Physics of Materials
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Lecture No. # 32
E Vs K, Brillouin zones and the Origin of Bands

Hello, welcome to our thirty second class in this course the physics of materials. So in this class, we are going to pull together lot of information that we have seen in the last few classes, and understand how we can predict material properties based on our analysis that we have developed, and these skills that we have developed to understand how the material behaves, how the constituents of the material behave. So, we finished off with the diagram which wherein I showed you the fact that you know on the same diagram we can put together the reciprocal lattice information as well as e verses k information. So, we will start our analysis just one step behind from there and then proceed forward.

We will look at how nearly free electrons interact with the lattice, and we will do this in considerable detail in one dimensions in one dimension, because that is easier to understand, and easier to represent on a on the plane of a board. So we will do that in significant detail; I will show you also on the board how the same information can now be represented in two dimensions. And finally, we will look on a at a few slides where we are looking at the same information, the same kind of interaction for a material in three dimensions.

Now, before we start drawing the diagrams and looking at the interaction, I am as tell you that you know when we actually finally built up this model using the Fermi dirac statistic. Importantly we identified something called the Fermi energy which is the energy of the highest energy level electrons right. So, we also noted that everything is filled up to that energy level, and that is this first set of the highest set of electrons present in the system in terms of energy. And therefore any interaction that you see with the outside world so to speak is based on what those electrons can do. So initially, we will draw the diagram without bringing in the Fermi energy, then we will show you where the Fermi energy is and then the let us look at what it represents. So let start from something that we are familiar with and will be proceed from there. I said that our we should understand clearly what we are drawing, so that is why I am going to show you something and reiterate something that I have mentioned before, and then you can follow the diagrams much more appropriately, fine.

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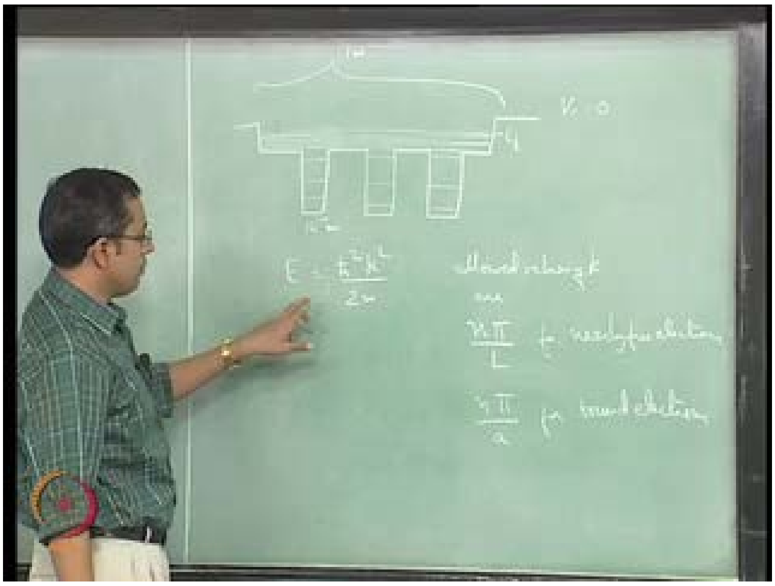

So this is the simplified model for our system that we are using and we have seen this few times right. So this is V equal to zero where in the electronic at infinity and therefore its potential is zero V 0 is 0 - 0 volts.

If you want to called it that, this is the potential well that corresponds to the extend of the solid, this represents electrons which are trapped within the solid, but still are free to move through the entire extend of the solid; they are not really confine to any one atom or any ionic core and then these potential wells represent the potential narrow potential wells which are potential wells corresponding to a each individual atom. And therefore, the electrons that are trapped here now are localized that is the term that is use they are localized to that particular atom right, and in terms of energy levels; these are some energy levels that they can have. So we have just these are all this just the schematic; so I am just showing you something here and then there are large number of energy levels here, which are very closely spaced this is the schematic.

We have to show something on the plane of the board and that is the way it shown to give you again, the widths here are ten power minus ten meters. The entire dimension here is of the order of a meter; I mean this is just a to give a scale of what we are looking at and regardless of… So, in fact if you look at one meters since this is only a schematic as you can imagine in one meter you can have ten power ten such atomic core. So to speak or may be half of that half as many if you are assuming the gaps are roughly similar, so I have just drawn three here; so obviously this is just the schematic. So this is not really, it is not that there are only three atoms in the one meter length; so there is the huge number of atoms it this is first schematic purposes. In terms of localization the basic concept of what happens when you localized is still that same regardless of the your talking here of the electrons at these energy levels or these energy levels.

And basically localization means the energies are now quantized which means only specific values of energy are permitted for each each of the electrons and those energy values can now be represented in terms of the allowed k values, because energy and k are related like this. Therefore, if only specific values of energy are allowed only specific values of k are allowed. In fact when we do the calculation it works out the other way we learned that, only specific values of k are allowed for the system once you localize it. Therefore, only corres those corresponding values of energy are allowed for this for those electrons.

Now the allowed values of k are two pi I am sorry are n pi by L for nearly free electrons and n pi by a for bound electrons and the difference is the as you can see the form is exactly the same n pi by some length dimension here, and the it is only the question of rather this length is one meter if it is for a nearly free electron or it is a which is sort of the atomic dimension which is here. So that is the difference between the two of them. So for both of them we can draw curves representing the allowed values of energy, so I will so they we now have a in a sense three cases two of them are listed here, the third one is for a nearly for a completely free electron which as escaped the solid. So for that all values of k are allowed there is no restriction any value of k. Therefore, all values of energy are low and this here the highest energy value here is E f the Fermi energy that we spoke about, so we will draw all the three of them and then will make a quick comparison.

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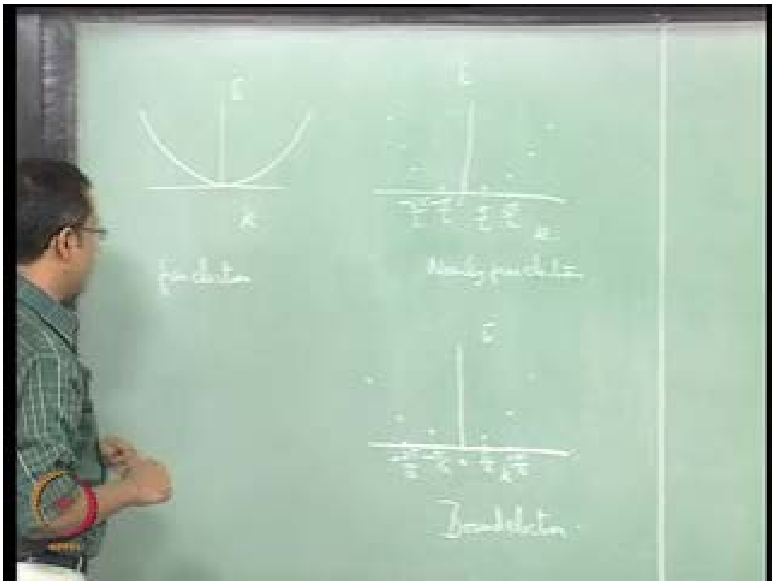

E verses k, here this is E this is allowed values of k, so for a free electron - so this is free electron, this is nearly free electron. So this is k again this is E now only discrete values are allowed and those values of k are n pi by L; so this is pi by L this is the two pi by L this is minus pi by L minus two pi by L and so on. And this is for a bound electron, so I just put it here E k bound electron so this is n pi by a allowed values of k, so this is pi by a this is two pi by a this is minus pi by a and this is minus two pi by a correspondingly you will have allowed values of k - I mean energy values, we can have further values somewhere there. Since the relationship is still h bar square k square by two m the energy the energy verses k the if you connect these dots you are going to get a parabola.

So the therefore, the shape is the same as that for a free electron except that several points here are now no longer valid; only specific points along this curve are valid and that is what we see both for a nearly free electron and for a bound electron. So this this is how these three figures relate to each other? Now the important thing to notice the scale of this is very different from the scale of this, so that is the important thing to note so for example, this pi by a, because this is a is of the order of ten power minus ten meters this is now in the denominator, so pi by a is actually very large value relative to pi by L which is where L is of the order of a meter.

In fact there are if you plot this figure on this scale then between the origin here which is zero here between the origin here and pi by a, there will be ten power ten points corresponding to allowed values of this nearly free electron. So that you just need to keep that mind for to understand the scale of these two figures I am not going to I am right now this is the separate figure this is the separate figure I am only drawing a comparison between the two so that you are aware of this scale of it. So you have to keep keep in mind the scale of it, the form of the equation is the same so you still get pi by L pi by a so that is still the same, except that a is ten power minus ten meters. So this is the and it is in the denominator so this is very large number so it is five times ten power ten this is simply pi.

So therefore, if you take the same this information and you plotted to this scale then you will find that there are ten power ten points between zero and pi by a, if you look at this figure or in other or put it an another way, if you look at pi by a here on this scale you have to go you have to add ten power ten points here I have only put two point here. So we have only put two or three four points drawn out here you have to go up to ten power ten points on that side, before you get the first pi by a here that is the difference in scale between this figure and this figure. So this is something we keep in mind, now so this is all with respect to the electron, what is our goal? Our goal is we will look go back to previous figure and we will see what we are trying to do.

We would like to understand what is the interaction between the allowed values of k corresponding to these nearly free electrons; so there are k values of this nearly free electrons. What is the interaction between the allowed values of the k values of this free electrons with the periodicity of the lattice? So lattice has some periodicity, so this is the different piece of information I write now a in imedi in our immediate in are dis in the discussion going to have, now we are not really concerned about these bound electrons, so we are not really concerned about bound electron. We only talk about the k values of the free electrons or nearly free electrons we only talk of the k values of the nearly free electrons, but we look at the interaction of those k values with the periodicity of this lattice which is still of the order of the a.

So the previous comparison I give true was simply that show you that the scale of a verses L, but I am show therefore, we are still going to use this a which is the periodicity of this lattice except that we are not talking in terms of bound electron, but this periodicity between the point and this point this point and this point it is still of the same sort of order of magnitude as these widths. So that is where the scale comes from roughly we get the scale. So that is how we look at it, so we are going to look at the periodicity which is now coming from which we are we discussed in the last few classes is being represented in reciprocal space using reciprocal lattice information reciprocal lattice designation - denotation. So the reciprocal lattice will capture the information of the periodicity of the lattice in that in the reciprocal dimensions the k vector will catch capture the information of the allowed wave vector in reciprocal dimensions and we will look at the interaction between the two of them.

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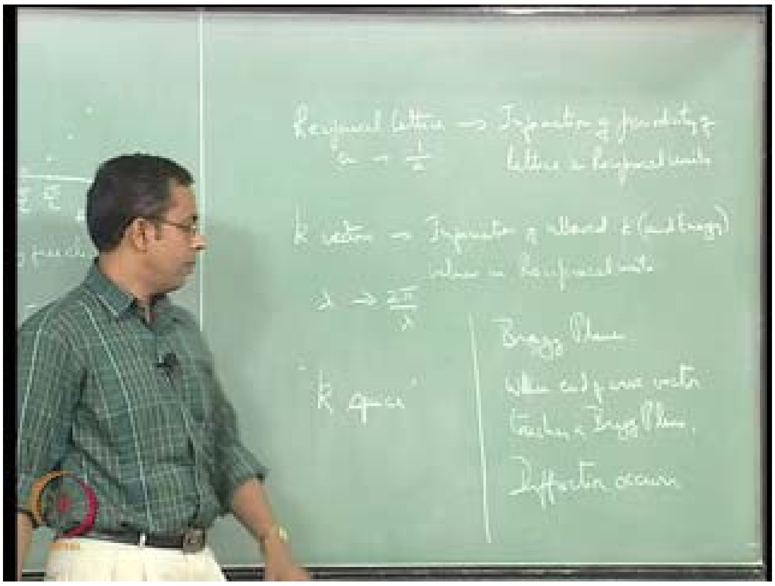

In this context we also saw put the down reciprocal lattice information of periodicity of lattice in reciprocal units and k vectors information of allowed k and energy values and therefore energy values in reciprocal units. So this is k vector captures information of allowed k and therefore, allowed energy values in reciprocal units and this is reciprocal lattice which captures information of the periodicity of lacite of the lattice in reciprocal unit of the structure right; only difference is in the in the manner in which discussed it this is lambda is being represented as two pi by lambda here and here a was being represented as one by a.

So the difference is that there is the scaling factor of two pie, so I will just put an arrow here, so lambda is to be represented as two pi by lambda a is represented as one by a. We talk of this interaction in in the context that we say that we are representing everything in k space, the diagram we will draw drawn in k space, what is k space? k space is one where the all the information is being represented in this form, therefore any dimension in any length that we see in real space we are plotting it as two pi by that length in reciprocal space, so that is the sort of the convention we are going to follow. Therefore, if you represent the reciprocal lattice information in k space again we will scale is by a factor of two pi and that is simply multiplicative factor, it simply means that you are only changing the you are multiplying you are not changing the the symmetry of the structure that you see.

you are simply changing the scale of the structure either in this case you magnifying it, because multiplying it by two pi and it is it does not change anything fundamentally, because we are representing two pieces of information on the same scale which is all we are really interested. We are able to look at the interaction only if all the information is the represented in the same scale, therefore it the necessary to do that. So we will represent reciprocal lattice also in k space and allowed way vectors also in k space and we will look at the interaction, so that is what we are going to do what is the additional thing we have done, we have seen that in reciprocal space we have identified what are known as Bragg Planes and we have said that when resi wave vector when end of a wave vector purchase the Bragg Plane purchase the Bragg Plane then diffraction occurs.

So when the end of a wave vector touches the Bragg Plane diffraction occurs. So this in fact captures the interaction that we are going to look at basically we are saying this Bragg Plane is coming from the reciprocal lattice. So that belongs to that represents, now the periodicity of the structure that we are discussing the wave vector that we are talking of belongs to the waves of any radiation or electrons that are represent in the system that are interacting with the system, in this case these way these are the wave vectors of those nearly free electrons present within the system. The interaction therefore, of these wave vectors with the periodicity of the lattice is capture by the fact that at specific values of wave vector when the wave vector touches the Bragg Plane diffraction occurs and corresponding to the diffraction process, what happens is, certain amount of certain values of energy now become forbidden. In fact what happens is when diffraction occurs that E verses k relationship gets distorted very, very near the diffraction condition as a result certain energy values get are prevented from occurring.

What we will do in this class is - we will look at this pictorially in the next class, we will actually put on values will look at how we can solve it sort of in analytical fashion we will see what equation we can put together? And see this in a mathematical sense so today write. Now you will look at it in a pictorial sense so that is how all this comes. Again wave vector now is in the two pi by L scale or n pi by L n pi by L is the scale for the this, this is Bragg Planes which are one by a and now two pi by a so again you see that it is something with a in the denominator on that scale where going to plot something with L in the denominator. So therefore, you will see this, so on this scale it look like a continuous set of points so that is what we are going to look at.

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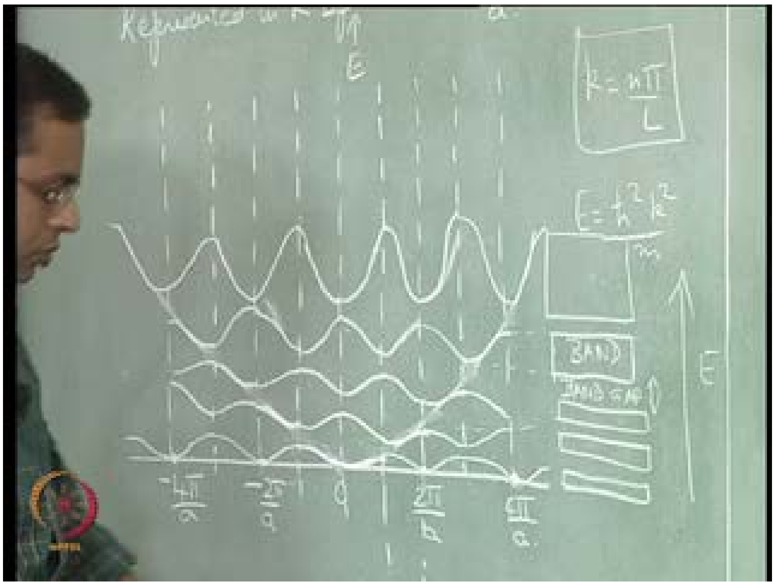

So now we will look at a one-dimensional lattice, one-dimensional lattice with spacing a inter atomic spacing a. Now to represent this in k space represented in k space, a will now get represented as two pi by a, if it was simply reciprocal space in the manner, we originally discussed it a would have been the represented as one by a, we are representing specifically in a particular scaled version of reciprocal space called the k space where the scaling factors two pi. So, a is going to be a represented as two pi by a. Therefore, reciprocal lattice vectors once you start - once you identify an origin for this k space reciprocal lattice vectors at occur at intervals of two pi by a. So, therefore we will we will plot that appear, so we will we will just say that this is your scale axis, this is the origin, so reciprocal lattice vectors occur at 2 pi by a 4 pi by a.

So for the moment we just take two two so that keeps the image rather clear again minus two pi by a and minus four pi by a. So this is the information - this is the representation of the periodicity of the lattice in k space lattice of periodicity a has now be represented in k space with these four points have just take an four of those point and represented them here. So that is all we have done we including one and they have to include the origin, so five points if you wish. Now we have we have a few things to do, we would now like to identify the Bragg Planes, so then we we know where it is that we can look for diffraction. So lets independent with respect to this periodicity lets identify the Bragg Planes. So, what is the Bragg Plane, Bragg Plane is is the plane that bisects - is the perpendicular bisector to a valid reciprocal lattice vector that is the Bragg Plane.

So, we look at the origin the valid reciprocal lattice first valid reciprocal lattice vector is two pi by a, so half of that is where the Bragg Plane will occur. So therefore, the Bragg Plane occurs at pi by a, so this is where the Bragg Plane occurs first Bragg Plane. So we will just draw dotted line which represents this Bragg Plane - so that is the Bragg Plane, in other words on this plot on in k space if we if we plotted all the allowed wave vectors when the wave vectors are arrive at wave vector at this value would now implied that the wave vector is touching this Bragg Plane implies diffraction is occurring and that causes distraction of distortion of that E verses k relationship and view starts seens some energy values which are not allowed in the system.

So now, so this is the information so we have the first Bragg Plane here the second Bragg Plane this is the four pi by a at half its so that is the next valid reciprocal lattice vector; so at half that distance you should have the second Bragg Plane which will actually come at two pi by a so that is where you will have the next Bragg Plane. Similarly, the next one will be at six pi by a, so therefore at three pi by a will have other Bragg Plane essentially at every n pi by a we are going to have a Bragg Plane, because at every two n pi by a we are having a lattice point; so this is what we have same thing we can do here so we will just mark this up for the origin. (No audio from 22:18 to 22:44)

So now I have plotted all the Bragg Planes in the system. I have plotted the periodicity of the lattice, because of the periodicity of the lattice I have plotted all the Bragg Plane. Now, so this is k space on this very same plot I can take the nearly free electrons and plot their wave vectors, so nearly free electrons are electrons where the allowed values of k are n pi by L. So we notice that this is n pi by L, here the same discussion that I had earlier which means you have ten power ten points of such ten power ten points of this n pi by L within this distance zero to two pi by a.

So therefore, even though I will which basically mean that you know on this scale when I show it you it will look like a continuous curve, the reason I am emphasizing this is I am going to draw a line that looks like I am going to draw something that looks like a continuous curve. But you must keep in mind that it is not a continuous curve it is the set of discrete points which are all spaced by this n pi by L except that they are slow closely space that we are unable to show them as discrete points on this scale that is all you need you need to keep remain that. These are discrete points the curve that I am going to draw consist of discrete points, but they are so closely spaced on this scale that it looks like a continuous curve, so that is what we have these are allowed values of n pi by L.

So the discrete set of points will now have this the original E verses k relationship is E equals h bar square k square by two m so that same parabolic curve like thing we will draw here;(No audio from 24:20 to 24:33) so this is an approximate parabola may not be the best parabola, but you can still see the basic idea here. So that is the parabola we have of allowed values of E verses k which are now drawn to this scale. So this is the parabola if you draw it properly will get in a nice parabola that corresponds to the E verses k relationship of the nearly free electrons.

So it consist of series of discrete points several several huge number of points all space by n pi by L which on this scale look like a continuous curve; so that is the what we have. Now based on what we have understood all the things that we have learn so for what we what we learn is that whenever this E verses k relationship such as these are all valid reciprocal, I am sorry these are all valid wave vectors whenever a wave vector touches Bragg Plane diffraction will occur, conditions for diffraction are fully satisfied. So therefore, diffraction occurs here here here and here - so what actually happens is this E verses k relationship now gets broken up at those locations where the diffraction is occurring and essentially it described by saying that you know travelling waves become standing wave so to speak, so what will happen is this relationship will now change and the diagram will begin to look like this. (No audio from 25:57 to 26:23)

So this is how the diagram now looks it means that suddenly you have a few locations where the E verses k relationship is now no longer what it used to before so we can just remove some of these points here and you can see it more clearly. (No audio from 26:39 to 26:50) So these now are the allowed values of E verses k. (No audio from 26:55 to 27:09)

So you see now what was a originally a parabola at regions where it comes close to the Bragg Plane that parabola is now being distorted and we end actually end of seeing some discontinuities you see the e verses k which would have just gone up this way because it is comes to close to a Bragg Plane distortion becomes like this. Similarly, it start from some value of here goes this way gets distorted and finishes of here start here finishes of here start here and finishes of here same thing occurs this way you say at, so in between where it was originally a continuous curve the interaction of the periodicity of the lattice with the k vectors representing the wave vectors allowed for the nearly free electrons. We find that the nearly free electrons, so in if in other words if you go back to this figure here the nearly free electrons the k vectors of these nearly free electrons undergo diffraction due to the periodicity of this lattice.

So here we capture the fact that you know when diffraction occurs we are looking at the interaction of electromagnetic waves with the periodic structure of the material lattice and we are somehow used to thinking that is the the the waves involved are coming somewhere from from external source that, because that is how we do that material characterization we look at electron microscopy or x ray diffraction. So those in those conditions the waves are coming from outside the sample however to the extent that you can look at electrons also as waves the electron within the solid themselves represent waves and wave vectors and they two can.

Therefore interact with the with the periodicity of the lattice using the same relationships that hold for the other material characterization techniques that we look at and therefore, that is the basically all that we have seen here diffraction is occurring at those Bragg Planes and as the result this energy verses and therefore, as a result this e verses k relationship is now getting distorted. So this is basically what we see, so as you can see now if you look at the the vertical axis is the energy axis all right.

So in this energy axis we now see that, because this E verses k relationship is getting disturbed we find that we have a set of energy values which are continuous which are now allowed then there is a gap here which represent an energy that is not allowed. So there is like a forbidden energy gap here and the and then again you have set of energy values that are allowed; the same thing can now be plotted like this is now represents a set of energies that are allowed corresponding to this height I just drawn that on the same energy scale here then there is a gap then there is another set of energy values that are allowed.

And then there is third set of energy values that are allowed this is the fourth set corresponding to this; (No audio from 30:04 to 30:20) so this is what we have, so what we see now is that from this picture you are able to see that there are set - specific set of energy values that are allowed and specific sets of energy values that are not allowed. This is the picture that we are conventionally use to when we describes saying that we that are bands in a solid - energy bands in a solid and there are allowed bands and there are band gaps so this is the band gap so that is the band gap and this is the band - allowed band.

So we we now see based on all the understanding that we have to pull together through this course we are able to see how fundamentally the interaction of electrons with the periodicity of the lattice creates a situation where bands and band gaps appear in the system; this kind of representation by the way is called a flat band diagram. Because lot of the detail of the allowed actual allowed k vector k vector and such are not actually shown in this kind of a diagram, but this is the kind of diagram that is typically shown to us in in high school physics, because it is much easier to follow and in fact for certain types of a activities where we looking at at transition and energy levels corresponding energy values associated and so on.

This figure, this kind of a representation is adequate there are certain other phenomena in the material where this representation is inadequate and we will see that it in a class or two in a couple of classes we will see that, that this level of detail that this figure represents actually gives us much better understanding of what is allowed in the system? And what is not allowed in the system? What is more likely to occur? And what is less likely to occur? And how two materials may differ from each other? So, these are the allowed bands and these are the band gaps in between them these are this is the band gap band gap band gap and band gap and these are all allowed bands. So this is how something that you have always you learned in high school now relates to something that is much more intricate much more detail about the system.

So we see now all the things that we have pull together and there represented it here I will also say that if you look at this diagram this kind of a representation is called the extended zone scheme extended zone scheme where you take one origin and you would draw the entire reciprocal lattice about that origin and then on that basis you actually draw this entire diagram. So this is called the extended zone scheme this is called the flat band diagram.

Now there are couple of other ways in which you can represent exactly the same information so I will on this diagram itself let see if we can pull that information together, so that you can see what we are meaning representing its basically the same information now the information is already on the board we are not really changing the information I am just showing you certain other aspect of the information which may not immediately be apparent, because of the wave we have drawn the diagram the information is that see this choice of origin is somewhat arbitrary it is our choice. We select by our convenience; so therefore, we can select the next lattice point also as the origin the next reciprocal lattice point also as the origin and so on right. So there is no real difference between these lattice points in that sense.

Therefore, the same diagram can be shifted to the right by one reciprocal lattice vector can be shifted to right two reciprocal lattice vectors and similarly, to the left by one or two reciprocal lattice vectors. So in fact it is correct to actually say that this exact same situation exist about every reciprocal lattice point, because there is our choice of origin is rather arbitrary we have just chosen one for our convenience, so what we will do is we will draw the exact same diagram about this lattice point as well as this lattice point this lattice point as well as this lattice point, then when you do that you will see what what will happen. So about this lattice points you see this curve here; the same cure will occur here and the same thing will occur about this lattice point, you will see that also same thing will occur here and will occur here fine. Now the next what you see here as a next feature will also occur similarly, across every lattice point.

So you will see that, so basically if you look at the second lattice point you have drawn this curve here the next structure will start here and go up here the next one will start here and go up here and the next one will start here and go up here and then next from starts here and goes up there (( )). So this is the same diagram now drawn from this point and similarly, you can take the next point here and it will come up here now I can draw the same diagram from here, the same way we have done which will look exactly like this.(No audio from 35:32 to 35:45) So that is what we will do and we can do similarly, from all those point from from this point we can do the same thing we have got this so the next curve will look like this the next curve look like this and the next curve will look like this right and we will do that also from this point here so you will see how this figure looping to look. (No audio from 36:17 to 36:32)

So, basically this curve now builds up across all positions that we have consider. So actually what you will see is, you will see series of curves that look like that coming from all different lattice locations. So that is how you will get it this will come all these diagrams at I am drawing now come from the adjacent positions that we have seen, you just have to continue the diagram use the same logic and you will start getting this kind of a diagram. So we have that and we you will see that this come down here, this is coming from some lattice point from that side you are coming you are bringing in that side that is how this will become, this is how it will come.

Now you see that same information what we originally drew up about to one lattice point which was the origin I have now drawn from every single lattice point that is across this structure and so they all begin to, they also show you some pattern here that is simply, because the same pattern is originating from all of those locations and this pattern now represent this band. So this is this bottom most thing which is going this way this way this way is represented by this band as a flat band diagram; the same thing here represented by this band what is here is represented by this band what is here is represented by this band and similarly, what is appear represented by this band in between you see this gap, these are all not energy values that are not allowed that is the band gap this is all not allowed another band gap again these are all not allowed third band gap and this is one more band band gap that you have.

So this is another way of basically the same information has now been shown to you from the entire lattice. So you can actually draw this across this entire lattice you will find such diagrams that is called a repeated zone scheme. This is called repeated zone keep representing this information from across all lattice points.

Finally, we will also notice that if you look at the what we originally defined as the Brillouin zone; the Brillouin zone is when you are when you the first Brillouin zone is the region in space which you can access from the origin without crossing a single Bragg Plane right. So therefore, if you look at the Bragg Planes here they are at the first Bragg

Plane is at plus pi by a and this side minus pi by a. So the first Brillouin zone is actually between… So we will write the Brillouin zones down here. (No audio from 39:12 to 39:34) So minus pi by a to plus pi by a is what the first Brillouin zone and we will… I show you that the second Brillouin zone is from minus two pi by a two minus pi by a as well as plus pi by a two plus two pi by a. In both cases you would across to one Bragg Plane, but not more Bragg Plane. So if you from here the first Bragg Plane is here.

So this region then is the first Brillouin zone; I just call it first B Z first Brillouin zone this region here plus this region here together are the second Brillouin zone right. So we have the first Brillouin zone and the second Brillouin zone if you add the two second Brillouin zone the total dimension is the same as the first Brillouin zone. So that way all the Brillouin zones when you look at them they may get fragmented into pieces when you collect all the pieces together the extent of it will be same as the extend of the first Brillouin zone. So any way if you see whatever information we have captured in this repeated zone scheme all that information actually exist within the first Brillouin zone itself right. So all the information in fact, because of symmetry you can actually look at just the first Brillouin zone and whatever conclusions you can draw from the first Brillouin zone will actually be represented will will be representative of the conclusion you can draw if you do it across the entire lattice and that occurs simply, because the structure is periodic and therefore, whatever is happening is happening periodically.

So if you gather all the information within one zone you will still get the same piece of information and you can that that way the diagrams have come you, if you look at just the diagram between this region and this region which is the first Brillouin zone you will look at it the same pattern only getting repeated everywhere right.

So this is called this in this way you can actually capture everything by just looking at one one Brillouin zone that is the that is the beauty of this representation. So that is called the reduced zone scheme. So if you capture it this way, this becomes for reduced zone scheme. If you only look at the first Brillouin zone, so if you look at only the first Brillouin zone which I am represent writing here as the first B Z the reduced zone scheme is representing all the information of the interaction of k vectors allowed k vectors in the system and allowed the the periodicity of the lattice all representated within the first Brillouin zone. So simply looking at if I will just drew this diagram only between these two lines and ignored everything that was on either side of those two lines essentially.

I am only showing you they information within the first Brillouin zone; it captures all the details of the system perfectly find. So therefore, this representation which is called the reduced zone scheme representation is also good enough for us. So in many books sometimes you will only see this first Brillouin zone picture shown to you and now you can understand form where that information is coming from sometimes they will show you the extended zone scheme.

So you you will see it based on one origin spread out across the entire structure sometimes they will show you the repeated zones in which case you will see this entire picture the way I have drawn it or ordinarily they are simply show you the first Brillouin zone. And you need to understand that it has been pull together into the first Brillouin zone simply, because of the periodicity of the lattice what the another way of describing it is you can move every information from every from every location back by valid reciprocal lattice vector and it will bring you back into the first Brillouin zone and that is how you can think of this diagram being push back into first Brillouin zone if you want.

So that is the third way of representing it all three are perfectly find you can use them based on your convenience and circumstances you can use them. In this I will also I also wish to add that we have only shown the E verses k relationship right. The other information that we have not shown here is where is the Fermi energy. These are all the values of E verses k that are permitted in the system in depending on particular atomic system that you have chosen the particular material you have chosen; the Fermi energy may be at some particular value.

So I will arbitrary say that the Fermi energy is this is the energy scale I will just say that the Fermi energy is here. It is just an arbitrary thing so you just have to recognize that along the energy axis this plot represent all represents all the possibilities given this structure and given the values of k vectors that could exist within the structure the Fermi energy, simply depends on what is the number of free electrons per unit volume how many is the what is the density of available states density of occupied states etcetra right. So some Fermi energy value is there now this Fermi energy value then therefore, represents the highest energy level that the electrons can have in the system; so this can be simply represented here.

So you see now how the structure and its interaction with the the wave vectors creates this band structure here the periodicit periodic structure of the material plus the wave vectors allowed creates the band structure and within this band structure you can identify the Fermi energy based on where this the Fermi energy appears. We are now able to say whether it is a metal it is a conductor or an insulator if it shows up here like the way. I have just shown here where it appears in the middle of a band then it the system is called metallic.

Metallic systems are once where the you have a half field band. So therefore, the electrons are very easily able to move, because enable to see just immediately above then there are empty locations they are able to freely move. On the other hand you could had a Fermi energy which finished off at just at the top of this band then that case we will look at the band gap ahead of it if that band gap is of the order of two electron volts are less then that is semi conductor; if it is of the order of four electron volts are higher we would called a insulator, so then we will look at the band gap. We will look at this discussion when we talk of semi conductors we will see that discussion is greater detail. So this is all the information that we have seen, so in fact the it is of interest to see in terms of the material property the position of the Fermi energy with respect to these bands is the very important piece of information; so that is what we we are able to conclude from this one dimensional detail look at the one dimensional structure.

I will very briefly show you a two dimensional structure and I will also show you the three dimensional structure very briefly so that you get a sense for how the same information is represented in two dimensions and three dimensions.(No audio from 46:14 to 46:27)

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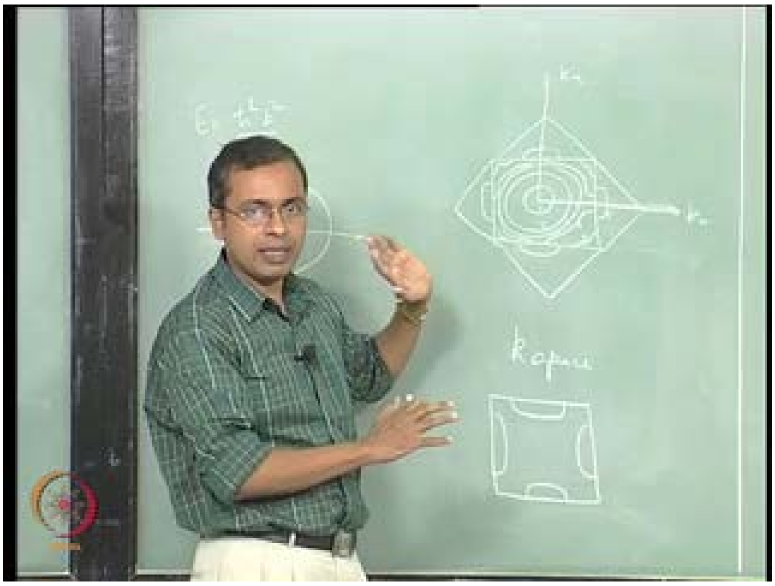

So we have already seen that E verses k relationship is E equals h bar square k square by two m this means in two dimensions we already saw that in two dimensions points of same energy are represented as a circle right. That is why the E equals h bar square k square by two m in two dimensions if you write the if you identify all the points are contain the same amount of energy are therefore, all the k vectors in k space, in k space k x k y k z in case space all values of energy corresponding to the… I mean all values of k corresponding to the same value of energy are is, I am sorry in two dimensions; it will only be k x and k y in two dimensions you have a circle and in three dimension is should become a sphere; so these are simply the two cases that we will very briefly look at.

So therefore, in a material if you are interested and what is happening to the Fermi energy then you are interested in the last circle that can be form using those electrons. We finish in one of the previous class we also looked at two dimensional square lattice and we found that its representation and reciprocal space is also a square, the first Brillouin zone is the square right then the second Brillouin zone becomes looks like that and so on. So we did this, we looked at all the Brillouin zones in in two dimensional space. So so these are the Brillouin zones if you draw it properly this will be the Brillouin zones for it square lattice being represented in a square form. So again we will assume that this is represented in the k vector dimensions, so this is therefore, this the diagram that we get here in if assume it is in k space that it is scaled properly. So that it is in k space this diagram comes from the periodicity of the structure from the crystal structure. Therefore, once you are have once you have a crystal structure this is fixed you have no choice on this so this is fixed.

However the number of free electrons available in the system may vary depending on that atom or even within the even for the same atom it may have it may depict the couple of different valencies so it the number of free electrons you have in the system could change therefore, the highest set of energy values that can the attained can differ the based on the are rather the Fermi energy that the our system might have which will directly depend on the density of available states and and the number of free electron avail per unit volume that can change if assume everything is the same and the density of available states is the same and you are simply changing the number of free electron per unit volume the circle that you can obtain can differ from material to material

So, if you have a material which has the very small number of free electrons if you simply have a circle that is like this in which case the this represents the Fermi surface. So this k space, so I just say this k x and k y and we we we say that you know the this circle does not interact to the first Brillouin zone; so everything is within one band. If the number of free electrons is going up, it it becomes the larger circle its starts getting close to the boundary of the of the brillouin Brillouin zone. You can have one more like this, if it becomes even larger what you will see is, it will start distorting; it will no longer become a circle close to the circle it will distort like this. So this is how the Fermi surface now interacts with the Brillouin zone and distorts in it is simply a attention of what we saw in the two in the one dimensional case where we look that it in one dimension and we found that it the k values began to distort and if you go even further you will see that the Brillouin the behavior is something like this, and it begins to appear in the next zone so you can if you go and look up you will find diagrams like this where basically.

So this is case one this is case two this is three this is four and this is five this is five these are not the numbers are simply to indicate which curve add sub to which are connects up with which so these are all the case where the Fermi surface of the just about touching the Brillouin zone and then finally, it begins go into the second the Brillouin zone again. We can do a reduce zone scheme representation where we basically move things in and represented. So you will actually see this is appearing on this side this will appear on this side that will appear on this side and so on.

So if you wanted to represent the second Brillouin zone in the within the first Brillouin zone in the above case, it will simply look like this in case four; so this is how you do this in two dimensions again the diagrams can get complicated if you look at more and more I mean, if you make it a longer diagram you include the all the subsequence zone and you continued to grow this I mean and look at different materials where the Fermi surface is larger and larger and you have you have to look at interaction between the Fermi surface and much large and higher Brillouin zones.

But the concept is exactly the same you have now got a very good idea of the concept in one d and two d; so that is exactly the same I will just finished off with the couple of minutes where we look at some slides where we are looking at the exact same interaction the way I have zone you here in three dimensions.

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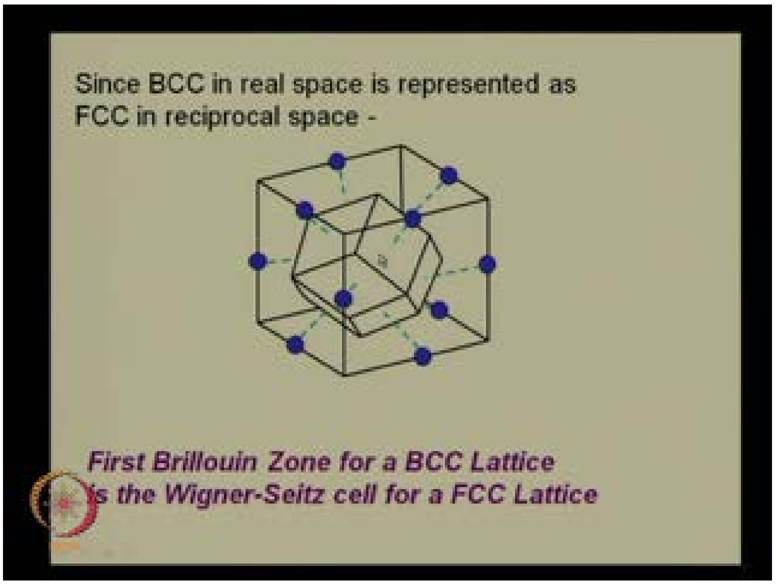

So we will do that so we will see now we saw that we have to now look at first of all the Brillouin zone itself and so we saw already that for BCC a material that is BCC in real space it is represented as FCC in reciprocal space and this is then the Brillouin zone. So of the the first Brillouin zone of the B C C is structure in real space which is now represented as the FCC in the reciprocal space.

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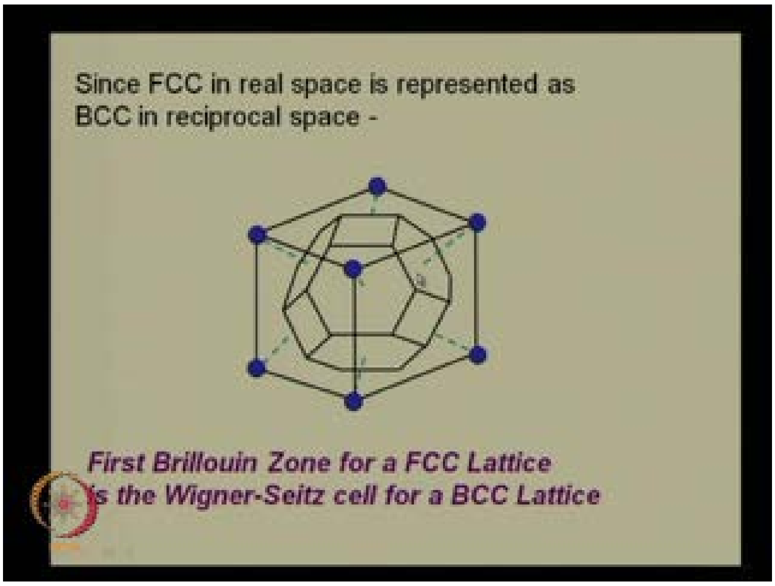

Similarly, we saw that something that FCC in real space is now represented as BCC in reciprocal space and this therefore, ends up being the Brillouin zone corresponding to that structure. So therefore now we will see here what with this stricture, we will assume that this is case where dealing with it is a face centered material that is face centered cubic in real space which has been represented and BCC in reciprocal space within the structure; we will put in the Fermi sphere. It is similar it is the same thing it is E equals h bar square k square by two m and therefore, all values of energy corresponding to I mean all values of k corresponding to the same energy are represented by a sphere so Fermies for surface is the sphere in k space here. So we will look at various possible Fermi surfaces within this which simply represent different materials having the same structure, but different number of free electrons per unit volume. So here is a case where you have a large Brillouin zone and a Fermi sphere which is the right in the middle which is kind of small, because the number of free electrons is less let say. We will look at another material - series of materials.

So, where the Fermi surface is getting to be larger and larger tell it begins to interact to the Brillouin zone and we will just see how that looks. This is the slightly larger Fermi surface still no interaction with the Brillouin zone even larger still no interaction with Brillouin zone even larger getting very close to the Brillouin zone, but not yet any interaction the Brillouin zone. And finally, you have and situation where it has got in very close to the surface of the Brillouin zone these locations of this sphere are getting very close this location this location and this location and correspondingly. The other side we are not seeing, we are seeing only one side of the figure these are regions including this front surface where it has got in very close to the surface of the Brillouin zone and therefore, the sphere as now distorted in the shape. It is spherical up to this point then distorts and touches the Fermi surface and again distorts here. Similarly, comes here distort here and so on and similarly, distorts them. So that is the same way in which we have already see in this in one dimension and two dimensions and I am now showing you the three dimension.

So, to end up to summarize in this class we have looked in detail at the interaction between the various energy levels allowed in the system and the periodicity of the structure. We have looked at the allowed k values and the allowed crystal lattice information we have looked at their interaction and we have seen how Brillouin zones result this interaction results in the band structure that evolves for the material and based on where the Fermi Energies with respect to this band structure, you see various properties of the materials so right. Now we have seen it only pictorially in the next class we will also look at that specifically at that gap that band gap that is appearing there we will look at that in the with little greater detail just to see if if mathematically we can see how that band gap up comes about and what is the extent of the band gap, so you will do that and then next class. Thank you.