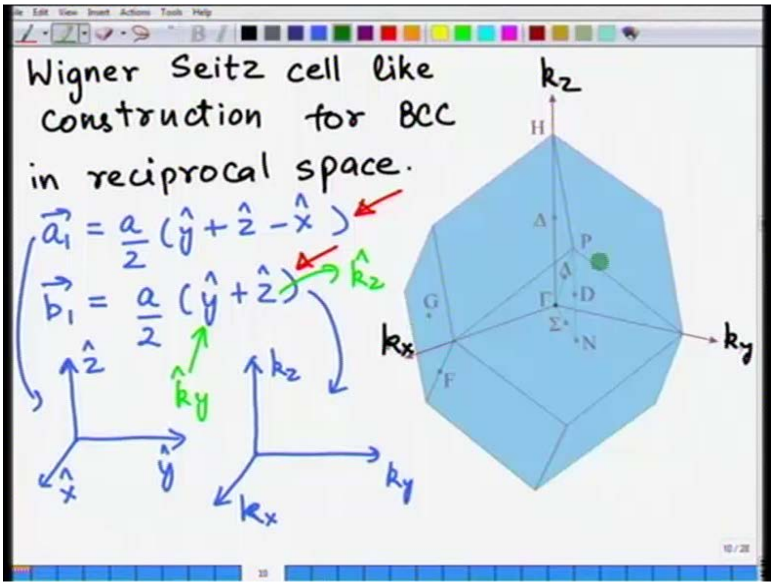

Now, this picture I will show you. So, this is what I am introducing brillouin zone now before I said I will do this brillouin zone 1 more time. But, just or instead I should say at this point of time Wigner. So, if you do a construction just like Wigner's itself which we did for direct lattice then if I do the then; obviously, whatever we did for F C C. If you go back and look at your Wigner's itself for F C C since in reciprocal space, F C C look like B C C.

Therefore, if I make a Wigner's itself in reciprocal of the reciprocal space, then it look like a F C C and it is exactly same cell which I have drawn here in this page, we have the cell which has been drawn. I will come back to this page and note that construction is already told, shown to you that take any lattice points draw lattice vectors. Take any lattice points, draw vectors to all possible infinite number of vectors to all infinite number of lattice points which are there.

So, you keep drawing them for every vector for every vector draw a perpendicular bisector plane perpendicular bisector plane. At the end of it, imagine you have drawn this infinite number of planes because infinite numbers of vectors and you have drawn perpendicular bisector to them. If you drawn them then after those at the end of the day there is a some volume enclosed the smallest volume which will be enclosed inside that volume which is enclose enclosed inside that that sorry that that small smallest volume.

There will be enclosed by some planes, some portions of those planes that was the Wigner's itself in direct lattice same construction here. Now, this in reciprocal lattice is called Brillouin zone. I will talk about this and in two dimensional I will show you the constructions eventually in a little bit. So, until then just hang on and more importantly well not more importantly, but equally importantly.

So, I should make a little change I should write this as small k, I hope you are comfortable with that this drawing. So, in the in the sense that remember I am using k x and k y and k z here. What is that mean? That means, that just like I was drawing this cells as remember a 1, let us do example here that will make your life easier you are able to understand.

So, if we look at this page let us just do a 1 and B C C was this quantity right here, write this a 1 as a 1 as equal to a by 2 y plus z minus x hat and we will write b 1 also which was a F C C, which is right here y plus z. So, a by 2 y hat plus z hat, so what was this a 1 and a 2 and a 3. So, remember what we are saying is that if you have a direct lattice somewhere like this and in that there is a x y and z. Similarly, I should have something in the reciprocal lattice for corresponding to this.

If I have this is the orientation then for this I should also have another, I should have orientation, that orientation we are now labeling as k x unit vector. So, this is sorry k x direction k y direction and k z direction, only to show that this is three possible directions in reciprocal in reciprocal space that is this k direction. So, in effect I could have replaced this quantity by k y hat and I could have place this by k z hat, I could have replaced this by k y hat and k z hat because they just unit vectors in that space. I have used both x y and z for both in the direct lattice also unit vectors in direct lattice also here and I have used x y z also as unit vectors in reciprocal space.

But, if you want to be very precise and consistent with this diagram here then you can replace in the reciprocal lattice, this as k x k y and k z unit vectors because that is in reciprocal direction. So, that is all; that means, and notice there are many g f h p d and R shown this relevant this picture. I will take later when I actually draw the band diagrams for you E versus k diagram.

I am going to use this to generate those diagrams. So, there will be the the relevance there. So, at this point of time just take a look at this picture from the point view the shape and that shape remember is exactly Wigner's itself in F C C, since in reciprocal lattice for the F C C of B C C. Therefore, this is the Wigner's itself in the reciprocal lattice whose name is of course Brillouin zone.

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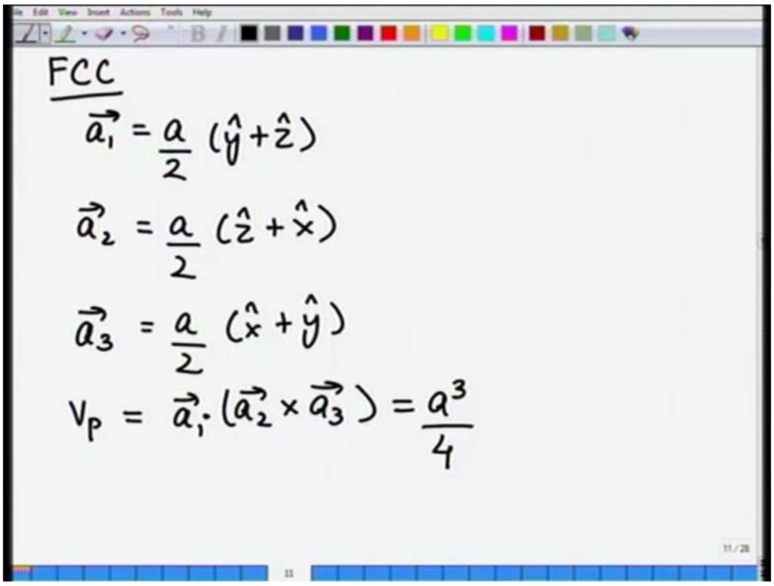

So, with that let us move on let us move on to also this, now we will take F C C. So, we have done simple cubic, now let us do face centered cubic. So, we do face centered cubic then we call again I am going to repeat what we are written in last page a 1 of course was equal to a by 2 y plus z a 2 was equal to a by 2 z plus x and a 3 was equal to a by 2 x plus y. So, therefore, what was the volume of this primitive cell, is the primitive vectors what will be the volume of the primitive sector dot a 2 cross a 3.

That is what we need to calculate and that quantity of course will be equal to, go ahead and check this a cube by 4, which I can write down really calculating it because we know in F C C, if you take conventional cell of cubic cell of lattice parameter a. So, therefore the volume will be a cube a will be a cube and since that has four lattice F C C s 4 lattice points per unit cell where as these vectors I have written here a 1 into a 3 are primitive vectors. That means, this the cell which will be constructed by this we will have only one lattice point. Therefore, it is volume must be at least one fourth of the conventional cell I have written it because of that reason you can verify by doing actually this calculations.

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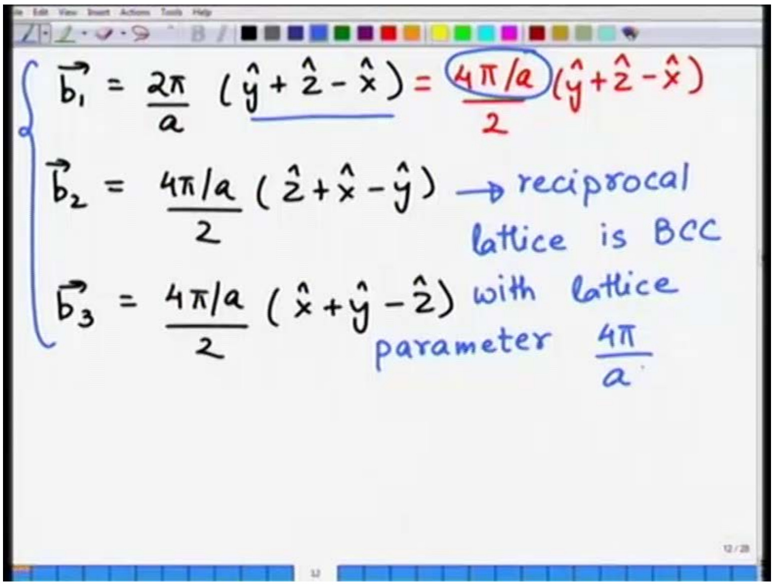

So, again with this you will find that if you do the same thing then find b 1 as equal to in this case 2 pi by a y plus z minus x which I will also write as 4 pi by a divided by 2 y plus z minus x. You will now clearly see why I am doing this since we already discussed this. So, I am going to write this again as 4 pi by a by 2, this is equal to z plus x minus y and b 3. this I am preserving because, now do very because formulas are there. It is matter of taking cross products nothing else, x plus y minus z.

Now, what does that look like. So, at this off course these lattice vectors review F C C. So, review F C C all this side face, right face, back face, front face, top face, bottom face. So, these are the lattice points in F C C what will be generated by this particular primitive cell. Of course, primitive cell will be different will look different and that shape I have shown you earlier in the previous lecture the primitive cell.

I shown primitive vector and I shown with the volume that primitive vector encloses that I have shown you. But, now notice when you use this primitive F C C, is this primitive vectors and we do the reciprocal lattice transformation then we get b 1 b 2 b 3 vectors. Now, b 1 b 2 b 3 vectors are. Now, look at the form, this form is much the same as B C C which we did right here, notice for body centered cubic, these vectors look as look as a by 2 y plus z minus x y plus z minus x. Now, notice here same thing y plus z minus x and now, but it is 4 pi by a by 2 rather than a by two in B C C.

Now, in reciprocal lattice, it is 4 pi by a, what does that mean? That means, I am generating reciprocal lattice B C C with lattice parameter, with lattice parameter 4 pi by a. That lattice parameter is 4 pi by a. So, that is how easy it is simple cubic transform into simple cubic body centered transform into a F C C reciprocal lattice a F C C lattice transform into B C C reciprocal lattice. You are welcome to try this for hexagonal lattice also or any other kind of lattices, you will find hexagonal transforms into hexagonal itself. Now, that exercise, now I think you get the idea how this reciprocal lattice transformation is done . So, once this transformation is done.

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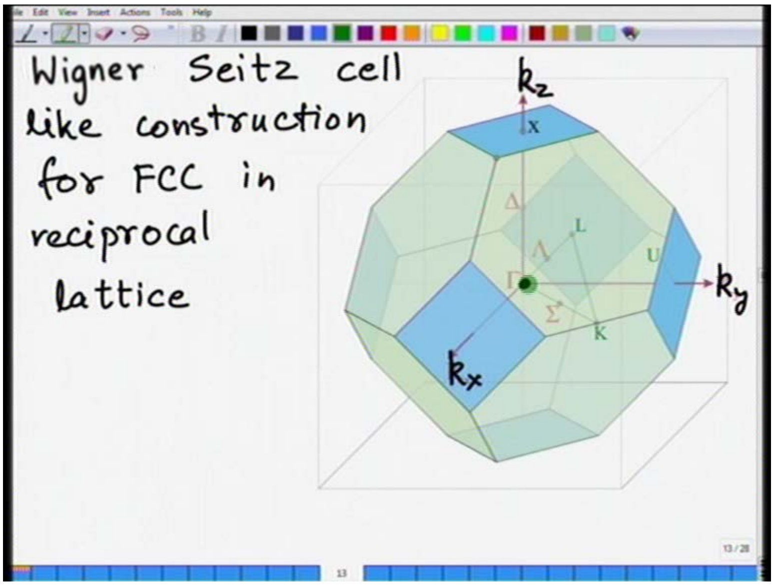

So, let me show you the Brillouin zone or the Wigner-Seitz cell Wigner-Seitz cell again I will write that wigner for F C C in reciprocal. So, now in reciprocal lattice, the thing look like B C C. Since it look like B C C, therefore let me make first make this again correct k x k y like that. The idea small k what I should write, now capital K must show the directions. So, now I have three directions k y k z and in this case you can see that since it transform to B C C. So, Wigner-Seitz will remember look like this for B C C construction again is the same take B C C reciprocal lattice from every from take one point lattice point draw vectors to all the infinite number of lattice point draw vector.

From this point, you have chosen from this point you have chosen draw lattice vectors and that point chosen is right here from this point, draw lattice vectors to all lattice points then draw perpendicular bisector planes to it. Then, the smallest volume that will form in this, we will have shape and obliviously, the lattice point will only be in the center then. Now, the lattice point like this and that is the Wigner-Seitz cell like construction and this in reciprocal space is called a in Brillouin zone.

Again, this is the Brillouin zone of a F C C lattice, if the F C C lattice is real lattice for then it is B C C in reciprocal lattice and that is the Brillouin zone. Therefore and in this zone again, I have shown you this different k point, k l u, this sigma, the gamma, delta all the symbols are there. These are again going to get used later not now. Later, they are going to be used in band diagram. So, be prepared to look at this picture again and again all right. So, with this I will close the chapter on the reciprocal lattice and I will go on to now next topic which is.

So, a which was the Brillouin zone, I have already mentioned what brillouin zone is, but what I am going to do now is show you the I am going to work with you and instead of in three dimension. I will do this a in 2 dimension to show you how Brillouin zone is constructed and what does it mean. So, let us do that part by first. So, brillouin zone remember.

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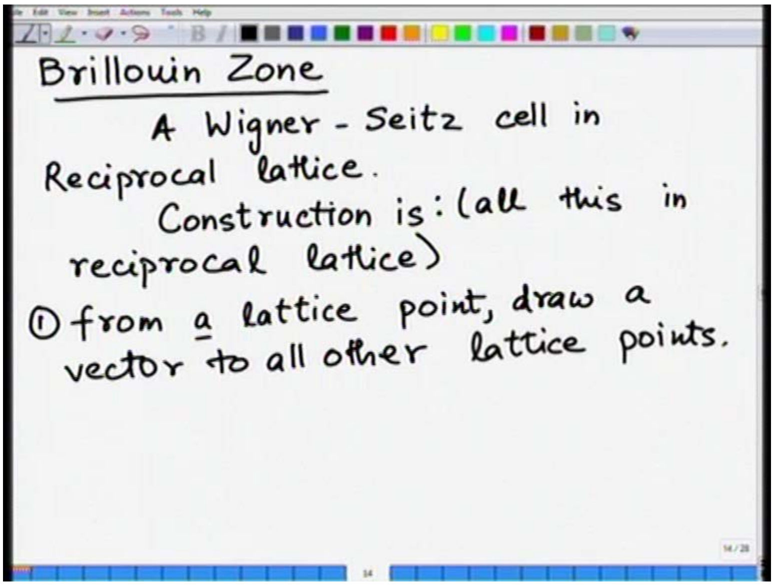

So, let us start with these Brillouin zones I have, as I have gone long, then I have already defined it to define what it is a Wigner cell in reciprocal lattice. Only thing I want to say right now is why we bother about it, this plays an important role. What I am going to show you is, now since three dimension construction for F C C, B C C gives a sort of imagine and I have already it to you. So, you can say imagine and I have already told you how this construction is done, but if you not really followed it then off course very difficult to do that in three dimension in a by a writing by hand.

So, what I am going to is I am going to do this construction for you in two dimension. I will do the same construction to make a Brillouin zone in two dimension and then hopefully you will understand how this Brillouin zone in three dimensions was constructed. Then, I will move on to show you the importance of it, first thing which I will show you is that something happens of the Brillouin zone at the zone sorry the zone boundary at the zone boundary.

I will show you that the Braggs diffraction condition gets satisfied and therefore, electron wave is strongly reflected at these zone boundaries. So, that is really the purpose, it becomes lot more easy to analyze things in the reciprocal space and this is where the importance of this comes. So, therefore, of course in the zone.

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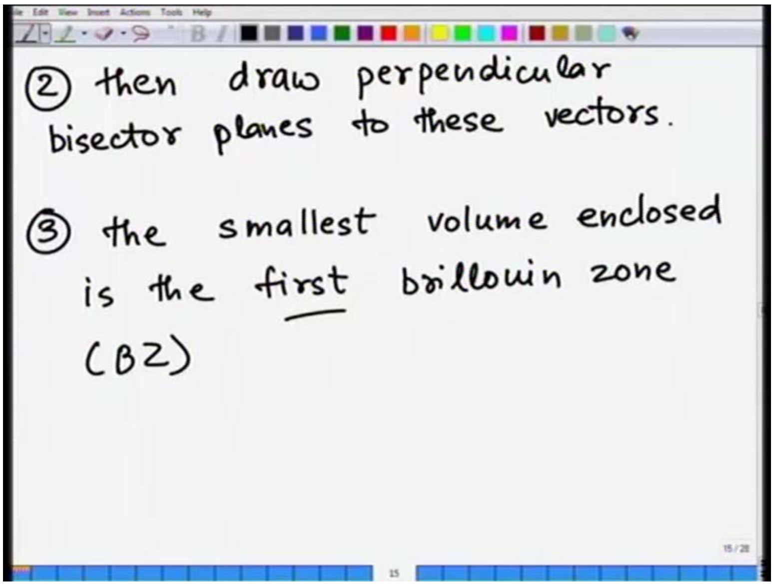

So, you have to plot this E k diagrams of course we will using for that purpose, but eventually when we move on and we include the potential in our from free electron theory. If you start including potential, we will see that there is a band gap originating like in semi conductors. It happens because of these reflections which are happening at electron reflection happening at Brillouin zones boundary. So, essentially the constriction is construct is from a lattice point. Draw a vector to all other lattice points by the way all this in reciprocal, all this in reciprocal lattice. So, from a lattice point draw a vector to all other lattice points.

Infinite number of vectors like this, then draw perpendicular bisector planes these vectors or in infinite number because infinite vectors are there the smallest volume enclosed is the first which I will form. Now, abbreviate as B Z that is the Brillouin zone and I will now introduce term first Brillouin zone. I might say Brillouin zone, I will mean; that means, for Brillouin zone which means there are second Brillouin zone, third brillouin zone, fourth brillouin zone etcetera, etcetera which you can see that that the smallest volume was first Brillouin zone.

So, now, if you take the next largest volume which is enclosed by this planes out of which you remove the all the portion of the first Brillouin zone, then whatever is remaining is called second Brillouin zone. So, you can keep developing this idea, but what we will be interested in is only the first Brillouin zone. So, that is the general construction. So, let me show you this construction.

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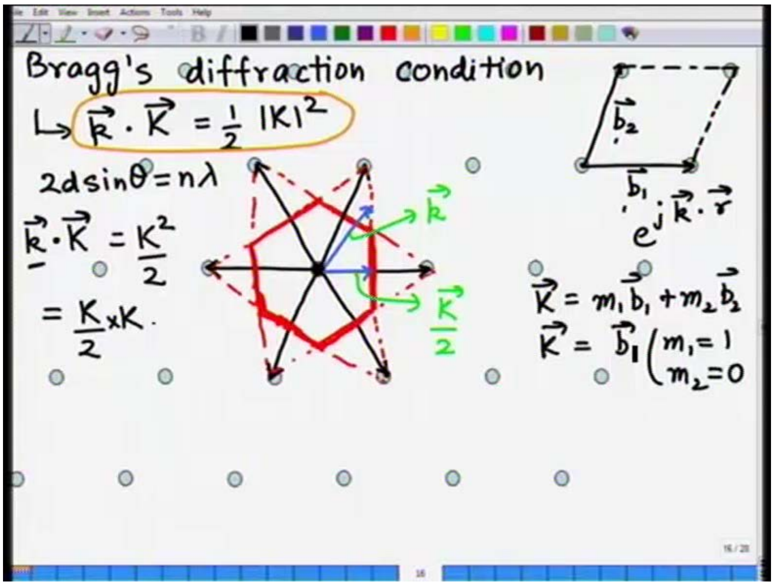

So, now what I am going to do is, now here is an array of point, now if you look at this point then you can clearly see it is a point lattice. Take any point and the environment around it and look at any direction, the environment is same, now it is two dimension. So, I am going to draw; now from these lattice points, I am going to draw vectors and then I am going to look perpendicular bisector. So, perpendicular bisectors to these vectors in three dimension would have been plains for perpendicular bisectors to any vector in this in this diagram will be lying. So, that is why it will become easier for me to draw.

So, first of all let us draw the lattice vectors, primitive lattice vectors. So, what is the unit cell in this for this point lattice and reciprocal space. So, here is my b 1 let us say, so this. So, here is b 1 vector, let us say this is the b 1 vector and let us say this is the b 2 vector. These are the two lattice vectors which we have, which therefore there are two vectors, only this is a plane.

So, therefore, they include enclosed area, that area is this, they form an area. So, this become our unit cell by defining this b 1 and b 2, remember no unique choice of b 1 and b 2 you can use many this is in reciprocal space and repeating unit of this cell. This unit cell then would generate all the lattice points. So, that is what this is. So, now let us generate a Brilliouin zone. So, let us use this as a center. So, let this is a center. So, now let us draw the vectors if I a draw a vector then all the neighboring vectors first I will draw.

So, one vector is right here, one vector is right here, one vector is right here, one vector is right here, one vector is right here, one vector right here etcetera. So, now if I draw a perpendicular bisector, perpendicular lines to it, then I will draw some perpendicular lines. So, here is a perpendicular bisector which I will draw or maybe I will use different color for perpendicular bisectors. So, here is perpendicular bisector for this particular vector for this particular vector there is a perpendicular bisector going somewhere like this for this particular vector a perpendicular bisector. I will draw from where I will draw perpendicular bisector somewhere like this some here is a perpendicular bisector.

So, somewhere like this is a perpendicular bisector. So, for this line vector I have perpendicular bisector like this going something like this for this particular line I have this particular line. I have a perpendicular bisector which is like this and so on. This particular has a perpendicular bisector which will look something like this. So, now what is the smallest area that is enclosed, let us draw that part. So, here is the smallest area which is enclosed in this. So, that is the first Brilluoin zone. So, that is the first brilluoin zone and of course vector to any lattice point any like I said you have draw this for also.

I could have drawn another vector like this black I should have drawn also a vector like this like I said draw vectors to all the lattice points and then you have to make the perpendicular bisectors to them. So, once you make the perpendicular bisector you would have made the perpendicular bisector for this like this you would have made the perpendicular bisector for this particular vector somewhere like this. But, you see that these would have been still outside, they would have not to come in play in defining the smallest volume. So, essentially if you draw this with few neighboring, sorry you can because I could see in this that all you need is neighboring a vectors only in the neighboring a lattice.

Therefore, I drew only those, but, in principle you should draw all of them and draw perpendicular bisector for all of them and then define the Brilluoin zone. So, here it is this is a Brilluoin zone. So, now in this Brilluoin zone to keep my picture little bit cleaner what I am going to do is first erase what I have just drawn again little bit later I want to erase these portions. Because I want to just otherwise make my stuff dirty, now I am going to show you something else. Now, I am going to show you, so this is how the Brilluoin zone is made. Once you understand what this Brilluoin zone is, then I am about to is tell you that on this Brilluoin zone boundaries.

On this Brilluoin zone boundaries actually anywhere on this bisector plains, even here even in this region here even at this point here or at this point here, this is the condition which is satisfied. So, I am going to write this Bragg's diffraction condition. Now, as I am going to write this as small k dot with capital K, small k what is small k, remember small k is the wave vector which appeared in e to power j. That was a kind of solution we had in a plain wave. So, that is a wave vector dot reciprocal lattice vector what is a reciprocal lattice vector, remember reciprocal k is equal to in this case m 1 b 1 plus m 2 b 2 where m 1 and m 2 are integers. So, that means, you can generate by having these b 1 b 2 this b 1 b 2, some multiples of m 1 and m 2 you will generate any lattice points.

So, from any origin here all these vectors black lines I have shown you essentially capital k vectors and they are using some value of integer value of m 1 and m 2 to reach to other lattice points. So, these are the k vector is equal to half k square is what is equal to and I am saying, this is a Bragg's diffraction condition which is equivalent to saying a the 2 d sin theta equal to n lambda. I will show you that in minute, but this is equivalent, I will show you that is equivalent. Now, let us see in vector form what happens. So, you look at vector form.

So, let us now take, I will use now red or some other color here and let us take any vector. Now, this let us say this is k. So, this is a small k some vector k any vector in reciprocal space is small k and then, now what is this vector. This vector is capital K by 2 vector, remember in this case this capital k which I have written it as equal to b 1; that means, I have chosen m 1 equal to 1 and I have chosen m 2 equal to 0. That is what I have chosen here, so therefore this is showing up as so k by 2 I am writing as k by 2 black line which is whole vector is capital K.

This line is only half of it because it perpendicular bisector. So, therefore, this is k by 2 now, look at what happens anywhere on this boundary small what is dot product between k and capital K. Now, you can see where this condition is satisfied or not satisfied on his boundary. If k is lies on this boundaries, so it is lying right here. If I take the dot product between these and these, now k small k dot capital K, what is that will be equal to that that will be equal to that k will be equal to. Essentially, now you can clearly see k square by 2, that is what this will be equal to. As you can see if I take the resolve small k on to this, so k of k dotted with a unit vector in this direction will be equal to k by 2.

If I take the component of small k in direction of k, that will be clearly k by 2 and of course then I multiplied by k itself and by dot product dot like this that will be or rather then I should write it as just simply as this quantity multiplied by this quantity. That will be k square by 2 that is what this quantity will be. So, clearly the Bragg’s diffraction condition therefore is satisfied on this particular plane from Brillouin zone boundaries, that is special the Bragg’s conditions are specified.

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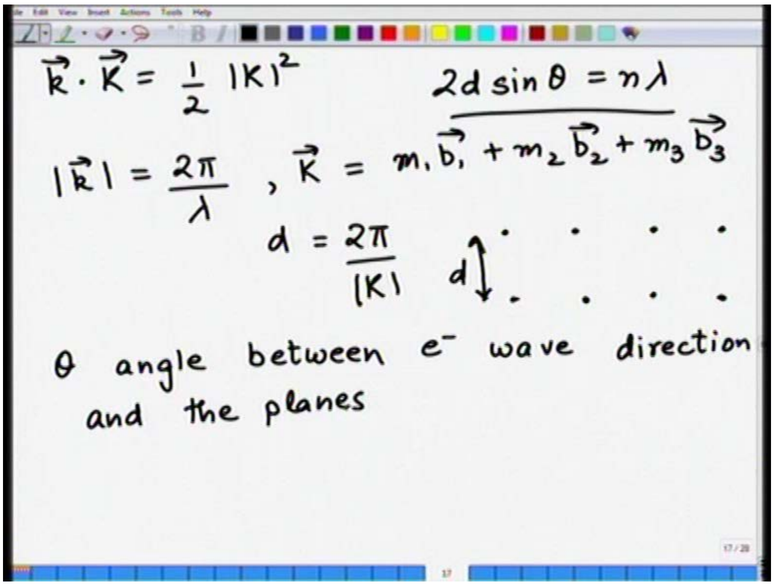

Now, only thing let me try to show you is that how k dot K is indeed equal to half k square. We could precisely define, it is equivalent to 2 d sin theta equal to n lambda, this is a more common form in which you are going to see the Bragg's diffraction condition. Let us for it is for straight forward small k off course is the wave vector, it is a simply small k is simply 2 pi by lambda, that is what this small k is.

Recall also that k off course is k vector is equal to m 1 b 1 plus m 2 b 2 plus m 3 b 3. In general I am writing in general form and d spacing between the planes. So, if I have these planes, atomic positions and this is a d spacing between them, then the d spacing between them of course is equal to 2 pi by k magnitude, that is the spacing between this. So, now if I have write this part, if I write k dot k to then, I will write this as and then what is the and then we say theta is angle between wave direction and the planes. That mean normal to the plane and k vector of course is normal to these planes this k vector is normal to the planes. So, they form the planes.

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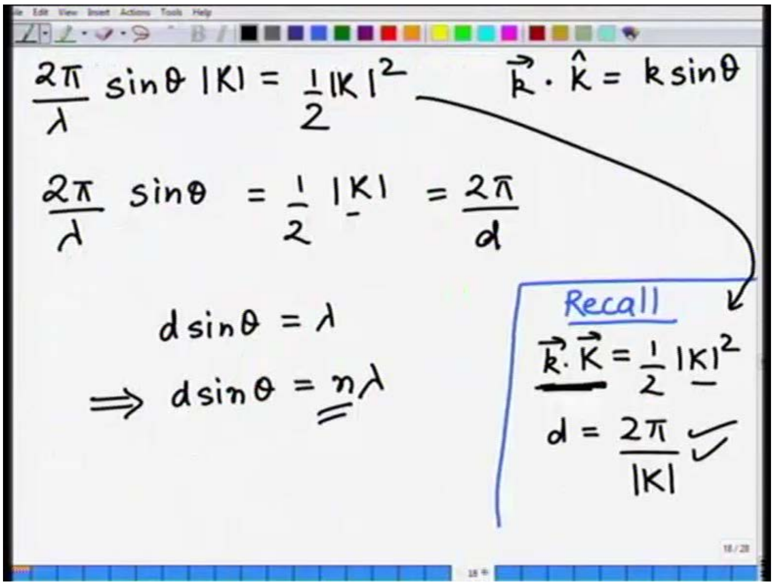

Therefore, I am going to write this as small k as 2 pi by lambda and I am going to write this as here. So, 2 pi by lambda into dot product with k I am going to cancel one k magnitude with the square here in terms of magnitude I will cancel it out. So, if you resolve k in direction of k only. So, if you take in the unit vector capital k then that angle this is the angle then this should become sin theta that should become sin theta k dot k should nil or k dot unit vector in direction of k would be k sin theta. That is what this quantity will be. So, that is actually that is what exactly that is how I have written here also.

So, what I have done is k in with the unit vector in direction of capital k and then a magnitude k their which would have cancel in the right hand side that would have an easier way of doing things which I will I am doing here. See that is the case, then this is k sin theta, then I have one another magnitude of k I should write here, and then I should write here half I am substituting into this equation. I mean in this equation I am substituting all this stuff. So, then half k magnitude, the square and then I should have written 2 pi by lambda sin theta equal to then half k magnitude, which I would have written I would what is k magnitude that comes from this equation right here.

So, that I can write as 2 pi by d spacing what is that mean that leads to d sin theta equal to lambda which of course we write as d sin theta equal to n lambda n n being the order of the equation. So, that is you can see, so I have shown you this that indeed on this

Brillouin zone boundaries. This Bragg's diffraction condition is satisfied and I will show you geometrically.

So, should I before I just quickly end I am happy with this kind of thing calculation I did. So, k dot K in this case is equal to you can see k capital K by 2. So, that is what I have substituted in here to get this equation which hopefully you can now see more carefully for you can see little bit better. With this let us close on the chapter on today's lecture on this Brillouin zones and now I am going to start moving into electrons in a crystal in the next lecture.

Thank you.