Semiconductor Optoelectronics
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Lecture - 5
The Density of States rho (k), E(k)(contd.)

The density of states rho of k and E of k, before I continue the discussion, let me briefly discuss the quiz that I had given yesterday the quiz question.

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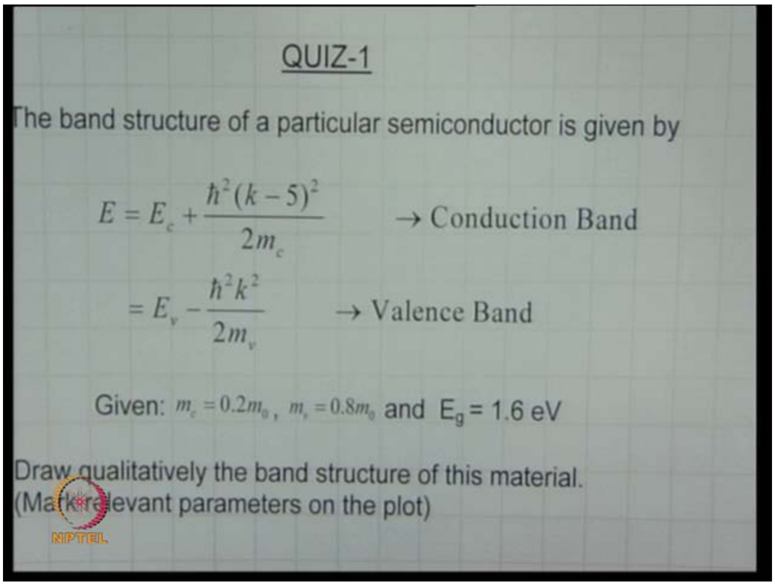

QUIZ-1

The band structure of a particular semiconductor is given by

$$E = E_c + \frac{\hbar^2 (k-5)^2}{2m_c} \quad \rightarrow \text{Conduction Band}$$

$$= E_v - \frac{\hbar^2 k^2}{2m_v} \quad \rightarrow \text{Valence Band}$$

Given: $m_c = 0.2m_0$, $m_v = 0.8m_0$ and $E_g = 1.6$ eV

Draw qualitatively the band structure of this material.
(Mark relevant parameters on the plot)

So, this was the quiz the band structure of a particular semiconductor is given by; there is an expression given to you and you were asked to draw the band structure qualitatively.

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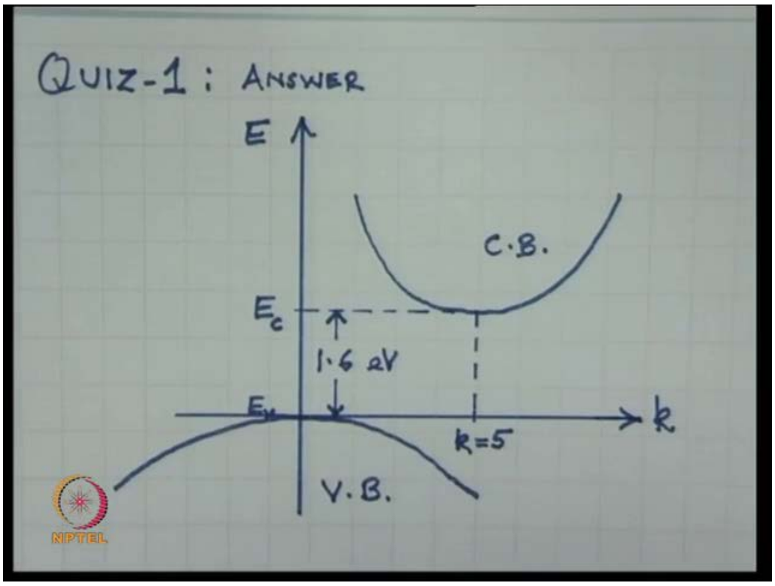

So, that is the answer. There are two things to note. One is that the valence band is shifted. That is why it was k minus 5 whole square. So, the valence band is shifted here and indeed this is nothing but an indirect band gap semiconductor. So, one of the objectives of giving the quiz was to how you will express the band structure mathematically for an indirect band gap semiconductor.

So, what you will have is k minus the shift, whatever is the shift. So, at k is equal to 5, we have the minima which is Ec; energy equal to Ec. The second thing that you know, which probably many of you have not noted is the fact that the mass of electrons in the valence band, in the conduction band and holes in the valence band were different. One must 0.2 m 0 and the other one was 0.8 m 0. That means four times heavier, the holes were four times heavier, the holes were four times heavier.

What is the implication of that? The implication is that the band here increases much rapidly, big energy access here. You can see here. As energy increases, the band goes here rapidly in this direction, whereas this one tends to go much slowly, but actually the energy here increases much slowly because m is in the denominator.

If you see the expression again and you see here that m is in the denominator. When m is larger, the constant which is h cross square by 2 m v here is a smaller constant. Therefore, it increases much slowly. In other words, they are not inverted parabola, identical parabola, but they are different. The variation is different. This is because of different effective masses of electrons and holes. So, these are two points to note in the quiz. We will continue with our discussion of the density of states.

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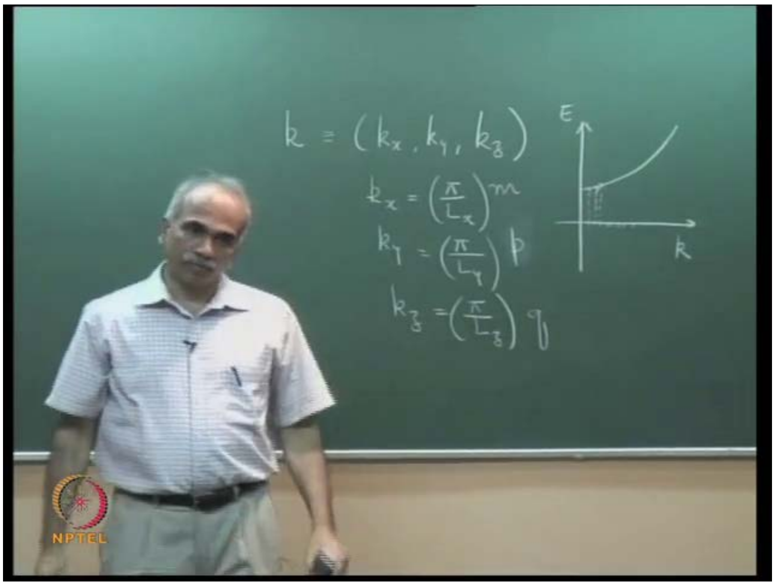

In the last lecture, we have seen that k, the state is characterized by k, which has three components k x, k y and k z. By applying the stationary state boundary condition, we have seen that k x, k y and k z is discretized. So, if you have a material of dimension L x into L y into L z, then k x is integral multiple of pi by L x, k y is equal to integral multiple of pi by L y and k z can take values which on integral multiple of pi by L z.

The point to note is, just a second, I made in mistake here. I used p. So, p and q, small p and q where m, p and q are integers, so the point to note the values of k x, k y and k z are discretized. Therefore, k is discretized. The implication is that in the E k diagram that we have the E k diagram, the values of k which we have here are discrete values and corresponding to the discrete values, we have discrete energy values. Corresponding to each k value, we have discrete energy values.

However, we have seen that the number of points here is very large. Each of this value varies come at the order one million. Therefore, the number of points is very large; essentially this forms it continuous. So, that is why, we normally draw E k diagram continuous, the E versus k.

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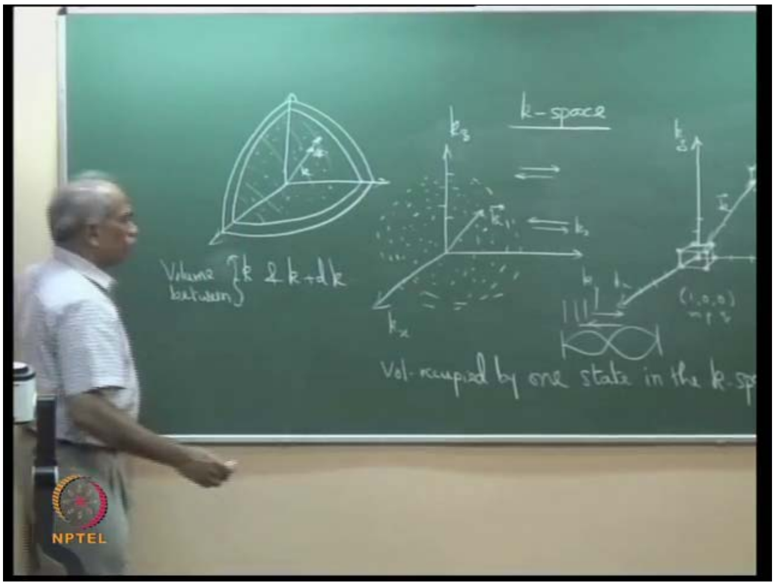

The second thing we have seen is therefore in the k space, E k, the k space or in the momentum space will have the number of permitted points. This is the k space, which means the axis are k x, k y and k z. The number of points that we have enormously large number of points and literally every points here represents an allowed k value. Our objective is to determine the density of states, which means the number of points between k and k plus of E k are unit volume of the material. So, how to determine that?

So, to determine this, the first thing we have applied stationary wave, standing wave boundary conditions, which means if I take k x value, a positive k x, the negative value k x direction is automatically taken care. k in general represents the direction along which the electrons is propagating if the propagation vector. Now, if I consider the positive direction, the negative direction is automatically taken care of because we had applied standing wave boundary conditions. Standing wave comprises of the wave which is moving in forward direction and backward direction resulting in the standing waves. Therefore, whenever I have taken plus k x, minus k x as already we have taken care.

Therefore, we need to, when we count the number of points that to get the density of states; we need to take the positive values of k x, k y and k z only. It means in the k space, which is the sphere; we need to consider only the positive octant, positive octant. We see a sphere, you have hemisphere and then one fourth of that is the octant, only the positive octant which means you need to consider an octant which is like this. An octant is generally represented like this, the sphere that is one eighth, the positive part of the sphere.

So, this is that portion of the sphere where you have only k x positive, k y and k z positive, this portion of the sphere. I hope you can imagine this is an octant, one-eighth of the sphere. You have half sphere, half hemisphere, which you divide into four quadrants. Then, you get one octant of the sphere. The octant will have positive k x and positive k y positive k z values. It is sufficient for us to consider only the positive k values, k components because the negative k components are already taken into account when we write the standing wave boundary condition.

Now, I want to count the number of points between k and k plus E k. Now, before I proceed to count the number of points in the k space, what is the volume of the pi by one point or what is the volume of the pi by one state. I should not say one point, one state. Please see that let me draw the third diagram to make it clearer because I will show here little bit spread out the points, the permitted values. I want to draw the q and this line. So, let be beneath height.

So, what I have drawn is each point here corresponds to a permitted value of k. You see what is this point. This point is 1, 0, and 0. This point that is k x where m is equal to this is m, p, q, so m equal to 1. So, this point is k x is pi by L x pi by L x and in this point, k y and k z are 0. If I take this point 0, 1, 0 and this point is 1, 1, 0 and this point here is 1, 1, 1, so different values of m, p and q will represent the different points, you can take anywhere in general.

So, if I take k value here, then there is a small spread to this side. There can be a small value. Let me show you first. See the picture what I have drawn is an infinite volume in the k space, in the k space, a small volume this is a k value. Just see the picture, if I change the k y, this is k y, this is k x and this is k z, if I change k y by this separation which is pi divide by L y pi divided by L y, then my k vector, the tip of the k vector can sit here.

The tip of the k vector can sit at any corner here, the tip of the k vector because the k vector is defined by m, p, q; values of m p q. If you keep m constant, change p constant and change q, then it will change by one unit in this direction. Do you follow? So, different values of m, p, q correspond to different points in the k space. One point here is shared by eight different cubes. One point is shared by different eight cubes. For example, this cube is this point is shared by this cube; there is a cube on this side and four cubes below. In other words, every point is shared by four cubes.

Assuming that L x equal to L y equal to L z in the cube, what is the volume of this cube here? The volume is pi by L x into pi by L y into pi by L z, pi by L z. So, this is the volume of the cube, the volume. I will make a statement and then you see. The volume of one state, one allowed state in the k space, the volume occupied by one allowed state in the k space is given by this, pi by L x pi by L y into pi by L z. Why one state? There are eight possible states here because there are eight corners. However, every corner here, every point here is shared by eight different cubes.

In other words, it is just like when you consider number of atoms in the cubic lattice, you have one atom shared by eight cubes, exactly like that; here it is not atom. These are simply points. What are these points? These points represent the allowed k values, which mean if you connect here to the origin to any of the point that will be an allowed k value, allowed state. Therefore, this is the volume occupied by one k state in the k space. So, this is we are all discussing in the k space, in the k space.

The statement is volume occupied by one statement, one state, one state in the k space, in the k space is equal to pi by L x into pi by L y into pi by L z. In the k space, if I find out what is the volume between the k and k plus d k, k and k plus d k, volume between the k and k plus d k, k and k plus d k, I find the volume and divided by volume occupied by one state will give me number of states between k and k plus d k. The volume in the k space between k and k plus d k divided by volume occupied by one state will give me number of states between k and k plus d k for unit volume will give me density of states.

So, the volume between k and k plus d k, please see this. It means I am looking at shell; volume between this shell, two shells. So, one is the shell which is k. This shell means the shell, the point is lying on the first shell a k, the second one is between k and k plus d k, so this is d k. This is the second one is here that is this point lying on the second shell. This is lying on the first shell. These imagine is an octant. So, one of them is one of the k is sitting on the one shell and the k plus d k is sitting on the next shell.

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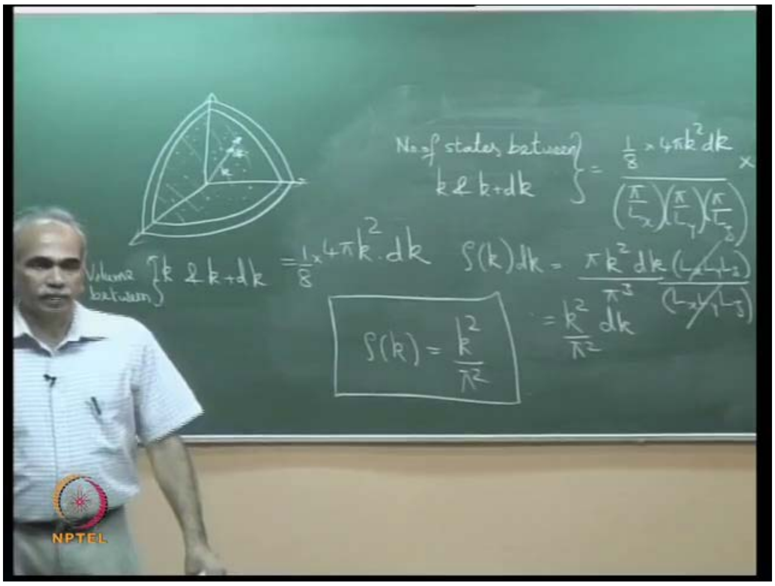

What is the volume between this and what is the volume between that? How do you get the volume? The volume between k and k plus d k, so this is equal to 4 pi k square into d k, 4 pi r square is the sphere surface area of the sphere multiplied by the thickness used to volume of the shell, so 4. But, we are considering only one octant of the sphere and therefore, one eighth into 4 pi k square d k. The volume between k and k plus d k of the shell of the positive octant of the sphere is one eighth of this volume divided by the volume occupied by one state will give me the number of states.

So, the number of states between k and k plus d k is equal to 1 by 8, 4 pi k square d k divided by volume occupied by one state that is pi by L x into pi by L y pi by L z. This gives me number of states. We have to add multiply this by a factor 2 because we are considering the momentum states of an electron. An electron can have two spin states, which also contributes to momentum states. Therefore, we have to multiply by the factor 2 because this state refers to the momentum state of the electron. It is the k space momentum state.

So, this is to a count spin of electron, this is a number of states between k and k plus d k. This is per unit volume is the density of states rho of k, the density of states rho of k d k is equal to this divided by L x L y L z that is the volume. So, you have one eighth of 4 into 2 that is already gone. We have pi k square d k divided by, in the denominator, there is pi cube and in the numerator, we have L x L y L z here divided by volume, which is also L x L y L z.

Please see this is volume occupied by one state in the k space. This L x L y L z is the physical volume. L x L y into L z is the volume of the material, the material of dimensions L x, L y, L z, volume, the actual volume this was volume in the k space. So, this gives me density of states. So, what you have left? This simply this is equal to k square divided by pi square into d k. I am sure many of you would have done this derivation earlier. Therefore, we have the density of states rho of k is equal to k square by pi square. Rho of k is equal to k square divided by pi square.

So, just if you know the definition correctly, this is elementary algebra, we have calculated volume and density by elementary so that you have the definition clear and the basic picture clear. There is nothing to remember here in this derivation; just the definition has to be correct and simply follow the procedure. It is just three four steps. Now, rho of k is the density of states in the k space, but normally we need the density in the energy space because all the rest of the parameters, which we get like the probability of occupation which is given by the Fermi function that also in the energy state. So, we would like to have the density of states in the energy states.

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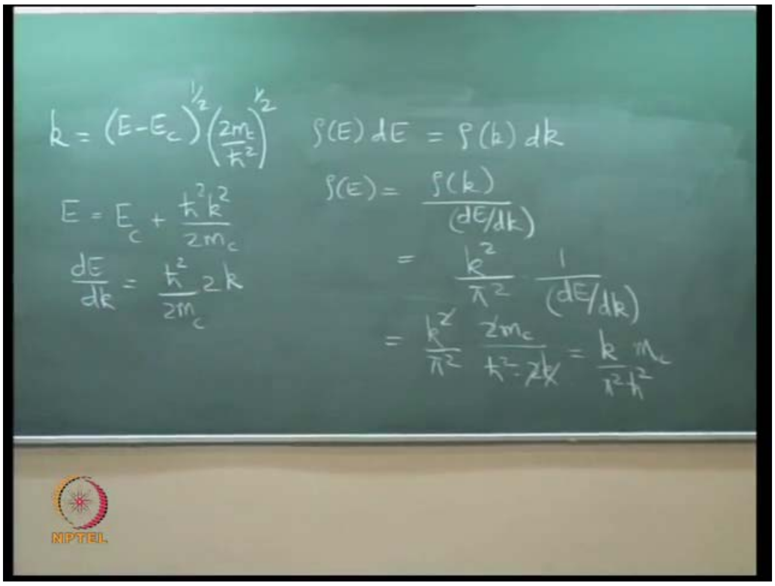

$$k = (E-E_c)^{1/2}\left(\frac{2m_c}{\hbar^2}\right)^{1/2}$$

$$E = E_c + \frac{\hbar^2 k^2}{2m_c}$$

$$\frac{dE}{dk} = \frac{\hbar^2}{2m_c}2k$$

$$\rho(E)\,dE = \rho(k)\,dk$$

$$\rho(E) = \frac{\rho(k)}{(dE/dk)}$$

$$= \frac{k^2}{\pi^2}\frac{1}{(dE/dk)}$$

$$= \frac{k^{\cancel{2}}}{\pi^2}\frac{\cancel{2}m_c}{\hbar^2 \cdot \cancel{2k}} = \frac{k\,m_c}{\pi^2\hbar^2}$$

This means rho of E. How to get rho of E? We know this, we have already seen rho of E is equal to rho of k d k. The number of states between k and k plus d k is equal to number of states between E and E plus d E. This was what we have seen in the last class from the E k diagram. Therefore, rho of E is equal to rho of k. I can write this as d E by d k. It is equal to k square divided by pi square into d E by d k, 1 over d E by d k. We make the use of parabolic approximation in very simple algebra. As I have been saying usually, we consider the electron and hole states where the parabolic approximation is very good approximation.

So, in the conduction band, we know energy of electrons is given by Ec plus h cross square k square divided by 2 m c. Therefore, E minus Ec or we do d E by d k here. So, d E by d k is, this is 0. So, we have h cross square by 2 m c 2 m c into 2 k and what is k from this expression? This is because I want to eliminate k completely from this expression, k equal to E minus Ec here E minus Ec into 2 m c by h cross square.

This is k square to the power of 2 m c by h cross square, this 2 the power half into this to the power half from the same expression, just rearranged k equal to this. So, I want to substitute for this k here. So, we have this. So, let me substitute here. Therefore, this equal to k square by pi square divided by d E by d k. So, that is just this. So, h cross square in the denominator into 2 k into 2 k divided by twice m c. So, 2 go here, one k goes here, one k goes here. So, we have m c by is it, so I simply substituted this k square by pi square divided by 2 k into this. So, this is equal to we have k by pi square h cross square into m c. I hope I have not made any mistake.

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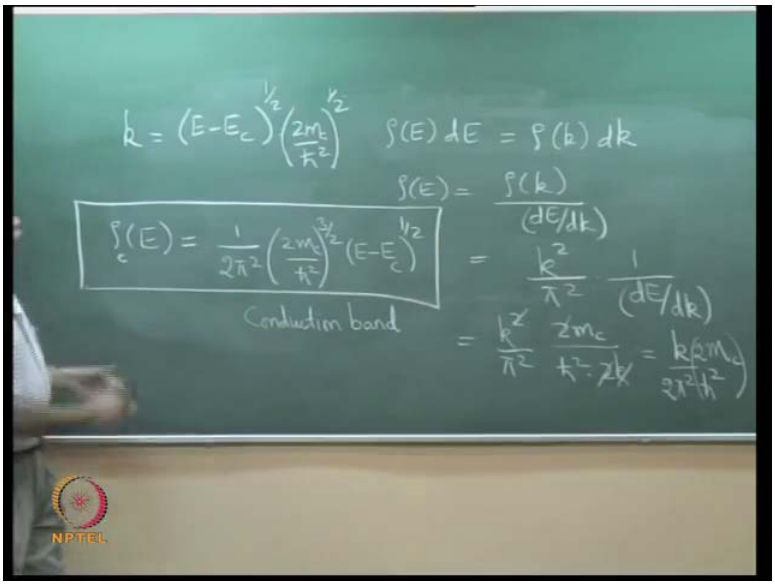

Substitute for k from here. So, we have rho of E is equal to for k, I will substitute this. So, I have 1 over pi square here, 1 over pi square, I want to do something here. Let me keep this two and two let us because I want to take this together, let me keep it as it is.

So, let me write this as 1 over 2 pi square, there is 2 m c by h cross square and there is 2 m c by h cross square to the power half. So, this is 2 m c by h cross square to the power 3 by 2 into E minus E c to the power half the expression for density of states for the density of states in the conduction band. So, normally this is rewritten as rho c of E equal to 1 by 2 pi square into 2 m c by h cross square to the power 3 by 2 into E minus E c to the power half. What is this E here? It is energy of electrons in the conduction band.

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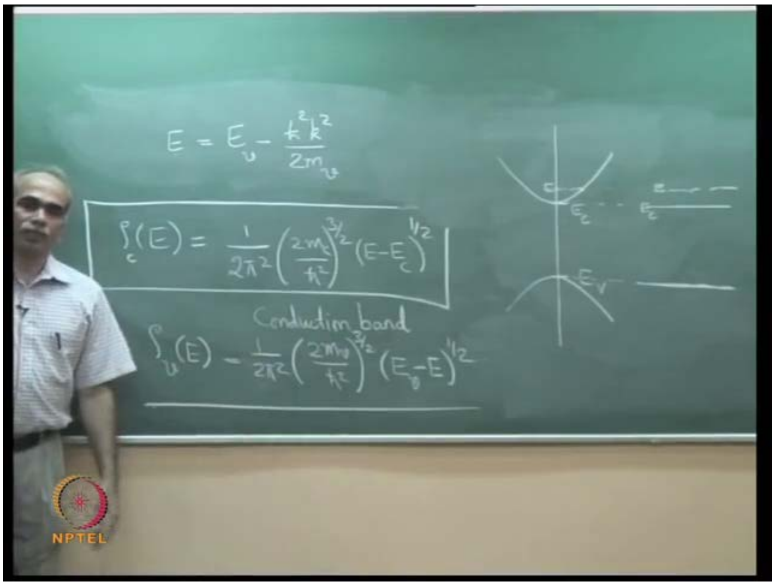

It means that if you look at the conduction band, if you look at the conduction band here where we had the E k diagram, we had the E k diagram like this. This is Ec, this is Ev. So, we are looking at the density of states in the conduction band for E greater than Ec. E is any value here in the conduction band, any value here E in the conduction band. So, E minus Ec is different for if you compare this with your old band diagram, then we are looking at the density of states available at an energy value E.

So, this is Ec, the band energy and we are looking at an energy value E in the conduction band. What is the density of states? So, the density of state is given by this expression. It could be more useful to see what is the variation of density of states with energy E, but before that if you follow exactly what we have done is to obtain the density of states in the conduction band. If you follow exactly the similar procedure starting with for the valence band, energy of holes in the valence band is Ev minus h cross square k square divided by twice m v.

Instead of using E equal to Ec plus h cross square k square by 2 m c, if you use this and find out the density of states for the valence band, you will get expression rho of v is equal to 1 over 2 pi square into 2 m v by h cross square to the power 3 by 2 into Ev minus E to the power half. Please derive this, make a simple exercise and you obtain the expression here.

Now, here we are talking of energy of electrons in the valence band here. So, E is less than Ev. That is why it is for Ev greater E less than Ev, this quantity is positive, otherwise it will become imaginary. So, E is less than Ev for the valence band. So, this is for the valence band. These are the two expressions for the density of states. Now, let me write this how the density of states would look like.

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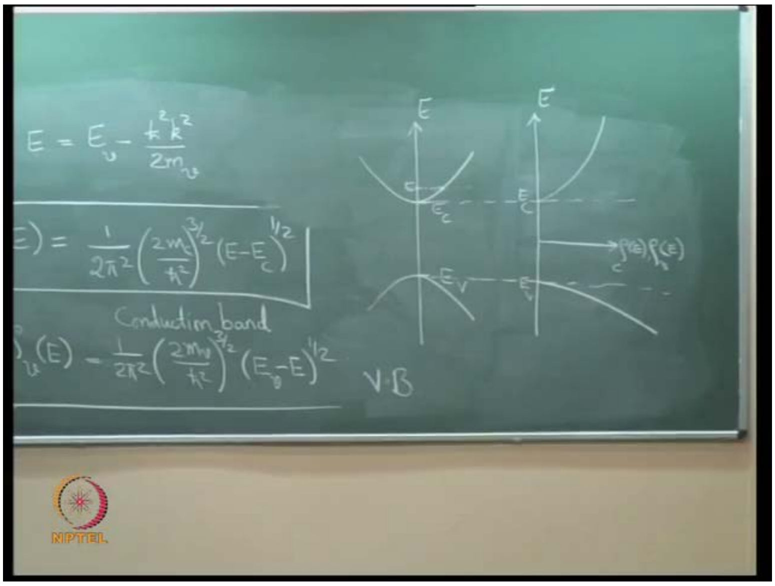

So, this is E, we are mentioning, we will always make E on this axis. So, we have all equivalent picturised here and I want to plot the rho of density of states rho of E and rho of E. So, this is this value here is Ev, this value, here is Ec. How does it vary with energy? All of these are constants. For the conduction, only energy is variable. So, it varies the square root of E, varies the square root of E, which means this should vary like this.

Similarly, for the valence band this should vary like this. Please see again. I have elaborated. This is going rapidly like this here it is going the slopes are different because assuming that m v is different from m c, m v is much greater than m c. Sometimes, you see in the books the density of states, plot density of states plotted like this.

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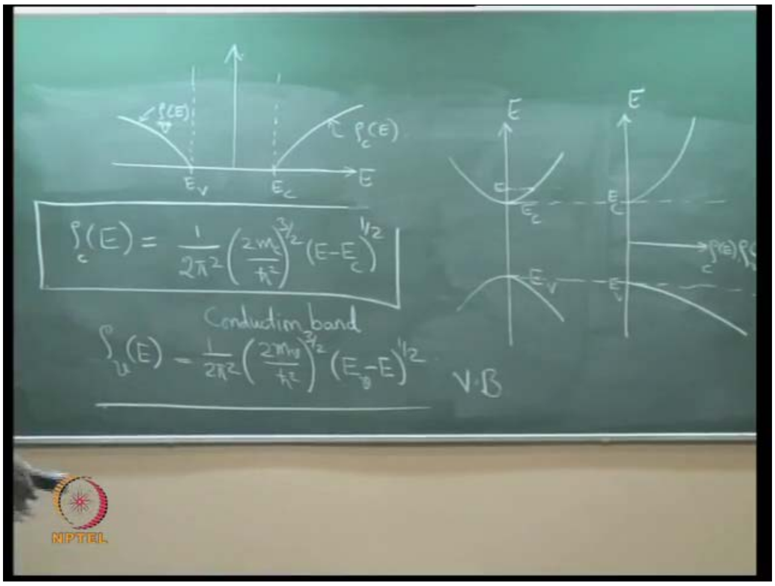

You have Ev and Ec like this. So, it is square root of E variation. So, this varies like this and this one varies. So, this is rho c of E, rho v of E and this is rho c of E. This is density of states. This is now on this axis, but to keep a consistence picture, we will plot always the vertical axis will remain the density of states energy. So, this variation is rho c of E, this variation is rho v of E. The variation again depends on the effective mass.

The density of states available depends on the effective mass of carriers. This is alright. So, these are the expressions that we will need to calculate the carrier concentration because as I already pointed out, the density of states multiplied by the probability of occupation will give you the carrier density and indicated over the band will give you carrier concentration. Before I proceed to determine the carrier concentration and discuss about the probability of occupation, I wish to draw your attention for to a small effect, which is right here. The major discussion, we will do anything later and that is related to the density of states in quantum well structures.

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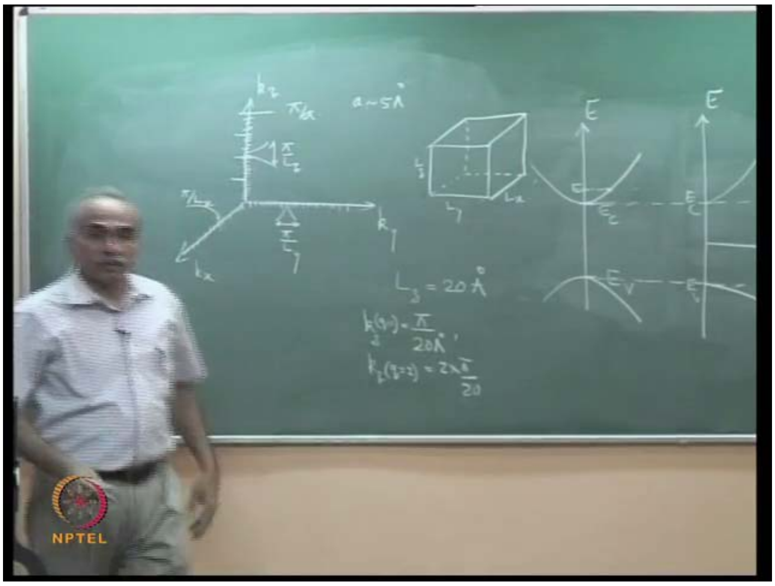

I consider a cuboid of dimensions, of dimensions L x, L y and L z. This is L z and this is L y and this dimension was L x, a piece of semiconductor with dimension this and correspondingly in the k space, we got allowed values of k y. This is k x, k y and k z. They are very closely separated points. So, start from above 1 million points within the first belongs and so very large number of points. The separation between two points here, so let me just zoom it and this is pi by L y, separation between two points here. This separation is pi by L z and separation between two points here is pi by L x.

Suppose I reduce this dimension. This was 1 millimeter. Let us say 1 millimeter. I want to reduce this. As if reduce this dimension that is we are reducing the vertical dimension here L z, what will happen? L z is reducing which means the separation is increasing. I reduce it further, the separation is increasing further and further the maximum value here was pi by a and a was approximately 4 Armstrong. That is why because L z was one millimeter and I had one million points here, but if I reduced L z, let us say L z equal to 20 Armstrong, I reduced one dimension, 20 Armstrong thin sheet of semiconductor.

What will happen? So, the first point will be pi divided by 20 Armstrong. This is k x, k z. The first point is k z with q equal to 1. So, the k z with q equal to 1, I have pi by L z. The second point k z, q equal to two two times pi by 20, so two times pi by 20 Armstrong, which is 2 by 10 Armstrong and q equal to 3 that is three times pi by 20 and q equal to 4 is four times pi by 20 which is 5 by 5 Armstrong. That is nothing but pi by a, the point is when have reduced this dimension to 20 Armstrong.

I have only four permitted values, 1, 2, 3, 4. The number of permitted values of k z are just four; from 1 million that has come down to 4. If you follow this, L x and L y is the same. Therefore, we have a large number of points for L y and L x, but here; it is completely discrete with just four allowed states. What is this implication? What will be the density of states?

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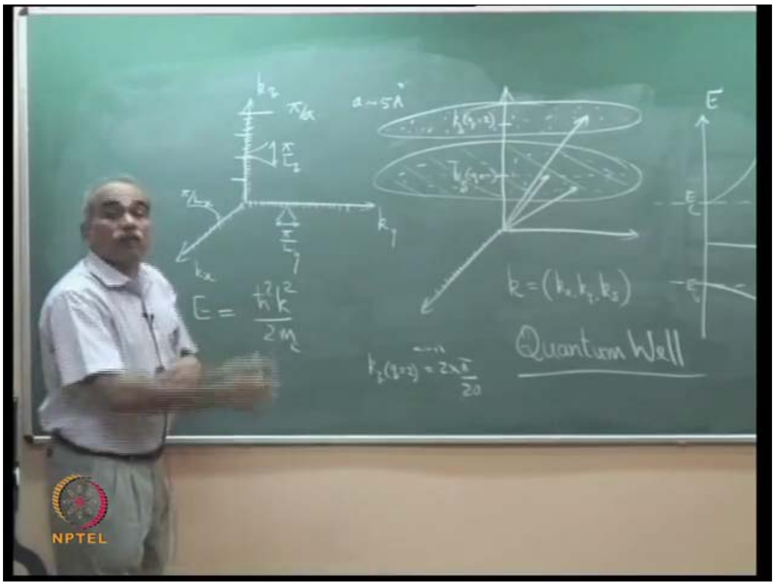

I draw it again in the k space. Now, I have first allowed points here and second allowed points here that as say this is k x for q equal to 1 k x, I am sorry k z, k z for q equal to 2, whereas these points can take, a very large number of points can take a very large values number of values permitted for k x and k y, but k z can take for simplicity, let us say there are only two values it can take. This is because its thickness is very small. This is a thin sheet of semiconductor turns out to the quantum value. We will discuss about the details of topic comes with the spike which comes especially later. But, at this point, you are assuming that it is quantum well, but we will discuss about this.

So, this sheet corresponds to quantum well as we will see, but the important point to see is the k values are highly discretized. What is in this implication? k comprises of k x, k y and k z. The first value of k z should be at this line. Earlier, we had sphere because a large number of k z values. Now, the first value of k z should be at this height, which means the k vector; the tip of the k vector must lie on plane. You see this is the axis, imagine on the plane where k and k x, this value, the first value the plane here let me show this as a disc.

So, on this disc, k, k can take any number of values any values, but the tip of this must lie on this disc. You see the disc. It is perpendicular to the z axis, the perpendicular to the k z axis. It has to lie on that because the first value of k z will be done, but the other values, it can have any value of k x, k y and k any value, but the tip must lie on this. Do you follow where will be the second value? When will be the q equal to 2? When it is q equal to 2? You will have the second disc. If you not follow, just see, it will become clear.

All k values must have non zero k x, k y and k z. So, your propagation, unless you are propagating exactly in this plane, when k z is 0, even if it is propagating at any angle, the first thing is k z must have value equal to this, which means it should lie on the first plane. Where else it can lie? If k is sufficiently large that means energy is sufficiently high.

Remember that energy is h cross square k square by 2 m c. So, if k is very large, it means energy, kinetic energy is large. So, the electrons have large kinetic energy. We can have k here; a tip of the vector can sit either in the first plane or in the second plane more or less unlike in the previous case, it was a sphere full of points anywhere you go.

That is why we have to take a volume of the sphere to find out the number of points, but now we can have because k can sit either, tip of the k vector in the k z propagation vector can sit either in the first plane or in the second plane. How to calculate the density of states and what will be the density of states in the quantum well, we will discuss in the next class.

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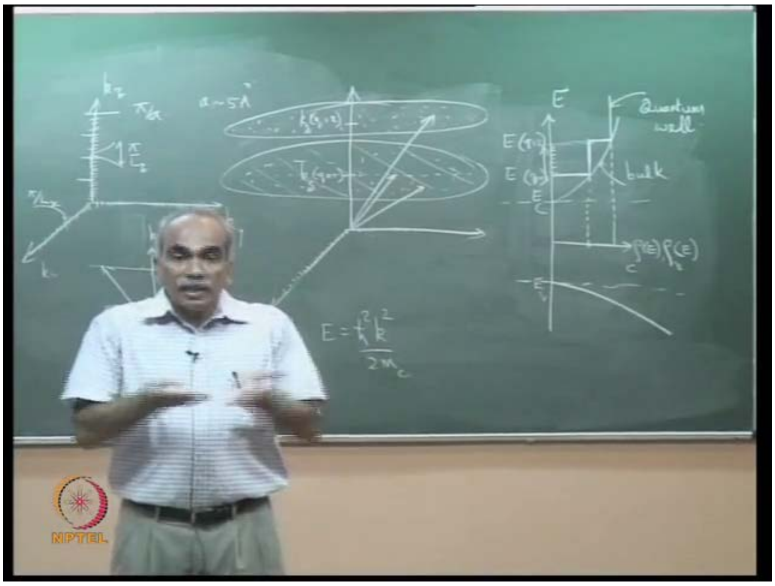

This is very important and the density of states let me, we will see the density of states in will behave like step function this is the bulk semiconductor and the density of states for a quantum well. So, in the k space, the allowed states will remain on this disc for different discrete values, corresponding to different discrete values of q. They are well separated or else q is also almost continuous, and therefore q could have been sitting anywhere.

If you see in one dimension just, if you see in one dimension, the k can have a value here, which means k vector can sit anywhere here like this. It could or k can sit here, tip can sit here because there are no other intermediate values. This is for q equal to 2, this is k z. This is for q equal to what? k cannot take any value in the intermediate. The states are discrete and the consequence of this, we will see the density of states will remain constant some value of energy.

So, below this, there are no states, density of states, this is density of this axis. This remains, it is constant here up to as you increase the energy here, the density of state remaining constant, it starts from here.

Please see the density of state here is constant in spite of the fact that you are increasing energy. When you reach an energy value here, this corresponds to q equal to 1 and when you reach energy value corresponding to q equal to 2 E, E corresponding to q equal to 2, suddenly there will be a jump. Why there will be a jump? This is because now the tip of the k vector can sit on the second disc. So, you have, it could have been sitting only on the first disc, but now it can also sit on the second disc.

If the magnitude of this is, see this length of the k vector is large, and then if you take the k vector like this, it can easily sit on the second disc. The length of the k vector large means the energy is large E is equal to h cross square k square by 2 m c kinetic energy. So, larger the value of k, it will get another disc to sit which means the permitted state becomes large.

Therefore, at larger energy values, the density of states will be here. In fact, it is double. Earlier, the density was here, here the density is double, but for all these energies, the density of states remains constant. This has an implication in the device characteristics as we will see later that when we see semiconductor optical amplifiers. The amplifier bandwidth will remain flat, if the density of states remains flat.

So, we will see these discussions in the next class.