Optoelectronic Materials and Devices
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Electronic Structure of Materials

Lecture - 07
Free electron band diagram in an empty lattice

Welcome to lecture number 7.

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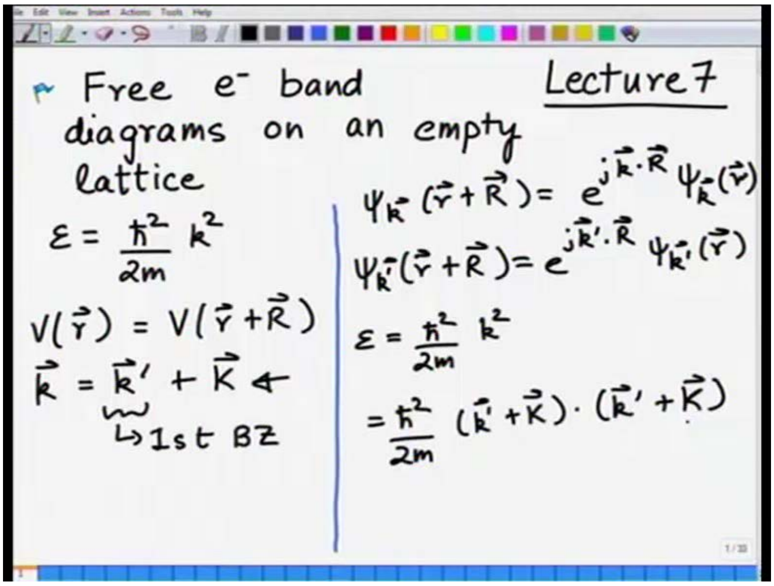

Let us today, what we are going to do is we going to plot this free electron band diagrams on an empty lattice. What that means? I will explain in a minute, but let us recall what we did. Let us see what we are trying to do; what we are trying to do is, we know that energy is equal to h square by 2 m k square. That is a free electron energy, see if I want to plot this then I can simply take e and k and plot it, but the problem remembered was that k is a vector.

So, what direction I should choose because when I am plotting e versus k then what direction dose k represents. That is question number 1, question number 2 was k of course, it is extent is from minus infinity to plus infinity now how do I plot it. So, now we have now remember what we did was, we derived equation for energy in free electrons without any regard to the underline lattice. Then, we introduce that if there is a lattice, there is a periodicity in the lattice, now what is the consequence. Then, next step we did was that if there is going to be any periodic potential though energy of free electron was derived with potential equal to 0.

So, yes we will have to correct for that also, eventually that energies also have to be calculated correctly, but for time being if you assume that energy indeed varies as e versus k square, then we will continue to it as free electron band diagram, there is just an assumption temporary assumption, but then in reality. Since, there is a periodic potential in the lattice which I will show in the next lecture one more time, but since even clearly sees in because periodic lattice were potential also, there is a potential also which would be periodic and as a result consequence of that that the Bloch.

There is a Bloch's theorem which allows to make some conclusion and that helps us in plotting band diagram that is my purpose of today's lectures that if I have a lattice, there is a periodic potential though energies have been calculated with 0 potential. We will just use those as numbers on the E scale, but on the k scale we will use what we learn from if the potential was periodic. What did we see that if potential was periodic in R, where had a period of capital R in that case we had shown. I had shown that is always possible that if you have will vector k then it is always possible to write it as a vector k prime plus some reciprocal lattice vector such that this k prime is in first Brillouin zone.

It is in first Brillouin zone because always find a capital k vector such that this k prime vector comes in first Brillouin zone. Now, this is one thing I had shown you geometrically, second thing I had shown you was in the previous lecture that there is no unique k which defines the wave function namely phi of k at R plus, R is simply equal to equal to E to power j k dot r phi r. I could also write it as phi k prime r plus r equal to e to power j k prime vector dot r phi of r. Now, I can see now I can see that it does not matter whether you choose k or k prime, is the same thing as long as k and k prime are different from each other by a reciprocal lattice vector here, so this is the trick.

So, now you see instead of this, since it does not matter to us what actual case I can always find a k prime whose limits are only within the first Brillouin zone. And hence I do not need to plot e k diagram all the way to infinity. I can plot it only up to k prime and when I plot it, then I mark it out that what k capital K I have used you have to do this transformation keeping track of it. I can always calculate energy as E h square by 2 m, that means if I know k prime and I know what k I have used to get to k then, since my energy is k square that is equal to h square by 2 m k prime plus k vector.

Explicitly, k prime plus this right this square like this that is same thing, so if I know a k prime so instead of plotting E verses k, I will plot E verses k prime whose limits are only within first Brillouin zone. When I plot, I will also write what k I am going to use, so that in case you want to calculate the energy you can simply add the k to k prime calculate small k and take square of it to calculate energy. So, that as an example let me show you as an example.

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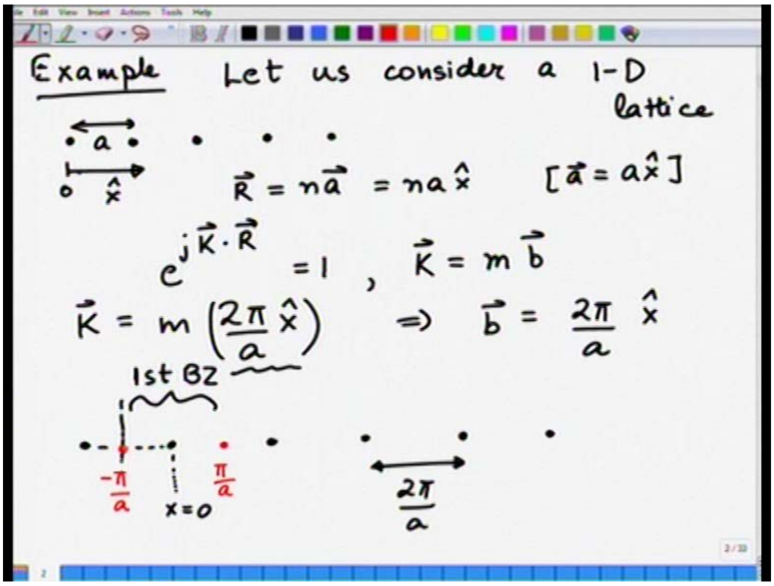

As an example, let us consider one dimensional lattice, what do that mean let us say that my lattice to make it simple, to keep it simple initial to understand what we are trying to do let us assume that lattice is one dimensional and then eventually, I will go to three dimensional real lattices. So, let us say this is what I mean let us say one, it is a one dimensional lattice with a lattice parameter of a.

So, this is the lattice parameter a if we consider this together origin and this is x direction in. If we consider this as x direction then I will define my lattice vector, what is the lattice vector for this then? In that case I can write this lattice vector as some n times a lattice vector which is same thing as n times a x hat meaning there by a vector is simply equal to the lattice vector is simply equal to a x hat.

So, a is a periodicity of this if so, let us now find the reciprocal lattice vector reciprocal lattice vector of course, now is has condition that if we find a reciprocal vectors. Let us vectors such that it for j k dot r should be equal to 1, if that is the case and if I define my k to be equal to some m times vector in that case you can clearly see that if I substitute r and k in there then what would I find. I will find k must behave as equal to something as equal to or maybe I use not m, but I use lets for time being or let me use.

So, I substitute in their what is that tell you that, says that I should have k which is e k vector should be simple equal to 2 pi by a x hat is what, this k should be implying that b should be equal to should be equal to for K should be equal to m times. I should say m multiples of it where b begin this quantity here this quantity being b, so that is what this quantity should be equal to. So, you can see that if I substitute R and K, I will get e to power j k dot R is 1. If I choose my reciprocal lattice vector as like this, what is that mean even an reciprocal lattice the lattice is one dimensional. And in that case if I plot it again the reciprocal lattice then reciprocal lattice looks something like this.

Again, one dimensional with a periodicity of 2 pi by a, now 2 pi by a is a periodicity of the reciprocal lattice. If I am looking for the Brillouin zone remember what do we do, what we do is sorry this is x equal to 0. Let us say x equal to 0 then in that case what do we do, we take perpendicular bisectors to this lattice vectors here is a lattice vectors for n equal to 1 and here is a lattice vector for m equal to minus 1. If I take perpendicular bisectors to it, here is a perpendicular bisectors then this is my first Brillouin zone same construct in one dimension in three dimension, these bisectors or plains in 2 D which I had shown you earlier these bisectors or lines.

In 1 D these bisectors are simply say these points I should use a different color here because this is not a lattice point. So, I should use this and here is the bisector points I write here a bisector points and this is therefore, pi by a, and this is minus pi by a. Since, the lattice parameter is 2 pi by a, now notice that now what that means is that if I want to plot e versus k diagram.

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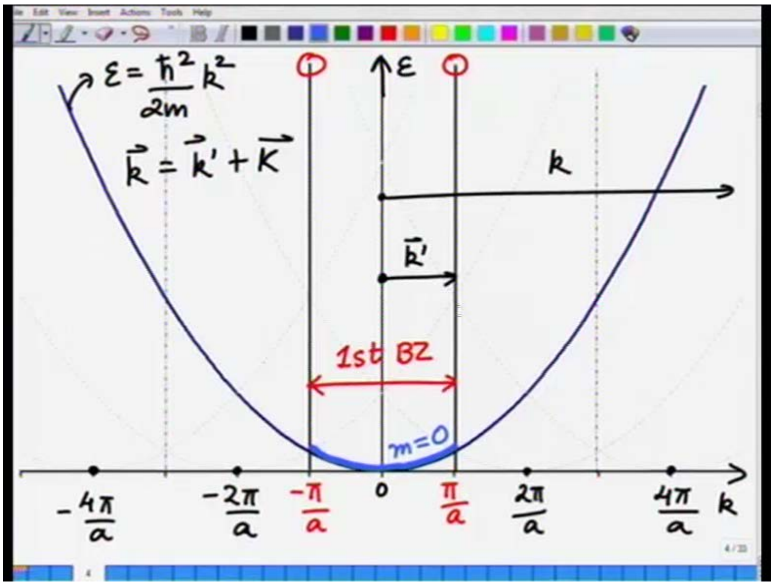

Let us say E now varies as h square k square by 2 m now of course, problem is straight forward since k is only in one direction. So, I can always take plot e versus k like this, I can take e versus k and let us say this is K which is simply x direction. Essentially, K x direction if you wish then in that case I can simply plot the parabola E versus k square, like this I can calculate and this is the energy. So, I keep calculating E versus k as a parabola, this because only one direction, but what I want to show you by in this one dimensional case is that we need.

Now, plot this parabola all the way to plus infinity and minus infinity, we can if this is 0 and we can think of 2 lines here, which is at pi by a first Brillouin zone minus pi by a and we can represent all this information by plotting this curve only within these two limits. Only within these two limits we can plot and we can show this entire diagram in these limits only. I want to show this for you to you one dimensional case and then move on to three dimension there, we will use this fact and plot it out for three dimensions.

So, let us should do that part and show it to you how this is will this will be done, so here I am you going to label this for you, this something what you need to show what you need to see is only the portion like keep labeling. So, here is a energy that I am plotting and this is k, which I am plotting, which I am trying to plot and this here is 0, here is the lattice point, right here another lattice point. Therefore, it is 2 pi by a, a lattice point here periodicity is 2 pi by a and reciprocal lattice, so 2 pi a minus then therefore, there is this

4 pi by a another lattice point and here is another lattice point, which is 4 pi by a there is a lattice point.

Now, if I plot e versus k diagram then I can simply plot this as this, this line which you see as a blue line right here, here is a parabola E versus k square, I am plotting this blue line shows a plot of e versus essentially h square by h square by 2 m k square. That is what basically this parabola has been plot it as this what I had been plotted out. Now, what I am showing you is I have drawn two lines right here are the two lines, I am plotting this line and this line. I am plotting and here is my pi by a and here is my minus pi by a, this is my first Brillouin zone which I showed you in just second above.

Now, this Brillouin zone and I want to show you that everything can be plotted in here. If that is the case let us think of another axis what we when think is like this that we will think of another axis running from here this is 0 and who is extended only up to here. This is my k prime axis here is my k prime axis, so this axis running from here to here which is k axis and there is a axis running from from 0 to pi by a or 0 to minus pi by a that is a limit and that is k prime. Remember k prime is a vector which belongs only in the first Brillouin zone why dose why so because k and k prime are always related by capital K.

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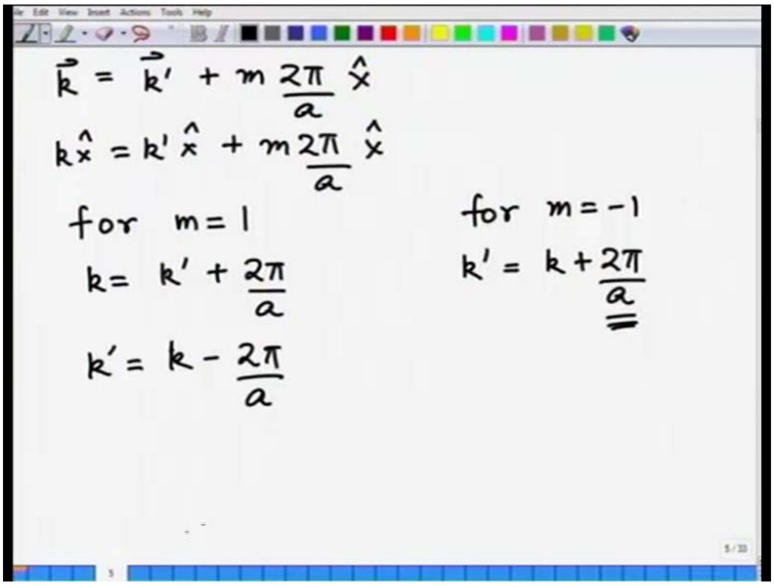

So, let us substitute this out, so then therefore, any vector k will be equal to will be equal to a small vector k prime plus some m times 2 pi by a x h and remember k and k, I am going to drop this vector inside in there because everything is in x direction. So, this k is also this k is also in x direction and this is this k prime is also in x direction everything is in x direction. Now, so when n is equal to 0, so let us use this blue line and I will darken it when let us say m is equal to 0 then I will double this line, thicken this line here from here to here.

I am going to plot it this is for m is equal to 0 hence m is equal to 0 for n is equal to 0 k is equal to k prime and I am going to plot k prime versus energy, so that is simply will go up to this point. Now, if I go at for the points beyond this that means, let us say I am looking for these points right here up to here from here to here.

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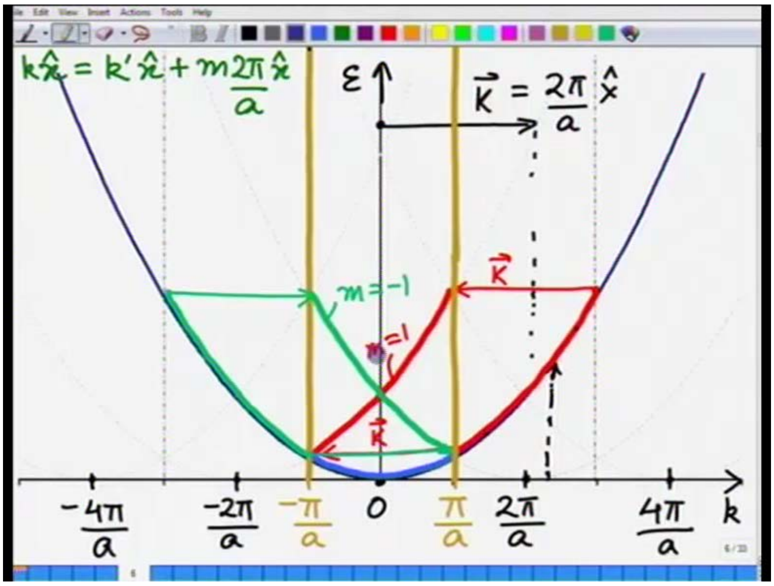

Let us use a another color lets use a red line let us say I have a line which is like this here is a red line which runs like this, this continuing line is the red one and use another color. Let us use green color which is this portion of the line curve. Remember I am saying this red and green portions now also have to be plotted in first Brillouin zone. So, what can we do what we can do is that suppose you now use m is equal to plus 1 and m equal to minus 1, if you use that what happens, let us use m equal to plus 1 for a minute. If m is for m equal to 1 what happens then k is equal to k prime plus 2 pi by a, which means k prime which means k prime.

So, you notice that if I use this lattice pointless k vector the n equal to 1 means. What n equal to 1 means that the lattice capital K vector I am using is this vector from here to here next lattice vector. This is the directive vector k equal to 2 pi by a. There is the lattice vector I am using capital K reciprocal lattice vector. If I use this lattice vector any k value here or here any of these k values can now be transformed into a k prime which belongs to first Brillouin zone by using this capital K.

If so, then if this is the value of k if say let us say this is the value k right here, if this is the value of k then what is the value of k prime say if I this is the value of k I can substitute that value of in there and calculate k prime as k minus 2 pi by a essentially. Now, if I calculate this if I use this so, I find a k prime by a form whatever the k value is if this is the k value if this is the k value from this cal k value, I subtract out 2 pi by a then I am basically back n I will you back n essentially, this whole curve then red curve can be represented in here like this, this red curve. Therefore, shifts from this point therefore, shifts to this point by capital K vector and this point shifts to this point by capital K vector, so by capital K vector we can shifts these two points.

Similarly, for green line this green line will shift same energy remains the same, but when you plot it by shifting this point like this and this point over to here. Essentially, what we have done is that used a minus m equal to m equal to minus 1 for m equal to 1 to transform all points into this same segment of the parabola which is shown here. Here this segment of the parabola into the first Brillouin zone, by doing this and I have shown you two green segment for m equal to minus 1, then k prime would be equal to k plus 2 pi by a which is essentially a parabola which is centered at minus 2 pi by a.

There is a parabola which is which center at minus pi by a. So, essentially you can see that whatever value you take if you subtract from that this k value subtract 2 pi by a all the red points get shifted into the first Brillouin zone. If you take all these points here add to it 2 pi by a, you add 2 pi by a to it and then you can see that that can be shifted into it is it can be shifted into this, this within the first Brillouin zone this green also can be shifted into the next Brillouin zone.

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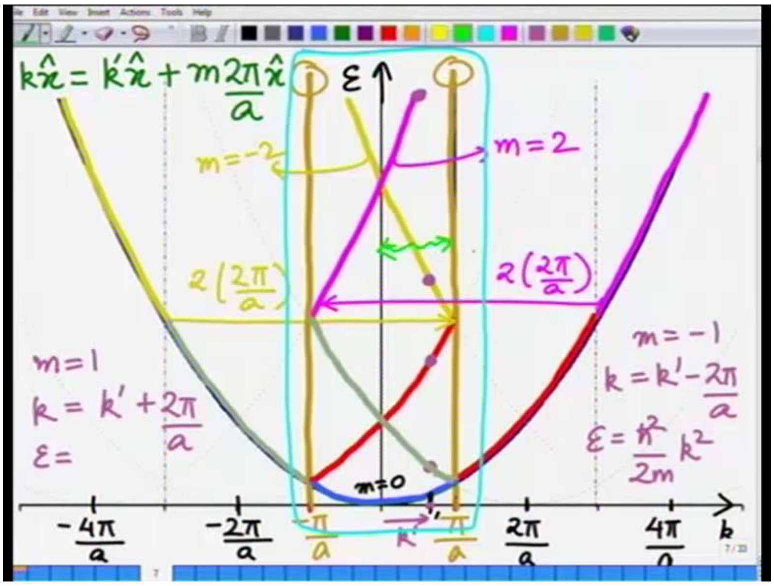

Now, if I look at further another portion of it let us say let us say we look at this portion of here going up to further up this portion if I see now I can use 2 k vector and this, this portion can again be transformed into. Now, I can again transform it into this particular curve and then this, this would be transferred as follows where this is equal to 2 k 2 times 2 pi by a. Similarly, this portion of curve let us use another color this portion of the curve which you see here can be transform right here. By the same way I can shift this quantity right here from here using two times 2 pi by a, so this curve is for m equal to 2 and this is for m equal to minus 2.

So, you can see that every potion of this parabola by this by in this in this form we can keep shifting to we can we can keep shifting this into the first Brillouin zone essentially. Therefore, if I now read as follows if I take a value of k prime if I take the k prime to be lets us say this value and I read m equal to 0 right here m equal to 0 then all I need to do is take the square of k prime and I can get this energy which I have just plotted out here. If I want to take this k equal to this point k prime k prime is this point which I am showing you here and if I use m equal to minus 1 then it is simply means that is k prime is equal to k prime k minus 1.

If I use my k 2 pi by a therefore, say at this point I can keep calculating k values which is k prime which is k prime is right marked here this is k prime I am talking about this is the value of k prime. Since I am reading this green curve m equal to minus 1, so then that means it should be equal to minus 2 pi by a I can take a square of this and calculate the energy still as E h square by 2 m k square now and I will find this energy to be equal to this point. Similarly, if for same k prime I took m equal to 1, then in that case in that second case the which I am now describing m equal to in this case minus 1 for m equal to 1, I would write then k and I will use this k prime here is the k prime value here plus 2 pi by a.

In that case again, energy will be calculated in same way and I will calculate the energy to be here and if I use similarly, m equal to minus 2 then right here if I use m equal to plus 2 then I will be right here in these 4 points. This way for all the entire this parabola this whole parabola which is going all the way up to infinity can be represented only within the confines of first Brillouin zone. I using this lines different lines within the first Brillouin zone and labeling them appropriated with the appropriately with a value of m if introduced in there.

Then you can see that we can we can basically confine this entire thing this entire band diagram essentially we what we need to do is confine this whole thing only within this region only. Within this region we can look at it and this is the band diagram really, now you can see that x axis is confined because of Bloch's theorem. Though energy when we are still using as the free electron energy which energy values may be incorrect, but I am just mainly trying to show you that x axis is not limited x axis can be limited to the extend only within the first Brillouin zones all for k points can. Since, the can be collapsed back into the Brillouin zone.

Therefore, we can represent that into first Brillouin zone essentially by plotting E versus k prime whose extent is from minus pi by a to pi by a with 0 in between. Not only that, you can see since it is symmetric about k equal to 0 therefore, you need to plot within the first Brillouin zone only one half of it that should be adequate. That means in fact if you plot only this half from here to here that should be adequate enough to represent the band diagram because we know the other side is simply the mirror image of it.

Therefore, there should be simply sufficient for write and see in actually in plot this band diagram only within the half of the Brillouin zone alright. This is the general idea how do we represent a band diagram in a confined space and why we are trying to do this because in this case new one dimension involved, when there multiple dimension involved what do we do. So, let us move on to this three dimensional now real systems and try to show you how band diagram band diagram using this principle constructed in that case, so with that then we will be able to understand how band diagrams are done. So, in order to do, so let us use this.

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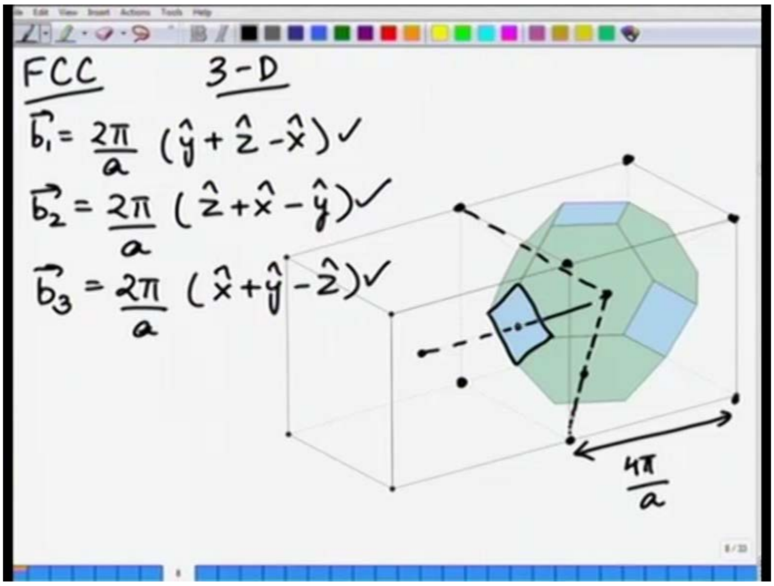

Let us use lets use the F C C, now three dimensional, let us do the 3 D, now let us consider F C C. If we look at F C C, then what happens in the case of F C C, F C C lattice is reciprocal lattice vector for F C C. I just given right here 2 pi by a y hat plus z h at minus x h at and then 2 pi by a z h at plus x hat minus y h at. Here v 2 v 3 2 pi by a x hat plus y hat minus z hat right here and how does this look like F C C reciprocal lattice looks like a B C C, so what is the B C C.

So, what I have shown you here in this picture is here are the lattice point B C C lattice points here are the B C C lattice points in one cell and this lattice parameter is 4 pi by a. Recall reciprocal lattice for F C C has a lattice parameter is B C C and its lattice parameter is 4 pi by a. So, here is 4 pi by a and then there’s n there is a lattice points right in the center about that then you take perpendicular take this right here like this.

Construct like this take perpendicular bisectors where is the perpendicular bisector you go there is a, another lattice point right here. For the another cell I have shown you here is the line running like this from to here and this is the perpendicular bisector for it right here is where it intersects.

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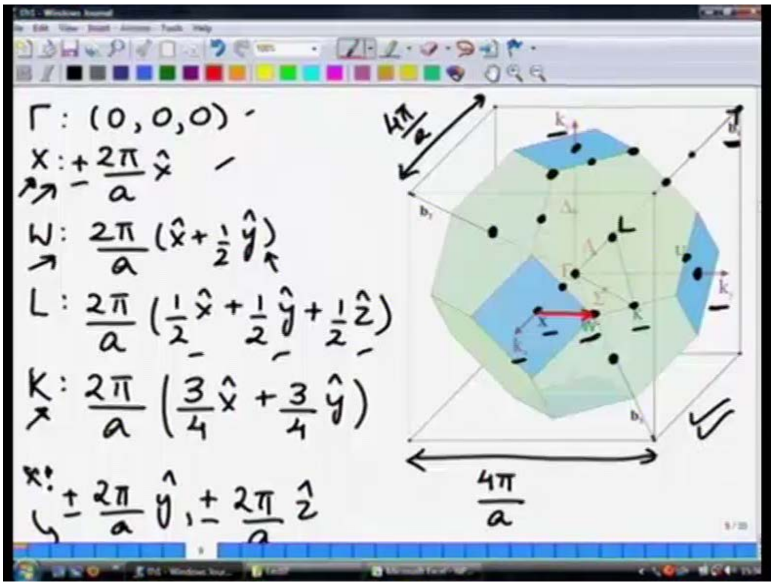

So, using that we have constructed this Brillouin zone, so this is the Brillouin zone, this Brillouin zone is now shown separately right here also. I had told you that there are some the centre point is called the gamma point and then a vector b 1. This vector b 1 is shown right here, b 1, remember is, this whole distance is lattice parameter 4 pi by a. Again remember that, so this is 4 pi by a, so that is the lattice parameter once this is the lattice parameter then you can see that I have taken x direction here is the k x direction here is k y direction here is k z direction 0.

This is z direction, if these are the x y and z directions then you can see b 1 vector, the b 2 vector, the b 3 vector which is corresponding to this which moves in y direction. Let us do one of them, say b 1 vector, if you want to do in y direction, move half in z direction move half and in minus x direction move half. So, let us move in from center right, here let us move half in y direction, so we reach here, let us move in z direction half. We route each here and let us move to minus x direction half, then we reach here, so that is form gamma point to this point right here is therefore, the b 2 vector. This gamma point of course, is just 0 0 0. There is a center of this, using this as the reference let us look at x point, x point is right here.

So, what is x point, this x point, therefore, is simply 2 pi by a x hat 4 pi by a is the lattice parameter, so x point this point coordinates of this point are 2 pi by a x h at 0 0 in y and z direction of course. So, whatever is what written x h at zero point, so that is the that is the vector here from gamma to x. This is the vector and if I look at w point remember x point is not one point, even this point is x point of same symmetry, even this point is x point.

So, I have written it in x direction, but x vector could be 2 pi by a, in fact plus minus I can put I have taken plus 1 by I can take minus 1. Also, you can take plus minus 2 pi by a, you can take 2 pi by a y h or you can take plus minus 2 pi by a z h. All these are x points, so you I have take shown you only one, but they could the all equal and symmetry so they all considered x point.

Similarly, look at w point which is right here, so these w points are equal and symmetry everywhere. So, this is also a w point etcetera, etcetera. So, these are equivalent points I will shown you one which is marked here at this particular point I had shown you this particular point is therefore, 2 pi by a x plus half y x at plus y half y h at. Try it out yourself, then the l point I have marked out this point this is also l point, all these are l points. These are all l point and I have right here the one I have marked here I am writing that particular one, but all the equivalent points.

So, those are 2 pi by a half in x direction half in y direction and half on z direction so that is what this one is. Similarly, k point, I am marked out I am marked out this k point, but whatever hexagons you are seeing their mid points of those all, all are equivalent points and they all therefore, there will be will k point and u point will also marked here.

So, all k points of equivalent symmetry, that means this will be a k point this will be a k point right here all this three will be k point. The other ones will be there four sided figure join is the six sided figure, those will be all u points so the that means this will be a u point and this will be a u point and so on. So, that is you get an idea what we going to do is now plot these band diagrams within certain directions particular direction for example.

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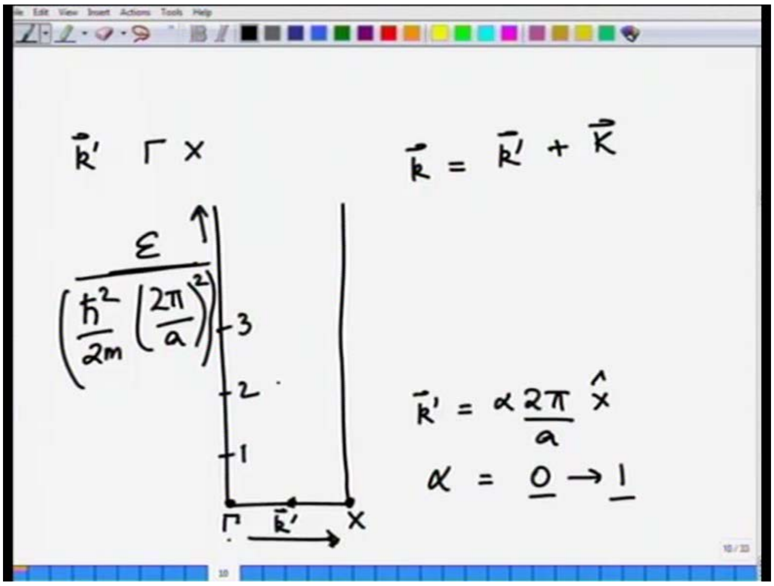

If you think that k prime will allow k prime to go from gamma to x. So, I want to plot the band diagram energy, energy versus some k prime is what essentially, I am going to plot and k prime. I will confine in the first Brillouin zone from gamma to x remember gamma is the center point and x is the edge of the Brillouin zone. So, I am going to plot from gamma to x and whatever is it is mirror image is in minus x direction a, therefore we do not need not plot that.

So, if I take this then I can plot these energies for this k prime, so I can take any k prime, so let us say this, this is k prime right here this is this value of k prime which is equal to let us say half the distance between gamma and x. So, let us plot that out now, how we plot this. So, once I know k prime remember I can always find a k which is k prime plus some capital K prime plus capital K vector. Now, what is the capital K vector, in this case that capital where k vector is m 1 b 1 plus m 2 b 2 plus m 3 b 3. So, what is this k vector lets expand it out by substituting b 1 b one b 2 and b 3 from right here. If you substitute in there what you get for F C C, you get this as 2 pi by a, so let us substitute in their value of b 1 in there, b 2 in there and b 3 vectors in there.

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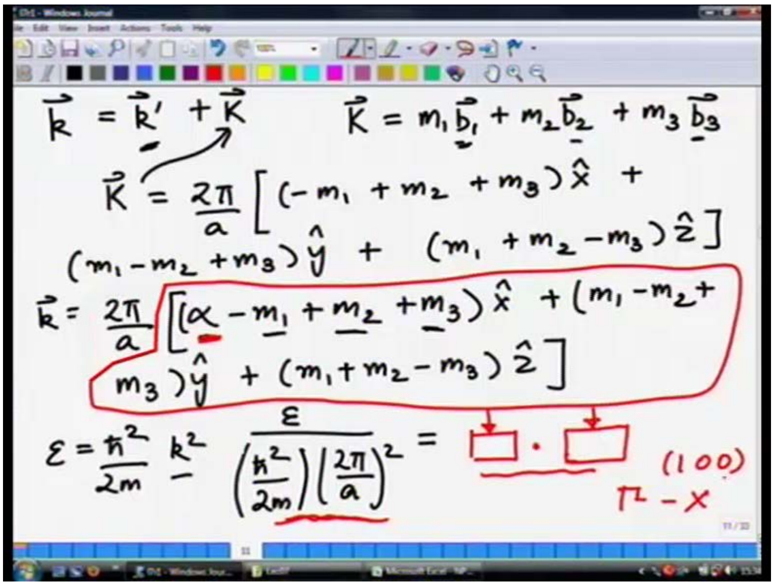

So, that k then becomes minus m one plus m 2 plus m 3 x vector m 1 minus m 2 plus m 3 a y vector plus m 1 plus m 2 minus m 3 z at. So, that is the K vector now and what is k prime vector for this particular k prime vector, what is this in from gamma to x direction. This k prime vector I can write it as something alpha times 2 pi by a x at. I can write it like this, where alpha goes from 0 to 1, alpha goes from 0 to 1. That means when alpha is 0 and then I am at gamma point when alpha is equal to 1.

Then I am at x point, then I reach this x point alright, if I do so then and alpha takes value from 0 to 1. So, if I substitute that k prime also in there then that case k simply becomes equal to 2 pi by a, so I am substituting this k prime in here and I am going to take this k which I have just written out. I am going to substitute that right in here and I calculate k, in that case k is equal to 2 pi by a alpha minus m 1 plus m 2 plus m 3 x h at plus m 1 minus m 2 plus m 3 y h at plus m 1 plus m 2 plus m 3 z h. Now, you see I calculate, I can substitute different values of m 1 m 2 and m 3 in this expression and calculate energy as h square 2 m and k square a, free electron energy I can calculate.

So, energy then once I calculate this a for different values say m 1 m 2 m 3, then remember alpha only values from 0 to 1, that means I will always be confined within the first Brillouin zone in direction of gamma to x point. So, as long as I am confined between these two points that is why I am going to plot I am going to take k prime value. That k prime value is defined by alpha, if i a alpha value whatever 0 or 1.

Accordingly k prime value gets fixed and I use different m 1 m 2 and m 3 and I can now plot out all different energies with this index m 1 m 2 m 3. Just like in one dimensional case we used 0 1 minus 1 2 and minus 2 here since three dimensional case, I will have to use 3 indexes m 1 m 2 m 3 to label the label different segments. Now, I have done this calculation for you, so let me first show you these calculations, which I have done for you.

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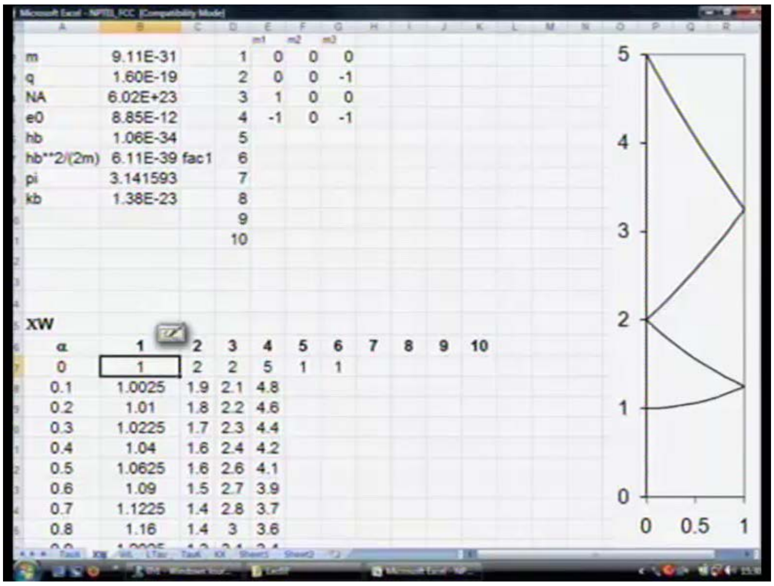

So, that that you will do see here is here is gamma point, here is the point, this is the gamma point, here is this point x, so what I am plotting is 0 to 1 means is basically value of alpha this value of alpha I am plotting here say 0.5 and 1. This energy that I am plotting here is energy equal to, so used energy is k less energy divided by h square by 2 m. This is the scaling I am using, nothing else, energy versus 2 pi by a whole squared, so that is the energy I am plotting. Essentially, this is a constant factor, remember a is a constant and everything else is a constant.

So, this is just normalization energy nothing else, so that is why I am able to use the word numbers like 1 2 3 here etcetera as a dimensionless right here because of this reason. So, I have made a dimensionless quantity other than that, there is no big deal about it. So, if I look at this, then that is what I am plotting this energy which I have just mentioned to you that is on the y axis.

What I have done is notice I am showing is this is a excel file, in excel file I am using these different values of m 1 m 2 and there is a values of m 1 m 2 and m 3. These m 1 m 2 m 3 for at different colors I am going to show you here 8 different curves where if when m 1 m 2 where m 3 is equal to 0 0 0, then m 1 and m 2 and m 3 are equal to 0 minus 1 and 0 and m 1 m 2 m 3 are 1 1 0 and so on. For these particular values 1 2 3 4 I have shown 8 different sets of value, for each set of value, this set is indicated right here 1 means this set here 2 means this set here 3 means this set here. So, I have 4 means, this set right here 0 1 1 etcetera. For these values I have calculated energies which you can see alpha is varying I am varying from 0 to 1.

Essentially, that means I am going from gamma to x is what I am going from there to there and what happens, then so x axis. Basically, I am plotting alpha, so energy therefore, is accordingly normalized and if I look at this point, this cell so what is the calculation I am doing you can see right here that here is the value of alpha minus. Look at the formula m 1 plus m 2 plus m 3 squared m 1 because it is k squared. Now, and m 1 minus m 2 plus m 3 squared and then m 1 plus m 2 minus m 3 squared.

This is the square of it and the in front is h square by 2 m into 2 pi by a square, I have take all that factor and divide energy divided use that for division of energy. Therefore, only thing that is left is square of this part, so I hope you understand this part and I hope understand what I have just said. So, with this now notice what happens here is the curve for this, if I calculate this formula, then here is the curve, this curve I had shown you here this is for m 1 m 2 m 3 equal to 0 0 0. Similarly, for these, well in this case I had plotted six different curves for 1 to 6, you can ignore this 7 and 8 then we ignored. So, 2 3 4 5 6 curves I have plotted here 1 2 3 4 5 and then six curve for these six curve corresponds to these different values which I had shown here, alright?

So, now as we are going to do this I am going to show you all the curves like this suppose, so this we had plotted from gamma to x suppose you want plot from x to w which I am going to show you did next. So, let us do that also, this is gamma to x actually let me write this out, so if I want to calculate this, so that there’s no confusion what I have done is. I am going to write this as if I take this factor if F can write this as energy by h square by 2 m 2 pi by a whole squared. I can use this and equal to then square of basically this entire factor from here to here and I will use different pen square of this factor only, use this factor, use this factor square of this red factor.

Basically, dot product of this particular factor is essentially square which I am plotting here, this factor is in here and this factor is in here there is a square of it. So, essentially that is why I was telling you I am just plotting the square of this number, this dot product of this number and I am plotting this quantity versus alpha is what I am plotting to you that gamma versus x.

Now, suppose you want to plot from even, so what we do is that way we plot is we go in some major directions, so for example, we in this particular case I just what I just shown you is that we are going from gamma to x which is a 1 0 0 direction. So, we go for 1 0 0 direction and then from x, I am going to go to w some from x, I want to go in this w in this direction, so next plot that I want to make therefore, is going from x to w.

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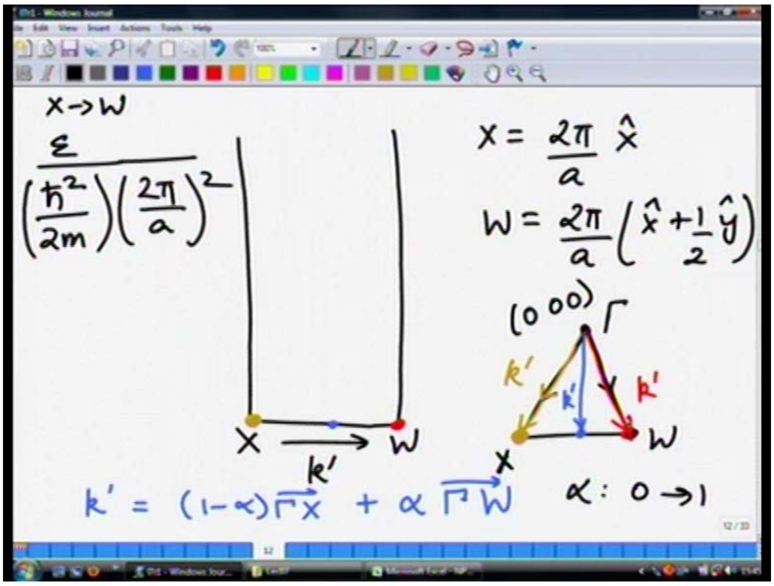

So, if I do so then let us go to next page, here now I am saying that suppose you want to go to x to w that means I want to plot. Similarly, this energy versus h square by 2 m 2 pi by a whole square is what I want to plot, when my points vary from x to w and remember x point was equal to let us do that x point was equal to remember 2 pi by a x h and w point was equal to. Remember it was equal to two pi by a x plus half y, so there was 2 pi by a x plus half y, say if I want to go from x point to w point, so I if I will again, if I am look at this way here gamma.

Here is x, here w, here is w point, I want to go from here to here, so if I want to do that, then let us see, then let us just plot it out. So, this three points from a plane, so here is gamma point, here is x point and here is w point, here is this gamma point which is the reference 0 0 0 that is the origin. Here is w point, so what I want do is I want to plot it as a function of this vector, this vector right here, I want to plot this k prime.

This k prime being plotted from here to here and this k prime I want to vary from this gamma. So, this is at this point right here at this point or lets use a color at this point this vector is equal to this vector, this is vector at x point k prime vector is this. This is the k prime vector and at this point right here which is corresponding to this point this point is this point and k prime vector in that in that case this vector.

So, at any point in between let us take this point in any point in between the k vector is k prime vector is this product or I am plotting basically k prime versus k prime vector is what I am plotting, so what is the k prime vector. Essentially, we can write it down for x w, so I can write this k prime vector as this k prime vector can simply be written as equal to 1 minus alpha times gamma to x vector gamma to x vector plus alpha times gamma to w vector. What is that mean, let us use a black pen itself if I want to plot this essentially k vector k prime vector, means this what is that means that means that even alpha will allow to again verify from 0 to 1.

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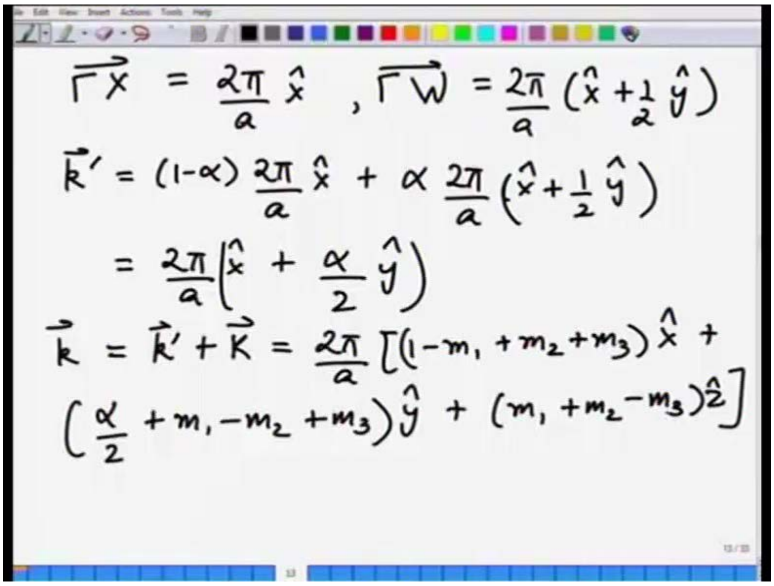

So, what is that mean that if alpha is equal to 0, then in that case I am essentially my k prime is this vector, this orange vector or yellow vector and that means it is we are in x point when alpha is equal to 1. When alpha is equal to 1, in that case I am really probing gamma to k vector is gamma w and in that case this red point is the position here is i. Now, right down my k prime vector, so if I write down my k prime vector, therefore since I know what this means.

So, as you can see what is gamma to x vector, gamma to x vector is of course, 2 pi by a x and gamma to w vector is what 2 pi by a x h at plus half y is as this vector. So this k prime vector k prime vector now is equal to simply, I can write this as 1 minus alpha 2 pi by a x h at plus alpha 2 pi by a times x h at plus half y h at which is equal to then 2 pi by a x hat plus alpha by 2 y h at. Therefore, I can now write k vector, this k vector then equal to is equal to k prime plus k vector and since k vector you already know. So, when add it up and you will get 2 pi by a 1 minus m 1 plus m 2 plus m 3 x h at plus alpha by 2 plus m 1 minus m 2 plus m 3 y h at plus m 1 plus m 2 minus m 3 z h at as this vector.

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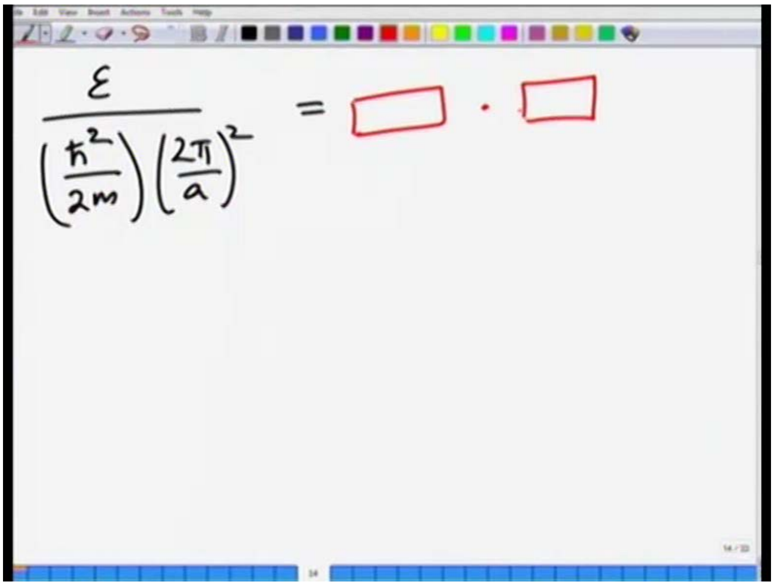

So, now I can calculate for different values of m 1 m 2 m 3 the same way I can calculate this energy versus h square by 2 m 2 pi by a whole squared l essentially equal to dot product of this. Again same just this term within the brackets whatever this term in the brackets I can take the square of it, so this term in the bracket dot this term in the bracket again I can do that part. And for different values of m 1 m 2 and m 3 I can now again plot this energy versus this curve, so the so let us do that again.

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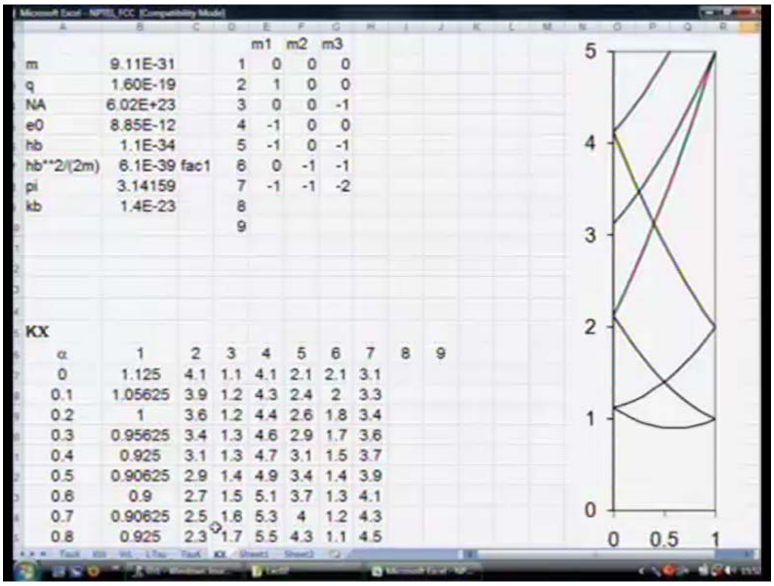

Here is for x to w, so this point is right here is x, this point is x and this point is w and again I have taken here four different values of m 1 m 1 m 2 m 3. This is set 1 set 2 set 3 set 4 and for this set 1 set 2 set 3, I can see here is the formula, here 1 minus m 1 plus m 2 plus m 3 squared. Then alpha, this is the alpha in a seventeen cell number of excel which is right here. This is a 17 cell a and this is 17 cell this value divided by 2 plus m 1 minus m 2 plus m 3 squared m 1 plus m 2 minus m 3 whole square though the values which, I have calculated here and plotted right here and four this different four sets I have plotted this and in principle.

I should be labeling this as 0 0 0 and I should be labeling all these values ok. The point is now, you can plot from x to w say I do that this is what I have done for from w to l, I have plotted w to l. I have plotted from l to tau I have plotted from tau to gamma, sorry l to gamma to k and k to x and all this plots I have plotted which I am going to show you now in one sheet I l them all to you together.

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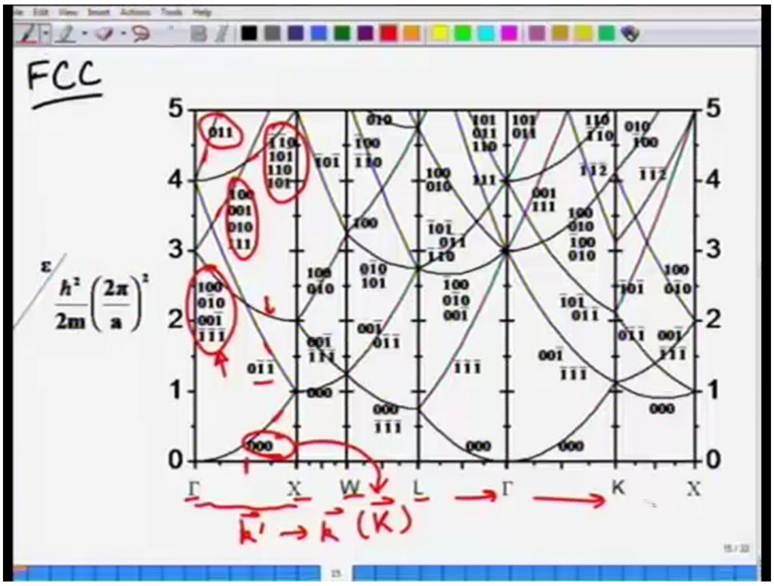

Like this right here is then a band diagram for F C C, which you can now see that in this particular case what do you see. So, here I had shown you plot of gamma to x so remember this is how its varying from x axis varying from gamma to x. I am using m 1 m 2 sorry in principle, therefore you are reading from any point we can read here k prime vector this is the k prime vector going from gamma to x.

The real k vector then is obtained by adding capital k vector to it and what is the capital K vector we are adding the capital l vector we are adding is using this index of m 1 m 2 and m 3 as 0 0 0. Once we do that then I can take the square of that to calculate the free electron energy in any case, whatever the energy corresponding energy is to that small k vector once from k prime. So, this is k prime k prime is transform to k by using this indexes which are written here for m 1 value m 2 value and m 3 value. That means, I tell you what k has been used this index, tells you what k has been used to transform from k prime to k.

This axis must be read as k prime vector, so you and k prime vector always belongs to first Brillouin zone. So, you can confine that and when I plot that you can see this has been obtained by using this particular part portion, the curve is this obtained by using this particular curve have been obtained by using any of these values. This particular curve has been obtained by using any of these values using this particular m 1, m 2, m 3.

Now, remember this happens only when I have chosen for example, k point as or x point as 2 pi by a in x direction, I could have chosen it in minus x direction, I could have chosen y direction, I could have chosen it in z direction. So, with that new set of indexes will show you up also, but very quickly if you see this direction m 1 m 2 m 3 you should be able to see that degeneracy also. This curves a degenerate curves saying that different m 1 and m 2 and m, three values are give you over lapping curves that showing you energy degeneracy.

There is a separate issue which we won't be addressing in this class but, what have we so this is plot the way this band diagram. Therefore, is shown is by going from one major point in the three Brillouin zone, one major point to another major point to another major point major points of symmetry on this Brillouin zone. So, for example, as we go from gamma point to x point, x point to w point, w point to l point, l back to gamma point and from gamma point to k point and k point to x point.

This is how this whole band diagram has been constructed and you can now see that for many, many directions, all different major directions for different k points, we are able to confine we are able to represent this band diagram. So, I will make some observations about utility of this band diagrams in a minute, but similarly, before I move on, let me also show the show this for you to you for B C C structure also.

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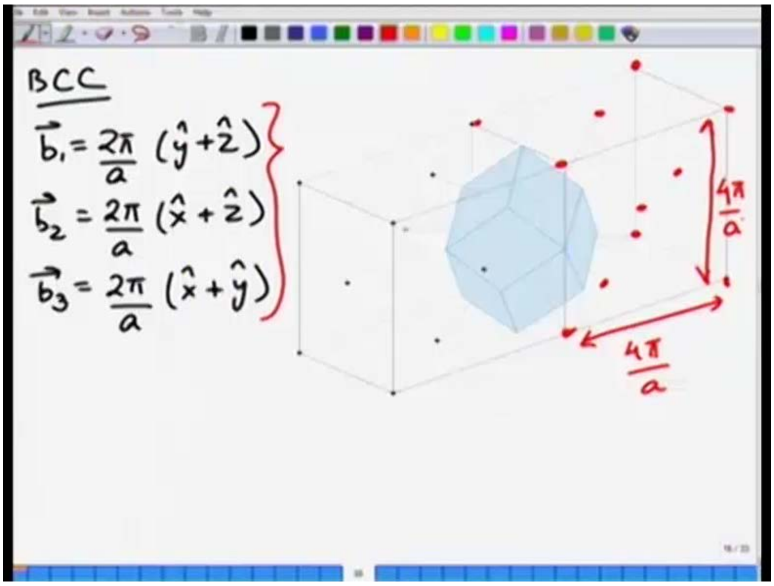

For B C C also I have shown you that B C C, b 1 b 2 b 3 vectors start looking like this, then that means in reciprocal lattice it is F C C. So, if I have shown you this F C C lattice points right here, these are the F C C lattice points, F C C lattice shown here and if I again take the perpendicular bisectors. I have shown in the constructor or the construction of the Brillouin zone that Brillouin zone looks like this again. I have a gamma point right here in the center, then there is a point like this which is a h point.

So, there is a h point right here, this is the h point right here which I have labeled here also which is equivalent h points. So, these are therefore, this h have been labeled as 2 pi by x, but you are welcome to write it as 2 pi by a, you could have chosen h as 2 pi by a y. You could have chosen 2 pi by a z, this periodicity of course, again is 4 pi by a is the lattice parameter of this red sell.

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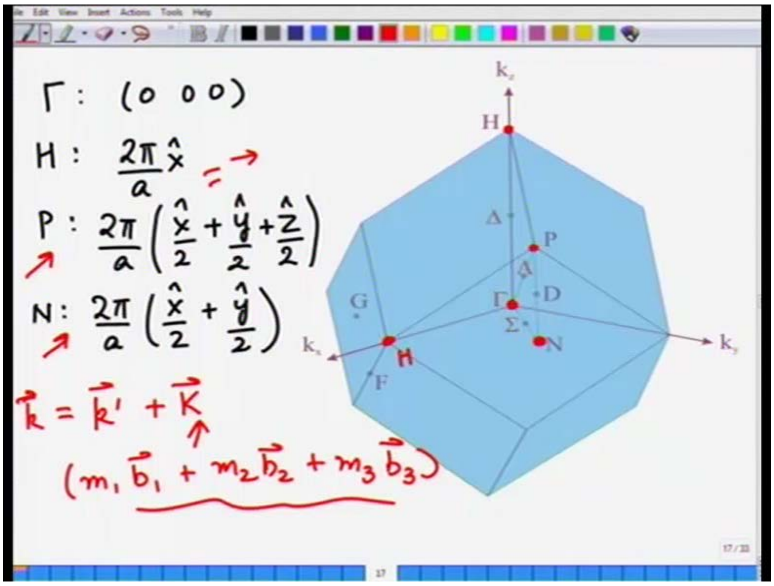

So, 4 pi by a, so I just 2 pi by a x you could have chosen h has 2 pi by a y, you could have chosen 2 pi by a z which they all equivalent points. Similarly, vector p or this point p is right here, whose coordinates are given here you can verify yourself and here is point n which is which you can verify here. Now, again for this structure also we can do the same exercise we can do the same exercise for this particular case also, where we write down for go for one direction from various directions from gamma to h h to p p to n and plus to gamma.

Write down the k prime vector K, we can write down the k prime vector correspondingly and to this k prime y vector, we can add this k vector with using different m 1 and remember m 1 b 1 plus m 2 b 2 plus m 3 b 3 is this. Essentially, this k vector, so by using different m 1 m 2 m 3 value, we can calculate k vector and once I calculate the k vector, I can calculate the energies. Once I calculate the energies, I can do the same plot for B C C also we do so then let me try to quickly show you before I end this lecture.

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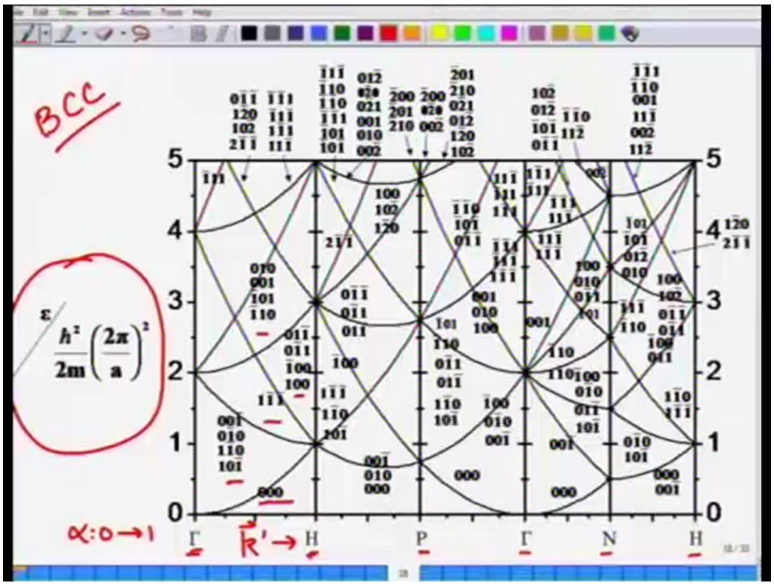

If we do that I have done, therefore, B C C also and for B C C, I have plotted it from gamma point gamma point to h point, and it looks as shown here for different m 1 m 2 m 3 values same way then form h to p. I am moving fast because now you understand how to do it and now, you can construct this is assignment problem for doing the B C C part yourself.

Then p to gamma point and then gamma to n point and I am going to show all this together and then from n to h points, so I have done this exercise in excel sheet myself. So, I will ask you to do this for B C C what I have done for F C C I have shown the details of how it is done for F C C exactly, the same thing has to be done for B C C which you can try out.

Let me show you how this will look like in that case and you can compare it whether you get the same thing or not. So, here is the curve again I am plotting this E versus h square by 2 m divided by 2 pi by a whole squared versus this is the k prime vector. Here is the k prime vector that I am plotting, here this is the k prime vector going from gamma to h. Of course, you can think of this as k prime vector or you can think of alpha going from 0 to 1 either way because the way we write it down. it is the used the parameter from alpha.

So, which I take I have shown you, so this is the same this is 0 0 0, I have written this indexes out, you can now what you should do is you should try out yourself the same exercise and plot this for B C C, this is for B C C. The previous one of course, which i form was F C C, so this was F C C and now this for B C C. I am not going to go over this but, gamma to h h to p p to gamma to n n to h. I will request you to plot this yourself, with this we should be able to understand.

Now, let us say take a minute or two to understand what are we done what we have done is that we have understood. Now, untimely what we want to do, we want to show E versus k diagram, E versus k diagram is what is we are calling as band diagram. We want to show band diagram for real semiconductors in up to which are good for optonet electronics.

Why do you want to do that not next lecture, but even after that I will show you what information you can get from E versus k diagram, this E versus k diagram give us lot of information which is good for optoelectronics and electronics in general. So, those I will show you one lecture hour from in the seventh. In the ninth lecture, I will start telling you about that E versus k real, E versus k diagram of semiconductors and what the utility of that is so in order to get to E versus k diagram. What we have done is there is a 1 axis e other axis is k we have figured out how to handle the k axis. We figure out k axis is a three dimensional axis once again its extent is infinite minus infinite to plus infinite in all three directions.

So, what we have done is, we have learned how to handle in this lecture and the previous using the Bloch's theorem. In this lecture we learned how to handle this x direction this k direction and represent it in this particular form as its on your screen right now. So, this k and we can confine this only within the first Brillouin zone, once you have done that then but, the E axis, the energy axis is still hypostatical energy values. That means we are assuming as if the energy is over free electron energies, those real systems are not the energy in the real systems since there is a potential, the energy was Schrodinger solution, Schrodinger equation must get must get modified and that energy should be different.

So, only thing left for me to do in the next lecture is to show to you that energy will get modified. If we can calculate this energy again, correct value then instead of plotting the free energy value of energy, we have plotted here instead of taking k square and h square by 2 m k square. Instead of that, if I can for different k prime values which I have shown you on this x axis right here or k values or k prime value, whichever way you want to talk about if a corresponding to that I can calculate the realistic energy. Then I can show you the realistic energy in here in this diagram, which you see on the screen and I will have my E versus k diagram.

So, in next lecture I am going to show you first as a approximate k is I am going to show you what will what will be consequence of periodic potential on energy, previous lecture I have shown you consequence of periodic potential on the k axis. Now, next time I will show you consequence of periodic potential on y axis, as a energy axis as a approximate calculation. Since, real calculation is very tuff. So, I will show you only the or else it is tuff and also cannot be done in a close form solutions, and there those require large programming large software and huge run time etcetera.

I explained to you why the problem is complicated problem, so what we going to do is we want to use the real calculations from literature and show it to you, but before that I will show you approximate calculation. I will show you what the consequence of periodic potential on the y axis energy axis will be and from that point on that will be eighth lecture. Ninth lecture will be then if we have a E k diagram, then what can we get out of it what is information, I can get out of it and in the tenth lecture then I will start showing you the realistic E versus k diagrams.

Thank you.