Semiconductor Optoelectronics
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Lecture - 4
The Density of States

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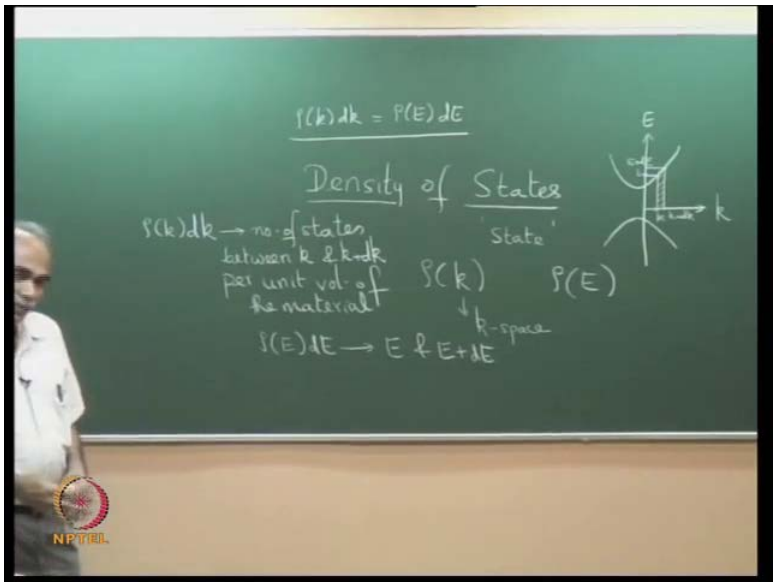

Good morning and we start with this lecture 4 the density of states, the topic is density of states density of states. Usually the name indicates what it refers to density of states. So density, this gives an idea that it must be something to do per unit volume, states - what is a state?. State is an allowed solution to the boundary value problem, state is that allowed solution which satisfies the boundary conditions. It is the general definition of a state or a solution an Eigen solution or a mode, different names are used, but a state is an allowed solution that satisfies the boundary conditions.

So we are referring to the density of states in semiconductors which is rho of k, denoted by rho of k or rho of E. This is in the k space rho of k, which is in the k space. What is this k and k space, we will see rho of k, rho of E. Now rho of k is defined as rho of k d k rho of k d k is the number of states number of states between k and k plus d k, it is the number of states between k and k plus d k per unit volume of the material, per unit volume of the material. This is the

definition of rho of k. Exactly like this you can also define rho of E that is rho of E d E is the number of states between E and E plus d E per unit volume of the material.

What are these E and k, E and k is the one which defines the band structure or the E k diagram that we have seen in the last class. So, if you see a typical E k diagram, so E here and k you can draw wherever E k. As you can see for every given value of k there is a corresponding value of E, there is a k here and there is a E here. Therefore if I go to the next step that is k plus d k, so k plus d k, then correspondingly I have E plus d E, this is k corresponding to that I have an E value and if I say that this is k plus d k, then corresponding to that I have E plus d E, the number of states between k and k plus d k here.

So, what is this, these are the allowed solutions, allowed energy value of as a function of k so the number of states means the number of points that we get. Here in the E k diagram between k and k plus d k is the same as number of points between E and E plus d E. So obviously, rho of k d k is equal to rho of E d E, we will use this shortly. This is the, this is the first picture of the density of states, before I proceeded with the density of states. What are the states, how many, what is the number of states which is available between k and k plus d k.

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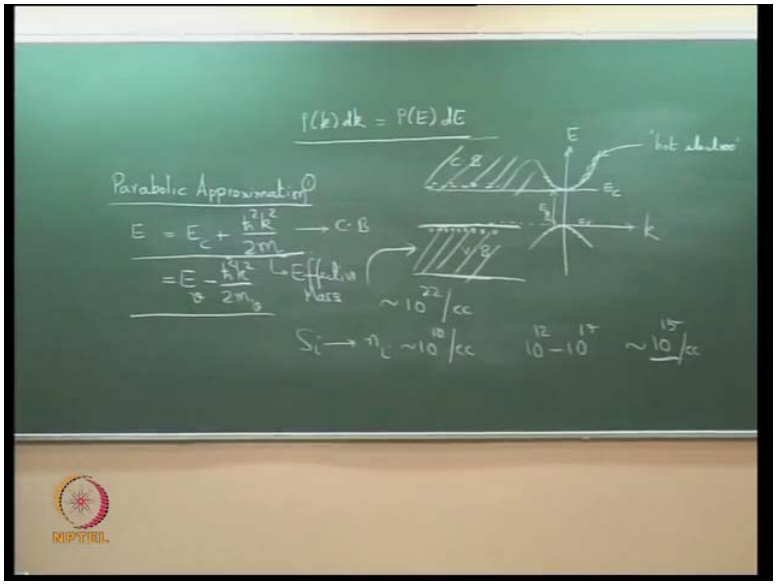

Let me recall a few things form the E k diagram that we have studied in the last class, k E. This corresponds to the, as I shown on already this corresponds to the valance band and this

corresponds to the conduction band that is, this is the energy value E c and here is the energy value E v and of course this is the band gap E g. So, this is the familiar band diagram, this is valance band and conduction band. We have seen that normally the typical number of electron in the valance band is of the same order of number of atoms in the valance band.

Which we are calculated in the earlier lecture is of the order of 10 to the power of 20 two per c c the number of electron in a band and generally, if you take silicon for example, intrinsic silicon then the intrinsic carrier concentration n i at room temperature is of the order of 10 to the power of 10 per c c 10 to the power of 10 per c c. As I discussed in the last class and depend on the band gap and typically intrinsic concentration is this much and if you dope a semiconductor to make a device, say p n junction device, typical doping concentration could be any were from 10 to the power of 12 to 10 to the power of 17, which means the number of carriers which are available is of this order or of the order of 10 to the power of 15.

The number of carriers which means the number of carriers available in the conduction band here is of the order of 10 to the power of 15 per c c. The, there are devices which are heavily doped were it may be 10 to the power of 18 or 10 to the power of 19 per c c, is the carrier concentration in a band. There are typically 10 to the power of 22 electrons and carriers which are available, which means the holes in a semiconductor, valance band holes in a valance band and electron in a conduction band is of the order here, which means it is much smaller compare to the total number of electrons in the band and therefore, if we consider the E k diagram this carrier which are available they are occupying only the bottom potion of the band we have holes here in the E k diagram and electrons here which are literally in the bottom potion of the band because the number is so small they always tend to remain near the bottom.

If you have a hot electron the term used, hot electrons hot electron means an electron with higher energy, it will come down, it will tinkle down by the phenomenon called thermalization. We will discuss more about this later when we introduce phonons it will thermalize and come back to the bottom. Therefore, in all device when you analyze device characteristics normally it is sufficient if you know this. The E k variation near the bottom itself because almost all carrier are poles and the electron accumulated near the bottom and the near the bottom. Here the variation is nearly parabolic, this variation here is nearly parabolic and we use what is called parabolic approximation of the band.

Parabolic approximation which means the energy E of electron in the conduction band is given by E is equal to E c plus h cross square k square divide by 2 m c. h cross square, were m c is the effective mass m c is the effective mass in the conduction band, effective mass of electrons in the conduction and E v that is energy in the valance band. This is for the conduction band and for the valance band this is given by E v minus h cross square k square divide by 2 m v. Were, m v is the effective mass in the valance band, effective mass poles in the valance band. This is called parabolic approximation because as you can see the dependence of E is parabolic depends on k square, it varies as k square, that is why you can see this variation is like k square. E c for any were if go here, a give value a particular value of k here, then you have E c plus this variation which is h cross square k square by 2 m c. In the last class we discussed that by using the effective mass you can treat the carrier as a free practical. Kinetic energy of a free practical is given by p square by 2 m p square by 2 m.

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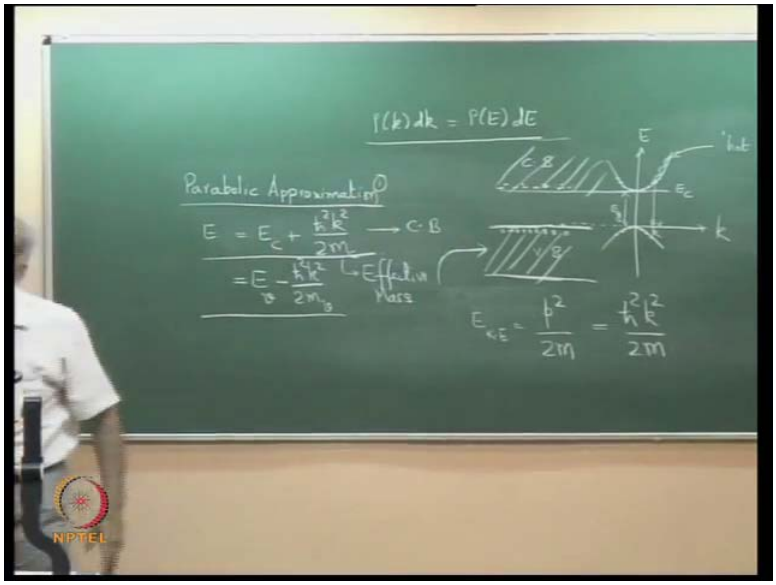

So, the kinetic energy is equal to p square by 2 m and p is h cross k, so that is why we have h cross square k square divided by 2 m. So here at the bottom of the band k equal to 0 and therefore there is no kinetic energy, but as you go to the finite k value you have h cross square k square divided by 2 m and this is called the parabolic approximation. If you see the whole band it

will not go parabolically, it will change if you see the whole band, but normally if you are interested in the bottom of the conduction band and the top of the valance band this approximation is very good approximation, parabolic approximation okay and we will use this parabolic approximation in deriving the density of states because in most practical cases that is sufficient and as practicing engineers, we do not worry about a rigger, but the second point that is discussed in the last class was the effective mass.

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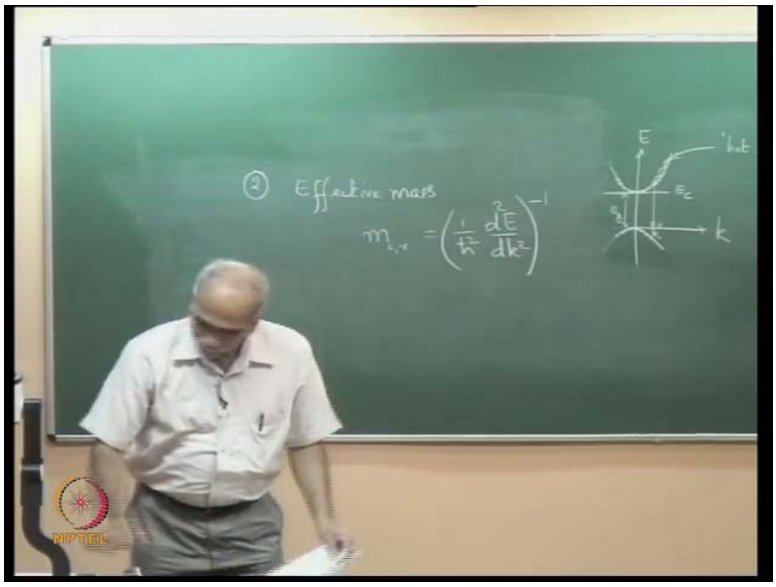

Which is also given by so m star that is m c or m v depending on which was 1 over h cross square d square E by d k square power minus 1, so I want to show you some typical values of typical values of the effective mass in semiconductor.

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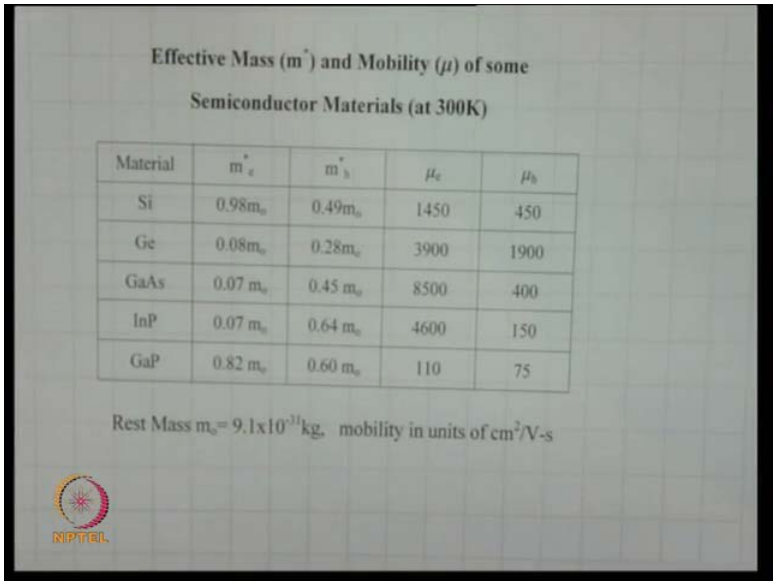

Effective mass in some of the semiconductors, some of the semiconductor materials Silicon, Germanium, Gallium arsenide, Indium phosphide, Gallium phosphide this are widely used materials in optoelectronics. There are many more semiconductor of course, in optoelectronics this are some of the important semiconductors which are used. What you noticed is that the effective mass the effective mass in silicon here, in the conduction band valance band, effective mass of poles in germanium here these are the values, in Gallium arsenide you note that this are the value, in fact there are something called light holes and heavy holes, but here we are mainly considering the heavy holes. I do not wish to introduce light holes and other bands at this stage, so what I would like you to know that smaller the effective mass, larger the mobility. You can see smaller the effective mass larger is the mobility mobility of electron is much more compare to mobility of holes for the band structure tells as an effective mass and it is also tells us what is the corresponding mobility.

Now what is the effective mass, let us have little bit more of this picture, the rest mass is m naught and effective mass is much smaller, it is like this effective mass is the mass experience or the mass exhibited by an electron the mass exhibited by an electron when inside the semiconductor. It is like this you have a long wooden log wooden log you try to drag it on the ground it is very heavy, really heavy, you are not, you are not really able to drag it that the log is very big. Now you put that log in water and now you pull it much easily because waters buoyant

force giving an upwards thrust and that log feeling much lighter and you can pull it without any difficulty. It is acting as if it as a light particle, why because it is in the medium, that log is in water.

Exactly like that when the electron is inside a semiconductor it is moving under the influence of the internal electric field the internal electric field with in the medium so it is like a cushioning effect, so there are potential variation and the electron as if it is cushioned and moving very smoothly. That is wise it is feeling very light and that is why the effective mass that you can see it is much smaller in the conduction band of electrons accordingly the mobility is much higher.

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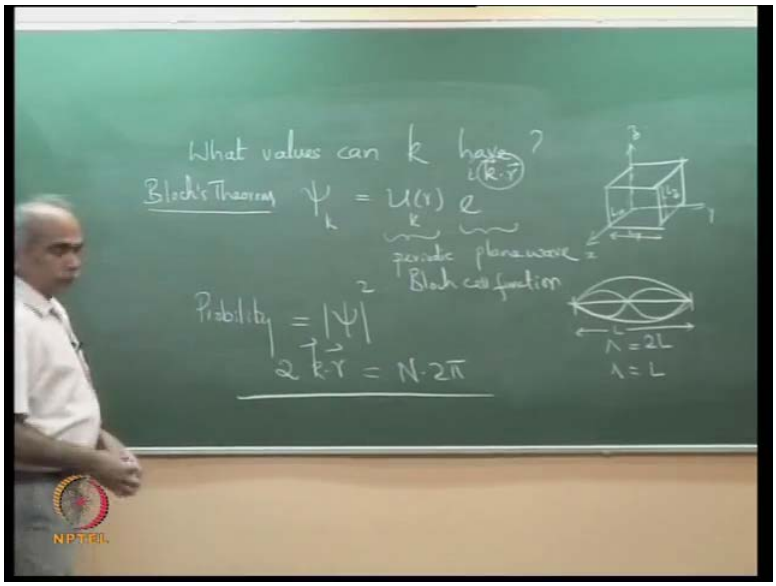

Now let me come back to the density of states, so now we have to understand what is this k and what is the values can k take. We know that for every value of k that is a corresponding E value, allowed energy value, but what is the values that k can take, what are the values that k can take. So the question is what values can k have, what is this k and what can k have.

Recall form Bloch's theorem that the wave function associated with electrons in semiconductor (( )) are given by u k of r into e to the power of i k dot r. k is a vector it is a propagation vector, I have not put the k notation here and this will bring more concepts about the k and the band structure itself because k is a propagation vector.

So, this is a plain wave it is a product of a plane wave and a Bloch cell function, which is a periodic Bloch cell function Bloch cell function. Therefore, phi k is periodic, now you know that probability of probability of finding an electron is equal to mod phi square. This is a periodic function, if we consider a semiconductor, let us say a small piece of semiconductor of dimensions, so let me mark the axis so this is x, y, z.

In space I have taken a small piece of semiconductor, let us say a cubic or a cuboid. So, this is of dimensions L x, L y and L z, this height here is L z, could be 1 mm by 1 mm, so that a cube L x equal to L y equal to L z. Let us say 1 mm cube size of semiconductor, is small piece of semiconductor. The electron is bound to the semiconductor, means you can find the electron inside but not outside. The electron is bound to the semiconductor so it is inside the semiconductor not outside, but we know about the probability of finding the electron is periodic, it is oscillatory function. Therefore, it is periodic, therefore if the electron has to be found inside and not outside the probability is 0 outside, which means size should go to 0 at the ends, at the boundaries. Sizes should go to 0 at the boundaries, which means the wave functions should form standing waves in the medium, this is called standing wave boundary condition.

There also periodic wave conditions or stationary wave boundary conditions, the logic is the field or the wave function has to go to 0 on the boundary of the semiconductor, which means if it has to go to 0 here and it has to go to 0 here and if it is periodic and oscillatory it means it must be forming standing waves. It is like this, you have a string which is (( )) at two ends, the displacement is 0 and it is given that it can oscillate periodically, the displacement has to go to 0, which means it will oscillate either like this or like this, which are modes of oscillation of string, which we studied in school, modes of oscillation of string.

What is the boundary condition that the displacement goes to 0 at the two ends, that immediately restricts the oscillation period or the wave length here, as you can see this the smallest wave length here, if I denote it by lambda, is equal to twice l because this l, this length is l, we see if I have a string length l, then this is half the wave length. And therefore lambda is equal to twice l. In this case lambda is equal to l lambda is equal to l, you can have many more such a modes of oscillation of a string.

Exactly like that, in this case if the wave function has to form standing waves inside the medium, it means the phase, the roundtrip phase, please see that this is the phase, k dot r is the phase, e to the power of i phi, phi is the phase. So, k dot r is the phase and therefore twice k dot r that is roundtrip phase must be an integral multiple of 2 pie. This is the condition for standing waves, roundtrip space must be an integral multiple of 2 pie, which means the wave going to here to there and coming back should add in phase again therefore in one round trip the accumulated phase should be an integral multiple of 2 pie. So, the condition is 2 k dot r is equal to N times 2 pie.

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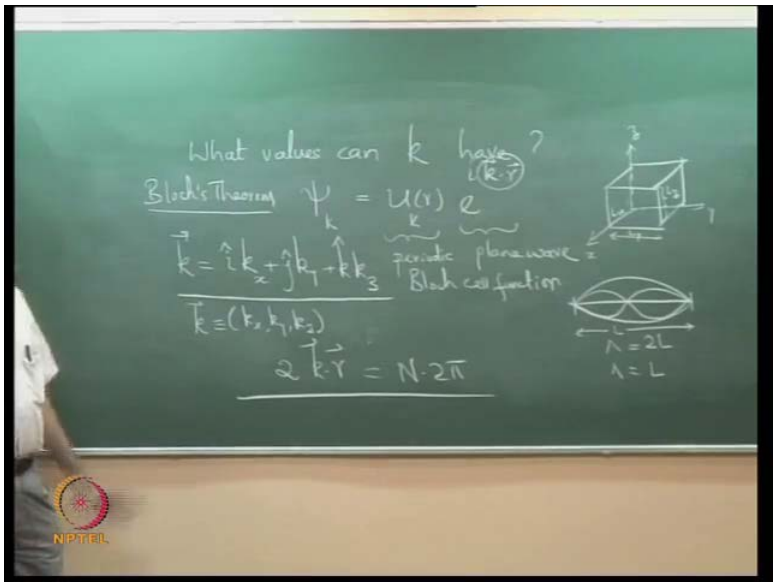

Now, k is a vector which means k is equal to i times k x plus j times k y plus, this is unit vector. Let me put k time k z. k has three components, k the vector k is equal to k x, k y, k z it is a propagation vector, please see the space, this is space. If the electron is moving in this direction, this is a k it have component in this direction in this direction and in this direction. So, it has x, y, z component the electron could move like this, could move like this, so depending on that it will have different x, y, z components. If k dot r is equal to N times 2 pie this means that, therefore, because k x, k y, k z are are orthogonal components of k orthogonal components of k.

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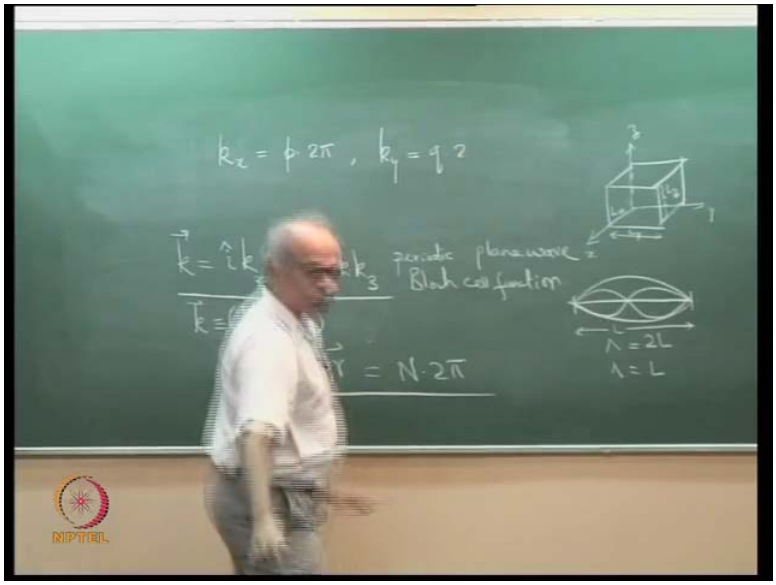

We must have k x is equal to p times 2 pie, k y equal to q times 2, one second one second.

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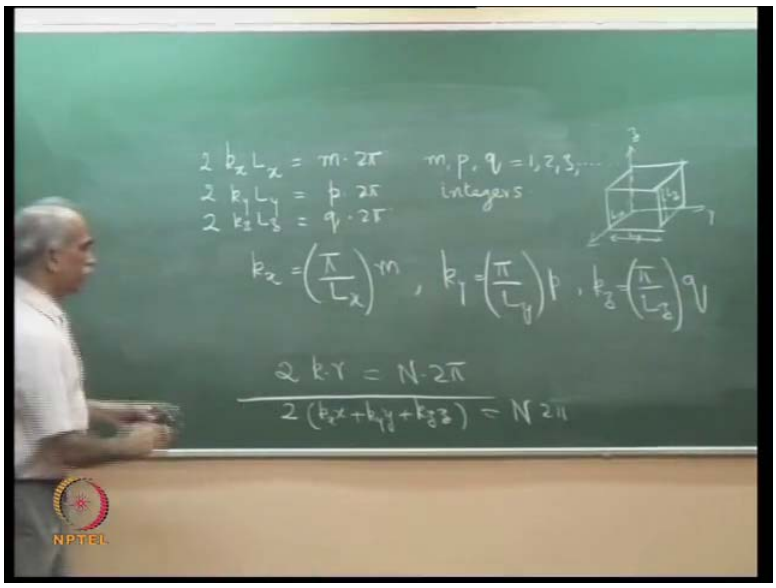

Let me use the notation as give in the books, let me correct this k dot r is equal to, please see what is k dot r, k dot r is k x x plus k y y plus k z z, it is a dot product k dot r is k x x, k y y, k z z the three compound are. Now if you consider this of dimension L x L y and L z, then i must have twice k x into L x, must be equal to m times integral multiple of 2 pie, twice k y into L y equal to

p times integral multiple of 2 pie and have twice k z into L z is equal to integral multiple q times 2 pie

This is for the vector and it has component x, y and z, which are orthogonal component. Therefore, if this is integral multiple of 2 pie it means each of the component must also satisfies m times 2 pie, p times two pie and q times two pie. Where m, p, q are, all of them cannot be 0. So, let me put 1, 2, 3 are integers are integers, yes.

Why all the components have to.

If this is equal to twice this, is equal to, if some integer times 2 pie, which means these are independent, the components are in orthogonal components. Therefore, everyone of then must be equal to an integer and of course this m, p, q is different form N, but because they are orthogonal components, every one of them, each of them has been satisfied roundtrip space of integral multiple of 2 pie. If you see in this picture, this is for a string that as been shown, yes it is applicable for all 3 axis, therefore each component must satisfied this equation, this means this means that k x is equal to pie divided by L x into m k y is equal to pie divided by L y into p and k z is equal to pie divided by L z into q.

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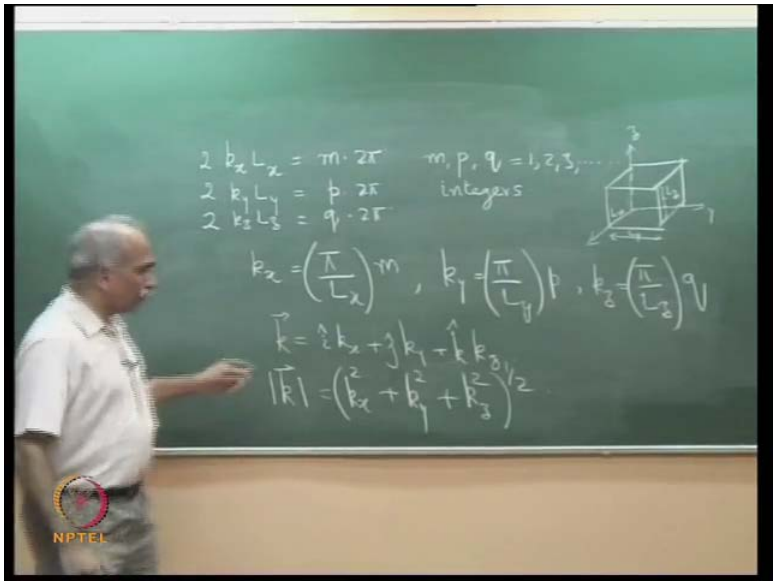

The propagation vector k is equal to x cap or i cap k x plus y cap j cap k y plus k cap k z. So k takes k can take this values and were k is this and more k, that is the magnitude of k is equal to k x square plus k y square plus k z square to the power half. Mod k is equal to k x square plus k y square k z square, what is the point, the important point to note is k comprises of three components and each of this components are now discretized they are discrete.

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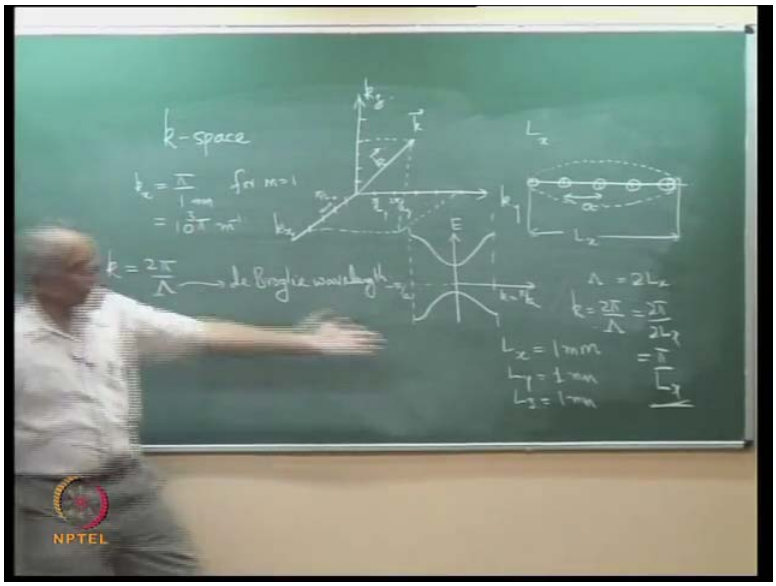

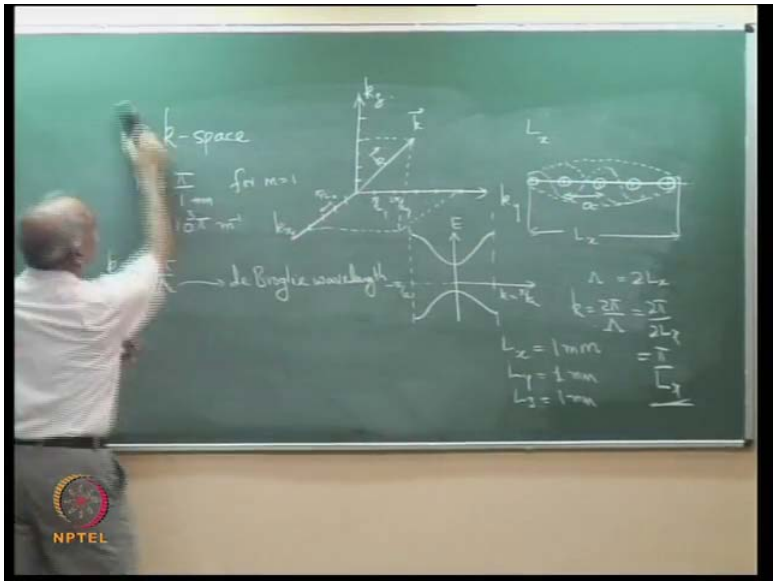

Which means the vector k itself is discrete, please see k x, k y, k z take discrete values because m, p and q are integers. If k x, k y, k z take discrete vector k will also be discrete, what it means

is if we go to the k space now, if we go to the k space, this is k space, which means this is k x, k y and k z. Any vector k can be represent by this 3 components, but the k value themselves take discrete values, the separation between this values is pie divided by L x because this is m equal to one pie by L x, 2 pie by L x, 3 pie by L x and so on, along y it is. So, this is pie by L y, this is twice pie by L y and so on and similarly this is also discretized . What is our objective, is to determine rho of k, the density of states the density of states is the number of states between k and k plus d k per unit volume of the material. So we want to find out what are the value that the k will take, so in general, let we take the vector k will here, then the x component then here y component it is this and z component is this.

So this is the k x value here for this vector k, so this is the vector k, k x, k y and k z, to proceed further let us have an idea what kind of numbers will these be, how many such points will be there and what kind of numbers is this. If L x for example, let us take the 1 dimensional case, atoms are with the inter atomic space in a, atoms are located periodically with a 1 dimensional laities with the inter atomic space a. What is L x if the dimensional L x is equal to one mm. Let us consider the dimension L x is equal to L y is equal to L z is equal to one mm. What is the smallest value of k x, m equal to 1. So pie divided by L x, so smallest value of k x is equal to pie divided by 1 mm, so one mm for m equal to 1 for m equal to 1 which is equal to 10 to the power of 3 because one mm, 10 power of minus 3 meter, 10 to the power of 3 meter inverse. This is the value of k, k has length inverse dimensions of length inverse and as you can see, this is the smallest value of k for a cube of size 1 mm k x.

What is the largest value of k, what do you think the largest value of k, because if we know that then what kind of numbers, how many points will be there, if like in the E k diagram, you recall in the E k diagram, we said that this is the boundary of the (( )) the first (( )). If you consider the the reduced zone picture then this value corresponds to k is equal to pie by a and this is k equal to minus pie by a. In the reduced (( )) picture this is the E k diagram, this is the E vs k, we have k equal to pie by a, the largest value of k equal to pie by a.

How did we get this k is equal to pie by a, if you see this what is k, k is equal to 2 pie by lambda where lambda is a de Broglie wave of electrons lambda is the de broglie waves. How do we imagine a lambda the electron, which is the wave dose this. If this entire length is L x L x is the

entire length then lambda, the wave length, you can see wavelength lambda is equal to twice L x or L x is half the wave length.

The dimension L x is equal to half the wave length or lambda is equal to twice L x. Therefore k is equal to 2 pie by lambda, is equal to 2 pie by 2 L x, is equal to pie by L x. You see that I have got, I am trying to give you a picture, what could be there, a simplistic picture, why that is the smallest value. Why L x, k x is equal to pie by L x is the smallest value because that corresponds to an electron de Broglie wavelength which is like this, form end to end, the fundamental mode in the case of a string, what is the largest value of, largest value of k it would corresponds to smallest permitted value of lambda, the smallest permitted value of lambda will be, you see this is an electron, the electron can do, it can do like this or the electron wave can do like this.

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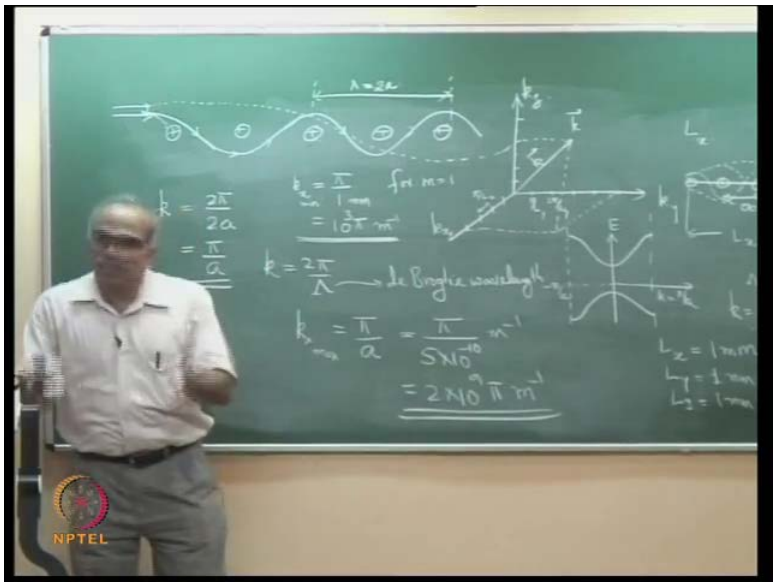

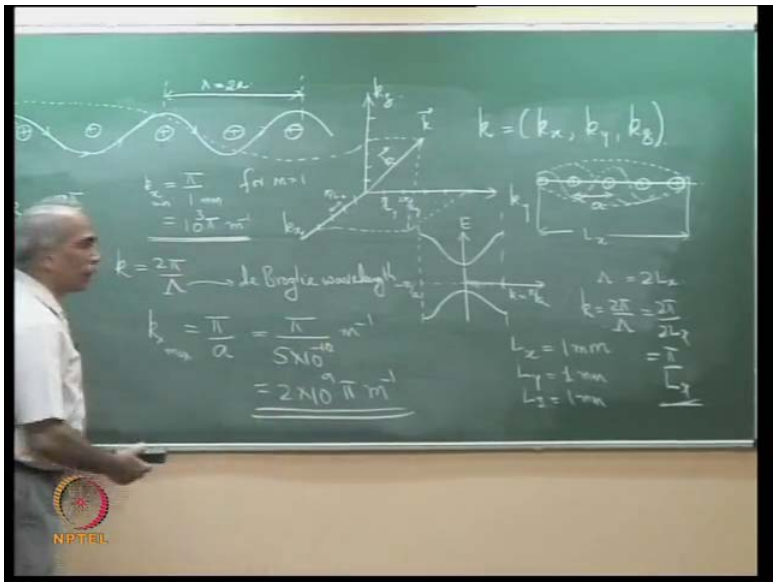

What do I mean by do like this? See this if you assume an electron which is entering form here, the particle electron, it get attracted towards the positive nuclear, so the electron went towards the nuclear but get scatted and it goes in this directions, when the electron go in this directions then the next positive nuclear which attracting it, so it is bending towards it. It is getting attracted towards the positive nucleus here. So, it takes, so it can take attracted so much so it would again gets scatted and going in this direction, but the next one will attract it and therefore the electron path, the path of the electron, as a particle can a best to this. The smallest path on the other hand other electron coming from here, it could slowly get attracted, but it may not bend so much, but it slowly get attracted and it may bend like this and then corresponds to this, that corresponds to a large wavelength, if it is attracted rapidly the potential is drawn, then it could do this, when it does this.

What is the wavelength, the wavelength here is corresponds to maxima to maxima, this distance and what is that this is inter atomic space a and therefore this is equal to twice a, the wave length lambda is equals to twice a. Please see this this is the wave length of electron which is this is inter atomic spacing a. Therefore, the smallest wavelength that you can have is this which means my k, the largest value of k which is equal to 2 pie divided by 2, a which is equal to pie by a.

Which is consist, with this picture the edge of the first Broglie zone is k is equal to pie by a, now why did I put this, the smallest value of k x is this much. What is the largest value of k, so k x this is min, minimum value, what is k x max is equal to pie by a, a is equal to phi Armstrong

which means pie divided by 5 into 10 to the power of minus 10 meter inverse is equal to 2 into 10 to the power of 9 pie meter inverse, k x varies from about 10 to the power of 3 pie to 10 to the power of 9 pie, it varies by six orders of magnitude.

When you go from the minimum value here, to the maximum value here, so from here 10 to the power of 3 coming up to 10 to the power of 9 in steps of 10 to the power of 3, pie by L x, in steps 10 to the power of 3. What does that mean, the number of points that you have here is a million, 10 to the power of 3 to 10 to the power of 9 in steps of 3, 1 million points, 1 million values of k x is permitted and similarly a million value of k y and million values of k z, so what is the point, every k is characterized by, every k is characterized by a value of k x, k y and k z. Each one can take a million values and therefore the combination can take billions of values.

So the number of k values with in on Broglie zoon that is in first band is billions, do you understand this points and that is wise I have put this number to tell you that the number of points permitted, number of k points permitted are of the order of billion.

Please pointed over this because you have all, most of you would have calculated the density of states and when you calculate you make an assumption that the number of points in the k space is extremely large. By putting this numbers, the minimum and maximum I have illustrated that, indeed that the number of k points permitted in this case is extremely large.

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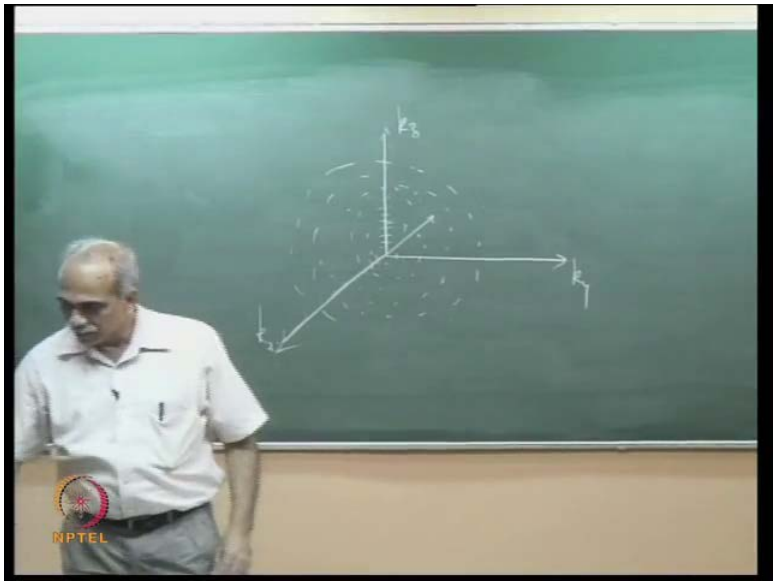

Therefore if you plot in the k space, k x, k y and k x, a billion points here, a million points here, a million points here, which means the permitted k values can be, there are enormous number of k values which are permitted in the k space. What am I making, every point here corresponds to a k value means the vector linking this to this point is an allowed value of k and such billions of points in the k space. We will continue from here in the next class okay. We go for a quick quiz, so take a piece of paper, it is the quiz.

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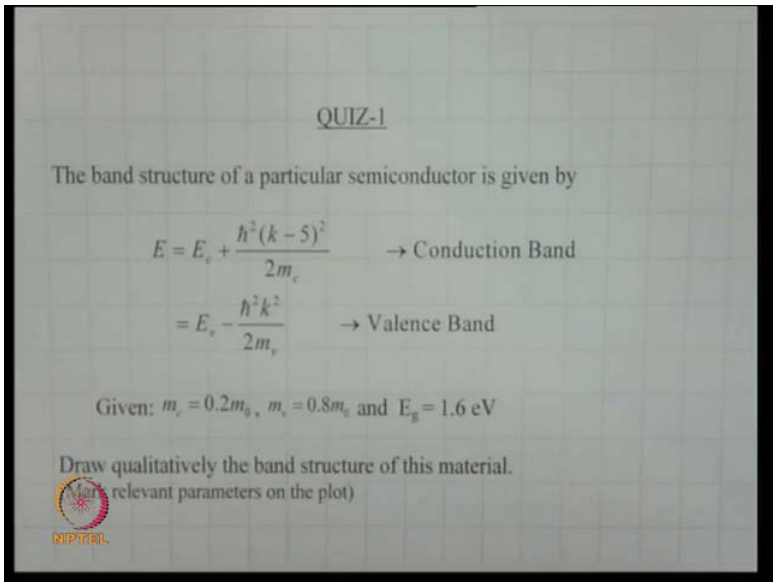

I hope you can see that but those of you in the last bench let me read it, the band structure of a particular semiconductor is given by this expression E is equal to E c plus h cross square k minus 5 whole square by 2 m m c, for the conduction band and E v minus h cross square k square by 2 m v for valence band. There are some parameters given m c, that is effective mass electron in the conduction band is the 0.2 times m naught, m v is 0.8 times m e and the band gap E g is 1.6 E v, the question is draw qualitatively the band structure of this material. The expression for band structure is given, you are asked to draw qualitatively the band structure. Making use of all the relevant data, which is given. Any question is it clear to, is it visible. So, I am reading again E is equal to E c plus h cross square k minus 5 whole square is divided by 2 m c and E v minus h cross square k square by 2 m v.

I thought that the size was sufficient, may be next time we will increase the size, the question is draw qualitatively the band structure of this material. No need to write the this question, just write the answer. That is just draw the band structure.