Semiconductor Device Modelling and Simulation

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Lecture – 11
Density of States

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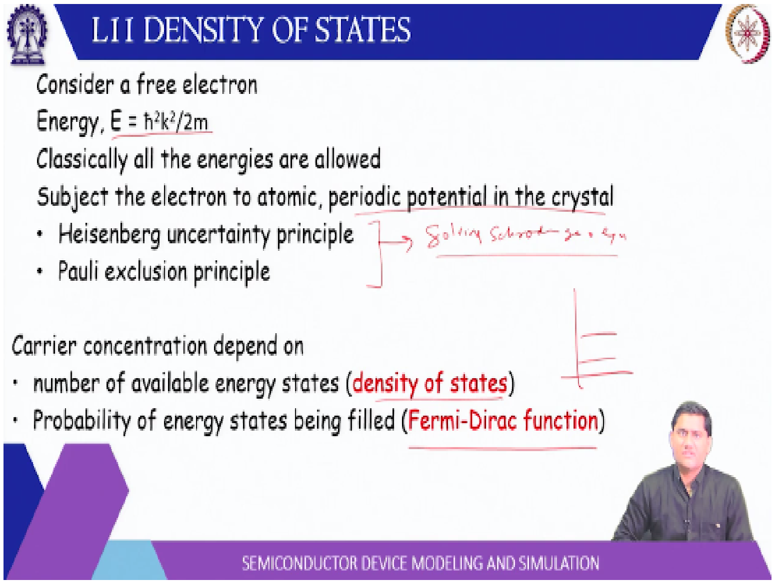

L11 DENSITY OF STATES

Consider a free electron
Energy, $E = \hbar^2k^2/2m$
Classically all the energies are allowed
Subject the electron to atomic, periodic potential in the crystal

- Heisenberg uncertainty principle
- Pauli exclusion principle

→ Solving Schrodinger eqn

Carrier concentration depend on

- number of available energy states (density of states)
- Probability of energy states being filled (Fermi-Dirac function)

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Hello, welcome to lecture number 11. In this lecture, we will discuss about the density of states. The states are basically kind of energy levels, which electron can occupy and these are discrete energy levels as we have seen in a crystal electron occupies a discrete energy levels and these energy levels forms certain state. So, a state is basically if you consider a building and there are houses are there and people can occupy them similarly, in our semiconductor crystal, these energy levels are the states that electron can occupy.

Now, consider a free electron. So, for free electron we know energy is h bar square k square / 2m and this energy is not discretized that means, electron can take any energy from 0 to infinity. So, classically all these energies are allowed now, when this electron is subjected to the periodic potential in the crystal then the quantum effect will appear basically. So, when we consider the quantum effect, we can apply Heisenberg uncertainty principle, Pauli Exclusion Principle.

So, this basically translates into the solving the Schrodinger equation and once we get the solution of the Schrodinger equation for a crystal they are discrete energy levels for the electrons. And what is the use of this density of states we can calculate the carrier concentration in a semiconductor. So, carrier concentration depends on 2 factors one is the density of state. So, how many states are there and what is the probability of the state being filled.

So, what is the probability that these states are filled. So, that is represented through a distribution function called Fermi Dirac distribution and this distribution is function is basically used for describing the occupation of Fermi fermions electrons are fermions therefore, we use this distribution function. Now, let us focus on the density of a state when electron is subjected to the periodic potential.

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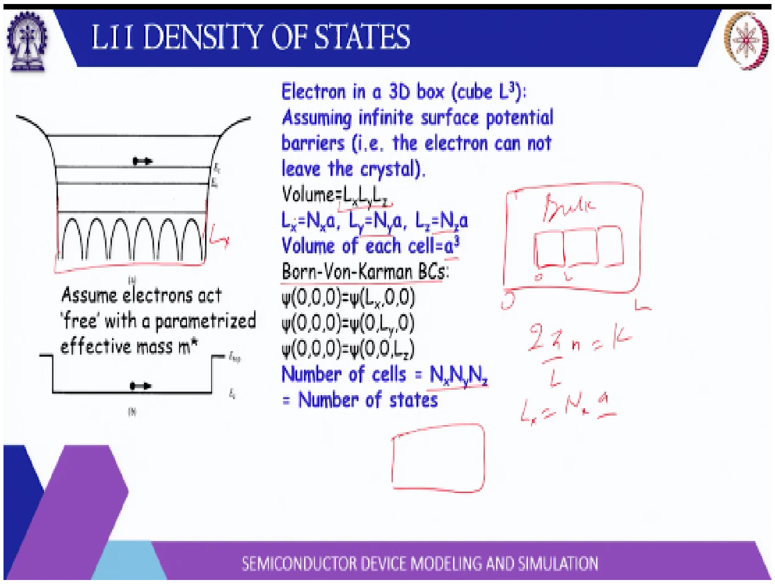

L11 DENSITY OF STATES

Assume electrons act 'free' with a parametrized effective mass m*

Electron in a 3D box (cube L^3):
Assuming infinite surface potential barriers (i.e. the electron can not leave the crystal).
Volume=$L_xL_yL_z$
$L_x=N_xa$, $L_y=N_ya$, $L_z=N_za$
Volume of each cell=a^3
Born-Von-Karman BCs:
$\psi(0,0,0)=\psi(L_x,0,0)$
$\psi(0,0,0)=\psi(0,L_y,0)$
$\psi(0,0,0)=\psi(0,0,L_z)$
Number of cells = $N_xN_yN_z$
= Number of states

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So, you can consider a crystal of length less L in each direction. So, in x direction is L x in y direction L y in z direction L z, so, the volume of this 3D structure will be L x L y L z and this electron is free to move around in this space. Now, when we apply Born Von Karman boundary conditions, so, the wave function what we do if we consider a bulk semiconductor and we consider a small section of this 0 to L and then we apply the periodic boundary conditions here or you can take a whole crystal and apply the periodic boundary conditions.

So, the waveform if we assume it is periodic, then that will give a condition that 2 pi / L times n will be k vector where n can vary from 1 2 3 like that. So, we can represent this L x is some N x times a where a is the latest constant and same thing for L y and L z. So, the volume of each cell is a cube. And this bulk structure can be thought of made up of several such units. And if there are n such units and if each unit has one state, then total number of sales will be equal to the total number of states that will be N x N y N z.

Now, if you take an overall semiconductor then we can use this concept to calculate the density of a states. So, and the electron mass, we will of course, replace via effective mass that concept we have already learned in the previous class.

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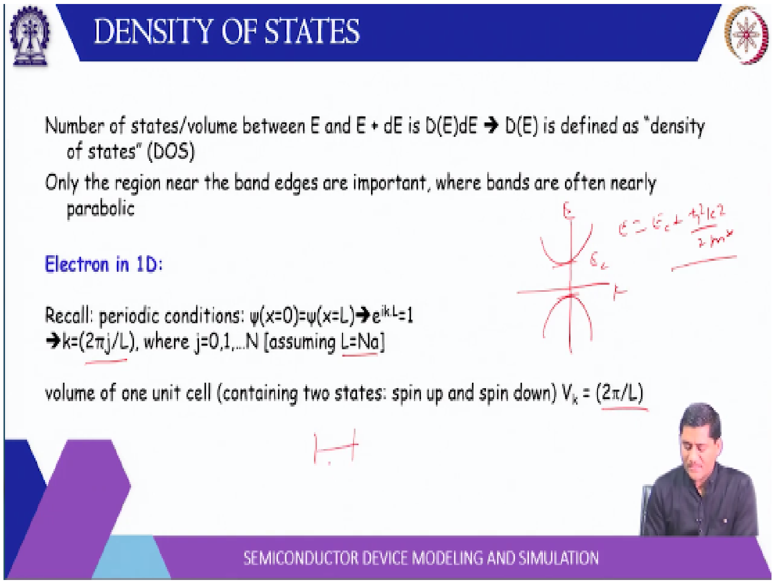

DENSITY OF STATES

Number of states/volume between E and E + dE is D(E)dE ➔ D(E) is defined as "density of states" (DOS)

Only the region near the band edges are important, where bands are often nearly parabolic

Electron in 1D:

Recall: periodic conditions: $\psi(x=0)=\psi(x=L) \rightarrow e^{ik.L}=1$
$\rightarrow k=(2\pi j/L)$, where j=0,1,…N [assuming L=Na]

volume of one unit cell (containing two states: spin up and spin down) $V_k = (2\pi/L)$

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

So, here we are restricting ourselves to the consideration that bands structures are parabolic, as you have already learned a parabolic bandy structure inside a crystal can be represented through the set this is E c. So, E is equal to this is y axis this is k. So, E = E c + h bar square k square / 2m star. So, where m is the effective mass so, that is for conduction vent for valence vent really E v minus h bar square k square / 2m effective mass.

Now, consider a 1d case. So, your k is 2 pi j / L times the integer 0 1 to N assuming L = N a. Now, volume of one unit cell is 2 Pi / L see in real lattice if the distance is L in reciprocal lattice it will become 2 pi / L.

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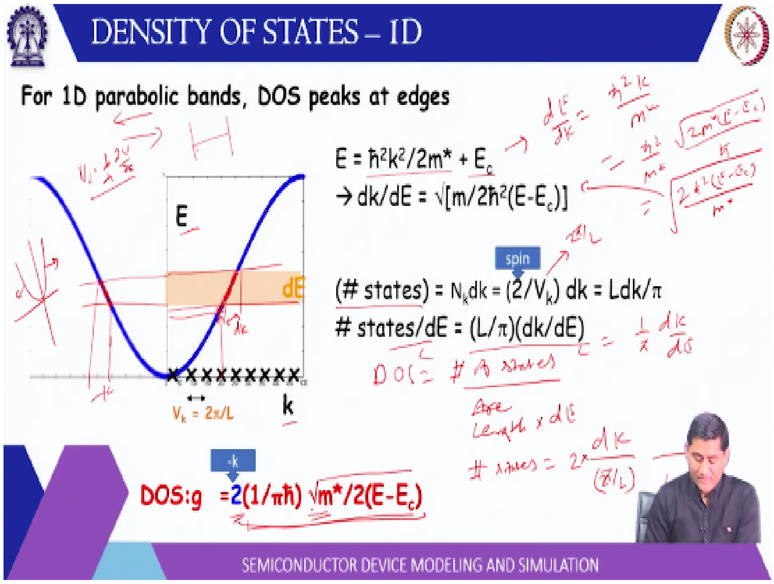

DENSITY OF STATES – ID

For 1D parabolic bands, DOS peaks at edges

$E = \hbar^2k^2/2m^* + E_c$

$\rightarrow dk/dE = \sqrt{[m/2\hbar^2(E-E_c)]}$

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

spin

$(\# \text{ states}) = N_k dk = (2/V_k)\, dk = L dk/\pi$

$\# \text{ states}/dE = (L/\pi)(dk/dE)$ $= \frac{1}{\pi}\frac{dk}{dE}$

$\text{DOS} = \frac{\# \text{ of states}}{\text{Length} \times dE}$

$\# \text{ states} = 2 \times \frac{dk}{(\pi/L)}$

$V_k = 2\pi/L$

-k

DOS:g $= 2(1/\pi\hbar)\sqrt{m^*/2(E-E_c)}$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

So, you can consider here this is the EK diagram. So, at y axis is the E x axis is K and E = h bar square k square / 2m + E c. So, number of states we can calculate. So, first let us understand what is the meaning of this EK diagram that means, if you tell me the K vector then corresponding allowed energy is this. So, that means, all the electrons will lay on this curve. So, if you tell me that E then I know what is the corresponding K or if you tell me the K what is the corresponding energy.

So, they all will lie on this curve. Now, if I want to find out what is the density of states, so, that was number of states now, DOS is defined as number of states per unit area or volume or length in 1D case it is length times dE per unit energy. So, you can consider a small section that says this is d. So, this is the reason here and how many is a steps are there. So, we can say that number of states will be now in this region the length decay is this.

So, number of a states dK divided by the volume So, volume is here the length is L so, volume is pi / L for 1D case. So, this V k pi / L 2 pi / L. Now, each state can have a maximum of 2 electrons. So, we will multiply this by 2. So, 2 times dK divided by pi / L. Now, if you want to calculate the DOS that this has to be divided by the length and dE. So, the expression you will get will be L by pi dK / dE and again divided by L. So, this will be basically if you divide this in L this will be 1 over pi dK / dE and dK / dE we can calculate from here from evaluate diagram.

So, dE / dK here is h bar square k / m star and we can substitute k here. So, h bar square / m star times k is the root of 2 m star E – E c divided by h bar and then you simplify it you get basically one h bar will remain here so, it will inside it was an h bar square. So 2 times h bar squared E - Ec divided by m star so, this is what you get here and then you can substitute to here. So, the expression you get is basically 1 over pi h bar times the square root m star write to E – E c.

Now, we have only considered this region, but this d region also corresponding to this section with where the wave vector is minus k. Now, k and k are the 2 different states, so, k is basically representing the wave vector. So, electron moving in one direction and electron moving in another direction these are 2 different states or you can think of it like this from the EK diagram we get v z is equal to 1 over h bar del v / del k and then so, this has one direction this has another direction.

So, you can visualize in terms of the group velocity also. So, if you consider this minus k also then we will insert this factor of 2. Now, we have to do this thing only in case of 1D in 2D what will happen, we will automatically consider these plus k and minus k. So, for 1D this is the expression for the density of states and you can see the density of each state is directly proportional to the square root of mass that means, if this curve is flat is it I erase it.

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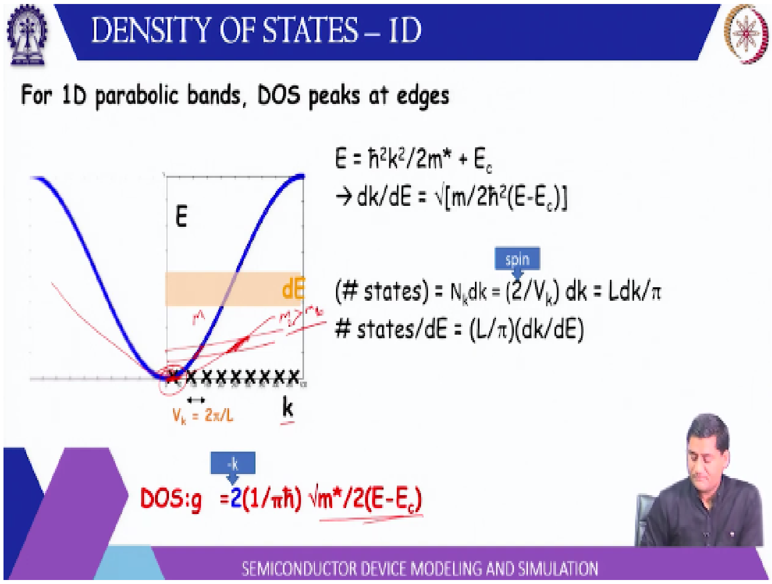

DENSITY OF STATES – 1D

For 1D parabolic bands, DOS peaks at edges

$E = \hbar^2k^2/2m^* + E_c$

$\rightarrow dk/dE = \sqrt{[m/2\hbar^2(E-E_c)]}$

spin

$(\#\ states) = N_k dk = (2/V_k)\ dk = L dk/\pi$

$\#\ states/dE = (L/\pi)(dk/dE)$

-k

DOS:g $= 2(1/\pi\hbar)\ \sqrt{m^*/2(E-E_c)}$

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So, that means, if this curve is flat then if you consider the same E number which is really more here. So, if m is more, that is it, this is m 2 this is m 1. So, m 2 is more than m 1 that means, the DOS will be more basically, you can see for the same number of same D number of states are more here, because this is more it has less flow basically. So, number of states will be more of course, given that 2 pi / L is same, another thing you can see it is inversely proportional to the square root of E – Ec.

That means state densities maximum here now why it is maximum if you see the slope here slope is 0 that is 0 slope means, if you take a small dE there is no change in k basically. So, for a small d or you can say almost 0 d there is some finite delta k. So, that is the density becomes infinite here or very large here. So, this is directly proportional to the effective mass and inversely proportional to the square root of E - Ec.

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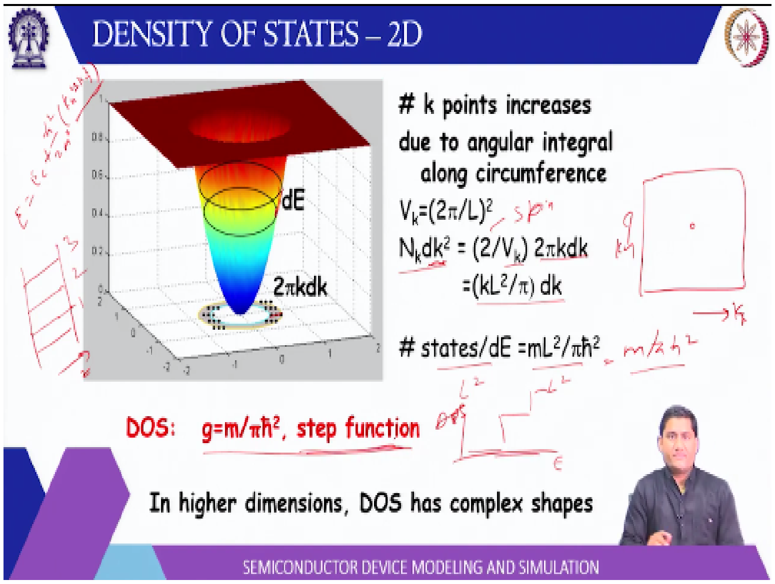

DENSITY OF STATES – 2D

k points increases due to angular integral along circumference

$V_k=(2\pi/L)^2$

$N_k dk^2 = (2/V_k)\, 2\pi k dk$

$=(kL^2/\pi)\, dk$

states/dE $=mL^2/\pi\hbar^2$

DOS: $g=m/\pi\hbar^2$, step function

In higher dimensions, DOS has complex shapes

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

Similarly, we can calculate the density of a state for 2D. In case of 2D you can visualise the state in terms of 2D diagram. So, let's say there's a K x here and there is k by here now, the area basically will be dK x dK y, but if it is parabolic so, that means E = E c + h bar square / 2m times k x square plus k y squared that is one way to write or you can write overall k vector square that also you can write. So, in this case the number of states N k dk.

So, this is dK square is basically the area and the area will be if you consider a circle here 2 pi k is the circumference and dk is the length alone. So, the small area is 2 pi k dk and there is a corresponding dE there. So, this is the basically area term. So, this is again 2 pi k dk divided by the volume multiplied by 2 like to further a spin, because each state can have 2 electrons. So, that basically gives you if you replace v by 2 / L square, you get k square by pi times dK.

And if you calculate the DOS density of states, then you states per dE per L square or per unit area. So, for L square and that is m / pi h bar square now, it does not depend on k or anything, it is constant. So, that is the 2D density of a state is a step function. Now, what will happen? This 2D basically arises from localize an enlisted z direction in one direction. So, what will happen? If you localize it in one direction, so, it is a plane here, let us say xy plane and this is less a z direction.

So, in xy plane K x and K y will be continuous, but in z direction, they will be discrete. So, 1 2 level 1 level 2 level 3 like that. So, this is a step function for each level. So, up to one this is a step function, then add one new term will come, so, it will increase and again we a step function, so, something like this. So, this will be DOS versus energy for 2D, I do not think you can see here, if you consider census area 2 pi k dk the number of state is constant regardless of the k.

So, that is unless there is a change in third dimension, the number of statement constant. So, in 2D density of a state is a step function.

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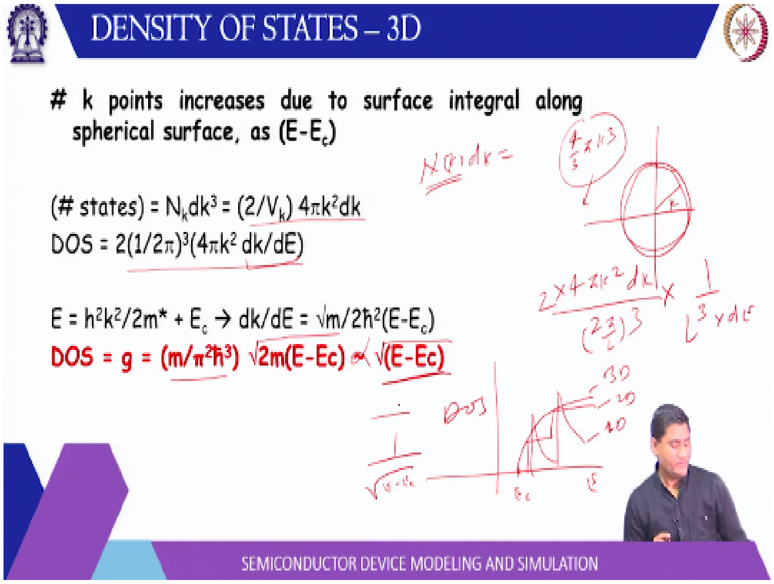

DENSITY OF STATES – 3D

k points increases due to surface integral along spherical surface, as $(E-E_c)$

$(\#\ \text{states}) = N_k dk^3 = (2/V_k)\, 4\pi k^2 dk$

$\text{DOS} = 2(1/2\pi)^3(4\pi k^2\, dk/dE)$

$E = h^2k^2/2m^* + E_c \rightarrow dk/dE = \sqrt{m/2\hbar^2(E-E_c)}$

$\text{DOS} = g = (m/\pi^2\hbar^3)\sqrt{2m(E-Ec)} \propto \sqrt{(E-Ec)}$

Now, let us consider a 3D case. So, here are the states N k dk will be you the volume, so, 4 / 3 pi k cube now, because this is the overall volume, if you consider a sphere the number of each state is varying as a function of k therefore, we are taking a small volume. So, what you will do instead of taking small volume what we are taking we take a part of the sphere with some radius k and that take the volume here.

So, that will be 4 pi k square that has a surface area times dk. So, that is a small volume of the sphere then again divided by the volume of each cell. So, that is 2 pi / L whole cube and 2 for a spin. So, you get this expression for the number of a states and density of estates you divide by L q and divided by dE. So, this expression for density of estates and again if you substitute dk by dE into it you will get basically density of a statistical do m / pi squared h bar cube times root 2m E – E c.

So, this is proportional to the square root of E minus E c. So, that means, the density of states this is E so, below E c this is 0 because this is square root of E – Ec. So, let us say this is easy. So, below it it will be 0 and above it, it is a square root of E c. So, it will something like this it will be parabolic but DOS squared is equal to E sub y squared equal to 4x the parabola equation so, that will be 3D. So, if this is 3D than 2D will be like this and 1D will be something like this.

So, this is 3D this will be 2D will be 1D. So, 3D is proportional to square root of E –E c 1D is proportional to 1 over square root of E – E c and 2D a step function or constant.

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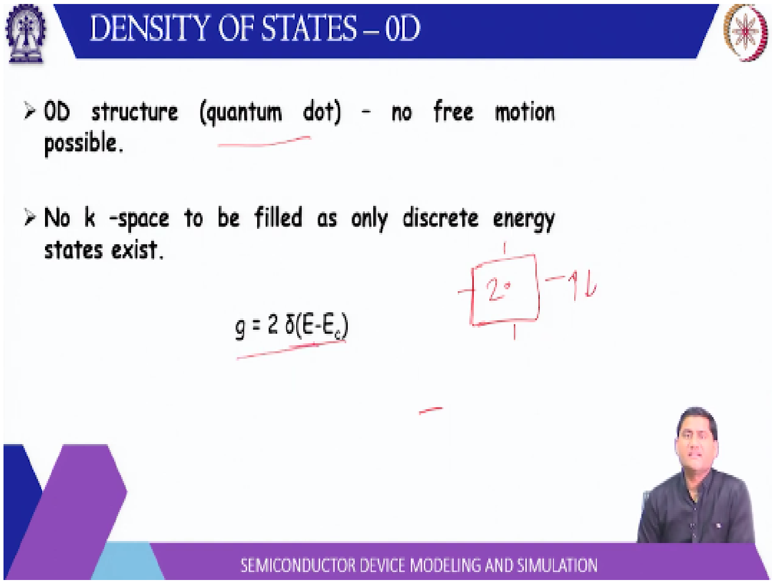

DENSITY OF STATES – 0D

- 0D structure (quantum dot) - no free motion possible.
- No k -space to be filled as only discrete energy states exist.

$$g = 2\,\delta(E-E_c)$$

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Now, let us get a more clear picture. What about 0 dimensional structure so that means if the region in a crystal is confined from all 3 directions and those are called quantum dots. So, in case of quantum dot the electron movement is restricted in all 3 dimensions. So, that means, it can only have some discrete energy. So, there is no moving wave can exist there. So, if the energy is easy, then it will be delta function basically.

So, that means, there is one a state with 2 electrons with up a spin and down spin. So, density of states 2 times delta E – E c so, that will be for quantum dot 0 dimensional space.

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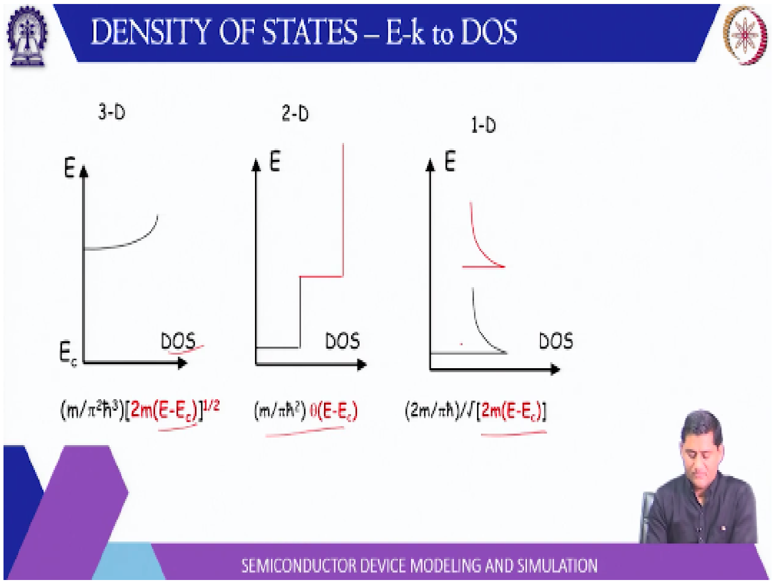

DENSITY OF STATES – E-k to DOS

$(m/\pi^2\hbar^3)[2m(E-E_c)]^{1/2}$ $(m/\pi\hbar^2)\,\theta(E-E_c)$ $(2m/\pi\hbar)/\sqrt{[2m(E-E_c)]}$

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So, this is a pictorial representation for 3D the density of states is proportional to the square root of E - E c for 2D is a constant and for 1D it is inversely proportional. So, here this DOS is x axis we can as well as plot it as y axis.

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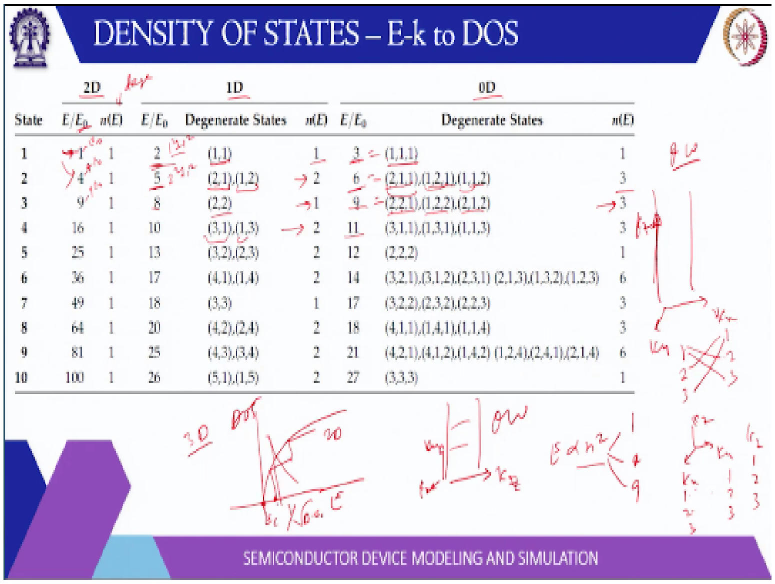

DENSITY OF STATES – E-k to DOS

	2D		1D			0D		
State	E/E_0	$n(E)$	E/E_0	Degenerate States	$n(E)$	E/E_0	Degenerate States	$n(E)$
1	1	1	2	(1,1)	1	3	(1,1,1)	1
2	4	1	5	(2,1),(1,2)	2	6	(2,1,1),(1,2,1),(1,1,2)	3
3	9	1	8	(2,2)	1	9	(2,2,1),(1,2,2),(2,1,2)	3
4	16	1	10	(3,1),(1,3)	2	11	(3,1,1),(1,3,1),(1,1,3)	3
5	25	1	13	(3,2),(2,3)	2	12	(2,2,2)	1
6	36	1	17	(4,1),(1,4)	2	14	(3,2,1),(3,1,2),(2,3,1) (2,1,3),(1,3,2),(1,2,3)	6
7	49	1	18	(3,3)	1	17	(3,2,2),(2,3,2),(2,2,3)	3
8	64	1	20	(4,2),(2,4)	2	18	(4,1,1),(1,4,1),(1,1,4)	3
9	81	1	25	(4,3),(3,4)	2	21	(4,2,1),(4,1,2),(1,4,2) (1,2,4),(2,4,1),(2,1,4)	6
10	100	1	26	(5,1),(1,5)	2	27	(3,3,3)	1

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

Now, here is a table to get a more clear picture from your textbook in case of 3D, it is not shown here the DOS is continuous the US versus the is continuous in case of 2D it is something like a quantum value. So, 2 dimensional as a K x and K y it is 3, but K z it is restricted. So, K z will be energy level 1 2 like this. And we know for when we solve Schrodinger equation for one dimensional we get energy proportional to 1 / N squared. So, for first a state let us say energy is one state is second state 1 / 4 third state 1 / 9.

So, you can see, if E 0 is the ground state energy, then ground state energy is one times E 0 the second will be 1 / 4 times E 0. So, in case of quantum one, we know that energy will be proportional to n squared. So, where n is the level so, first level energy will be 1 for second level it will be 4 times for third level it will be relativity 9 times. So, you can see 2D here E by E 0 for first level is 1, so, this energy is E 0 for second level is 4. So, then as is 4 times E 0 for third level 9 times E 0 and there is only one such state.

So, what will happen for 2D for boundary state it will be 1 then we will go like this, then second degree increase by 4 E 0. So, then it will go like this and so on. So, that is what 2D. In case of 1D this is constrained in 2 directions. So, it is basically something like quantum wire. So, let us say x dot x is constant and then y direction it constant, let us say z direction is free. So, in K x direction, it can have state 1 2 3 So, on in K y directional, so, it can have state 1 2 3 and so on. So, the lowest will be state where K x is 1 and k y is 1. So, that is 1 1.

So, the energy will be 1 the second lowest will be 1 2 and 2 1. So, the energy will be 6, so, how it is that, so, for 1 1 is E E 0. So, that is E 1 squared + E 2 e square it is 3 times E 0 for Second one, 2, so, 2 + 1 is 3 then third is to 2. So, that is basically 9 then the 4th one is 1 3 and 3 1. So, that gives you the 11. So, these are the energy levels for 1D space and you can also see the dmdc So, for 1 1 there is only one state possible for 1 2, there are 2 states are possible.

So, either 1 2 or 2 1. So, there dE energy 2 basically for 2 2 and one set so, the dE energies is 1, similarly, 1 3 and 3 1 there are 2 sets, so, that dE energies 2. So, what will happen in case of 1D The energy will increase basically and then it decreases is a square root of E - E c 1 over the square root of E – E c in case of quantum.dot is constant in all 3 directions, so, k x k y and k z it so, 111 the degenerate is 1 then the 1 2 3 1 2 3 so here also 1 2 3.

So, then 2 1 1 1 2 1 and 1 1 2 so, these the degenerate is basically 3. So, that these 3 have the same energy, because energy is proportional to the n squared and up to that 2 2 1 1 2 2 and 2 1 2.

So, again the degeneracy is 3. So, if you plot it, now, if you compare the energy, the energy is E 0 here, and here the energy is this n is the degeneracy basically so, for 1D this is 2 the was 1 square + 1 is square, for this one 2 squared + 1 squared is 5, and so on. For 0D is 1 so, 1 is squared + 1 squared + 1 square equal to 3 2 squared plus + 1 squared + 1 square = 6.

2 squared + 2 squared + 1 square = 9. So, the energy corresponding to the 3D DOS just starting from E c where the DOS is 0 because equal E c DOS is 0 here for 2D, it is starts at equal to 0, then at E equal to this is 2E 0 basically this 5 E 0 8 E 0 and for 1D 258 for 0D is 3, 6 and 9. So, it does start at 3, this is start at 2 and this is start at 1. So, that 2D DOS will start here. So, this is let us say 1, this is 2 here, and this is 3 here, so, 2 for 1D and 3 for 2D.

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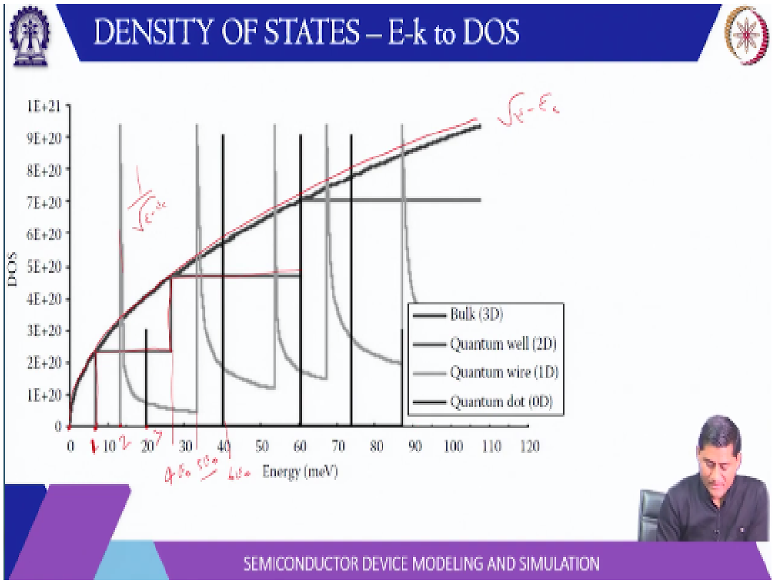

DENSITY OF STATES – E-k to DOS

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

So, you can see the picture here this starts at 0, this starts at 2 and this is starts at 3. So, this starts at 1, 2 and 3. So, this starts at 2 2 D starts at 1 and 1D starts at 2 this is E this is 2E and 1 2, and 0D is on here, this is here. So, 0D starts at 3 this is 3. So, this is 1E 2E and 3E. Then the second one you can see here it starts at 5. So, this will be at 4. So, this will be for E naught. And for 1D it is starts at 5. So, this is 1D day it will start at 5 E naught and then 0D to start a 6.

So to start at 6 E naught and you can see the nature for 3D Does the square root of E – E c for 2D is constant, it takes a step at n equal to 1 goes up, then n = 4 again goes up and so on, then for 1D, it takes a peek at 2 then comes down, it decays export as 1 over square root of E – Ec then again peaks at 5 E naught and drop down and for 0D it is at 3 then at 6 and so on you can compare with the table. So, I hope you understood the table.

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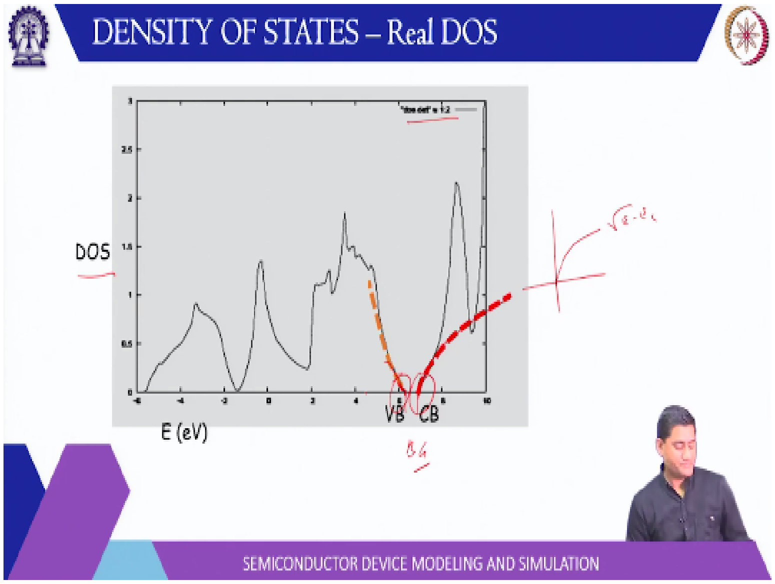

DENSITY OF STATES – Real DOS

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

Now, in real crystals the EK diagrams have not parabolic so, you will something like when you measure the density of a state you will get something like this. So, if you see here between this x axis at 6 and 8 there is a gap here. So, this is your band gap then if you see here you can fit it with some parabola basically. So, E k diagram really parabolic so, this is density of state it is a 3D basically. So, your EK diagram as to something like this is square root of E – E c. So, this is the E c this is E v.

So, you can fit it basically in terms of these curves here. So, it is parabolic somewhere here then it basically loses that parabolic characteristic and what we do here we measure the effective mass here from the parabolic curve.

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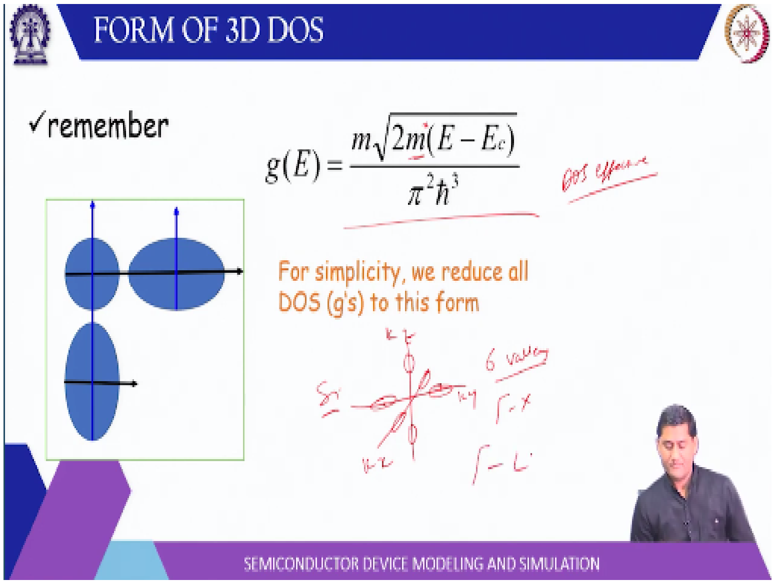

FORM OF 3D DOS

✓remember

$$g(E) = \frac{m\sqrt{2m(E-E_c)}}{\pi^2\hbar^3}$$

For simplicity, we reduce all DOS (g's) to this form

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

We should remember that for 3D density of state is this form where m is the effective mass. Now, as we have already learned that in case of silicon, germanium, these states are not parabolic or they are not a spherical whether I would say they have some ellipsoid like constant energy surfaces. So, we know that for silicon it has 6 so, this is x direction y direction z direction, so, k x k y k z. So, there is a ellipsoid here ellipsoid here ellipse here ellipsoid here ellipsoid here the ellipsoid here.

So, there are 6 such values along gamma x direction. So, for such a scenario, how will you give the effective mass. So, what we will do basically, we have a concept called DOS effective mass. So, we will give effective mass such that the density of a state remains same. So, what we will do? We will calculate overall density and compare with the equivalent sphere and the equivalent is sphere whose which can be represented with some other m effective.

So, if they give the same number of states, then we say this is a DOS effective mass for silicon and it is similar in the case of germanium, there are 8 such ellipsoids along gamma L direction.

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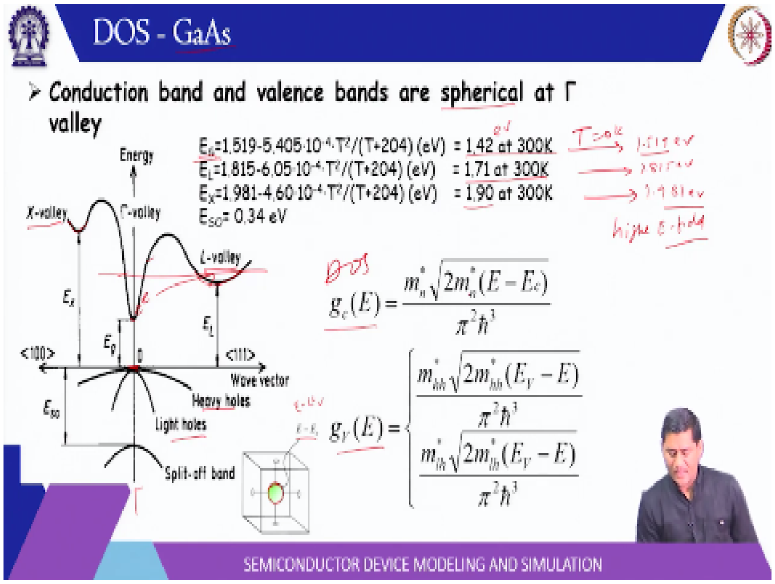

DOS - GaAs

- Conduction band and valence bands are spherical at Γ valley

$E_G = 1.519 - 5.405 \cdot 10^{-4} \cdot T^2/(T+204)$ (eV) = 1.42 eV at 300K $\xrightarrow{T=0K}$ 1.519 eV

$E_L = 1.815 - 6.05 \cdot 10^{-4} \cdot T^2/(T+204)$ (eV) = 1.71 at 300K → 1.815 eV

$E_X = 1.981 - 4.60 \cdot 10^{-4} \cdot T^2/(T+204)$ (eV) = 1.90 at 300K → 1.981 eV

$E_{SO} = 0.34$ eV

higher E-field

DOS

$$g_c(E) = \frac{m_n^* \sqrt{2m_n^*(E - E_c)}}{\pi^2 \hbar^3}$$

$$g_V(E) = \begin{cases} \dfrac{m_{hh}^* \sqrt{2m_{hh}^*(E_V - E)}}{\pi^2 \hbar^3} \\ \dfrac{m_{lh}^* \sqrt{2m_{lh}^*(E_V - E)}}{\pi^2 \hbar^3} \end{cases}$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

First let us consider a simple case where bands are spherical. So, in case of gallium arsenide the conduction band is spherical quincentenary surface in near gamma Valley, this gamma Valley and the valence band is also spherical near gamma Valley and of course, we can use the expression that we have derived. So, the conduction went DOS is m root 2m E – E c / pi square h bar cube and same way for the valence band again we have 2 bands here heavy holes and the light hole.

So, we can use the effective mass correspond to heavy hole and light hole. So, m heavy hole root 2m E y E / pi square h bar cube and for light hole m lh light hole root 2m light hole E v – E / pi square h bar cube. So, the quantimized surface looks like this in this you see in this figure is E – E c and same for E – E v and the bandgap is basically the energy difference. So, these are top of the valance band and top of the conduction band. So, this is a both are at gamma Valley.

So, it is called E g at gamma also. And this value if you notice here is a function of temperature. So, at 300 Kelvin it is 1.42 as you can see from the picture here at T = 0 Kelvin, this band gap is 1.519 electron volt. So, the unit is electron volt. So, when you increase the temperature, the band gap decreases, because at high temperature these atoms tend to vibrate, they are given sufficient energy and these bands kind of expand and the bandgap actually reduces.

Now, apart from the band gap, we also have band gap corresponding to L Valley and the X Valley. So, for L valley the bandgap is 1.71 at 300 Kelvin and at 0 Kelvin 1.815 electron volt similarly, x Valley is 1.9 at 300 Kelvin at 0 Kelvin 1.981 electron volt. So, these are different bandgap characteristic for different valleys. Now, these higher valleys become important at higher electric field. Because as you increase the electric field, the electrons here they got sufficient energy to occupy higher energy levels.

And because energy levels are same here they can as well go to other Valley this process called a scattering they get scattered to another valley. And you can notice here these valleys have different curvatures. So, that means their masses are different and that gives rise to some interesting phenomena that we will learn. So, in case of such simple bendy structures, where bendy structures spherical we can directly write expression like this for density of a state.

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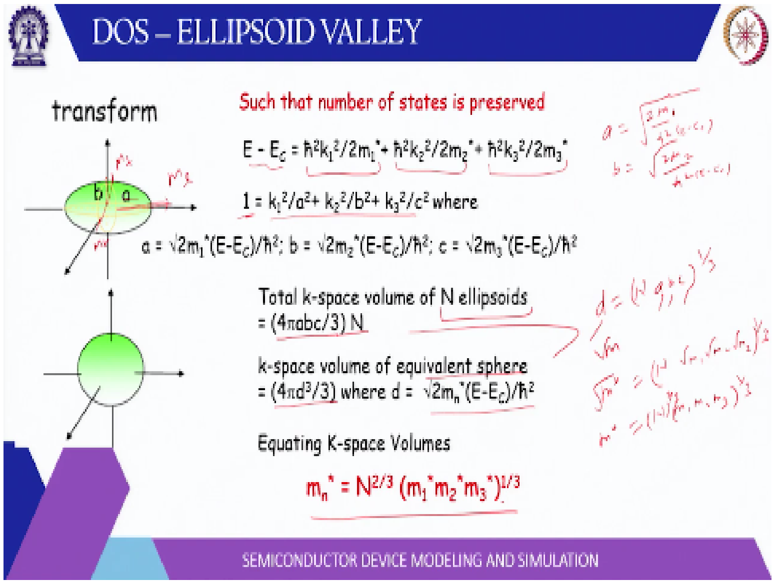

DOS – ELLIPSOID VALLEY

transform

Such that number of states is preserved

$E - E_c = \hbar^2 k_1^2/2m_1^* + \hbar^2 k_2^2/2m_2^* + \hbar^2 k_3^2/2m_3^*$

$1 = k_1^2/a^2 + k_2^2/b^2 + k_3^2/c^2$ where

$a = \sqrt{2m_1^*(E-E_c)/\hbar^2}$; $b = \sqrt{2m_2^*(E-E_c)/\hbar^2}$; $c = \sqrt{2m_3^*(E-E_c)/\hbar^2}$

Total k-space volume of N ellipsoids

$= (4\pi abc/3)\,N$

k-space volume of equivalent sphere

$= (4\pi d^3/3)$ where $d = \sqrt{2m_n^*(E-E_c)/\hbar^2}$

Equating K-space Volumes

$m_n^* = N^{2/3}(m_1^* m_2^* m_3^*)^{1/3}$

$a = \sqrt{\frac{2m_1}{\hbar^2}(E-E_c)}$

$b = \sqrt{\frac{2m_2}{\hbar^2}(E-E_c)}$

$d = (N\,abc)^{1/3}$

$\sqrt{m^*} = (N\sqrt{m_1}\sqrt{m_2}\sqrt{m_3})^{1/3}$

$m^* = (N)^{2/3}(m_1 m_2 m_3)^{1/3}$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

In case of is ellipsoid Valley let us say this is the ellipsoid. So, we are plus his long x axis is a and then transfer axis is b. So, the volume of this ellipsoid will be 4 / 3 pi abc, if there are n such ellipsoids then the total volume is n times the volume of each ellipsoid and that should be equal to the volume of equivalent sphere. That is 4 / 3 pi d cube. So, by comparing the 2 we can find out by comparing these 2 we can find out that d = N times abc power 1 / 3, so how we get it?

For ellipsoid you can write E = E c + h bar square k square / 2m 1 h square k squared 2m 2 h bar k square / 2m 3. So, these are the 3 directions x direction, y direction, z direction, so, it is ellipsoid. So, in x direction, let us say you have m l longitudinal in y and z direction it has same curvature. So, we call it m t 4 for y and m t for z. So, there is a transfer effective mass transfers effective mass and so, this can be represented by a ellipsoid here a is 2m / h bar square the square root.

So b this is m 1 similarly, b is root of 2m 2 y h bar square. So, this is what is done here basically and left side is again divided by and normalized to 1 where is this E – E c is also absorbed here. Now, when we consider N ellipsoids the volume is 4 / 3 pi abc times N. So, now if you consider d, this is root 2m E – E c y h bar squared. So, if you see here d and abc they are proportional to the square root of m. So, if you replace this by m, so, here m effective = N times root m 1 root m 2 root m 3 power 1 / 3 and this is also root m.

So, m you can write take i squared is equal to N m 1 m 2 m 3 so, you can take them separate. So, this becomes 1 / 3 and this becomes 2 / 3 so, you get this expression same thing can we done for heavy hole and light hole also.

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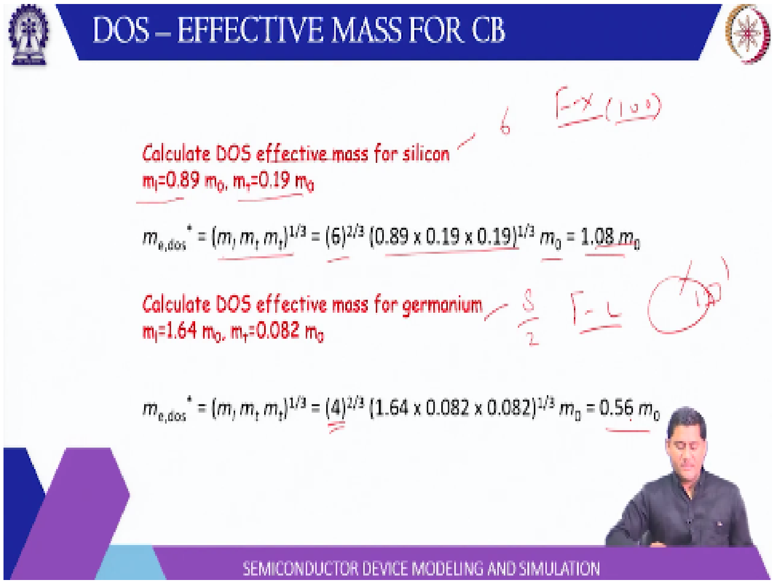

DOS – EFFECTIVE MASS FOR CB

Calculate DOS effective mass for silicon

m_l=0.89 m_0, m_t=0.19 m_0

$$m_{e,dos}^* = (m_l m_t m_t)^{1/3} = (6)^{2/3} (0.89 \times 0.19 \times 0.19)^{1/3} m_0 = 1.08\, m_0$$

Calculate DOS effective mass for germanium

m_l=1.64 m_0, m_t=0.082 m_0

$$m_{e,dos}^* = (m_l m_t m_t)^{1/3} = (4)^{2/3} (1.64 \times 0.082 \times 0.082)^{1/3} m_0 = 0.56\, m_0$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

So, now, here is a little exercise, you can pause the video here calculate it and compare the answer. So, m effective is m 1 m 2 m 3 because this elliptical, so, one longitudinal and 2 transverse so, m l m t m t power 1 / 3. Now, there are 6 6 equivalent valleys because this is a long gamma x directions now, x is 100 so, 6 to the power 2 / 3 m 1 m 2 m 3 times m naught. So, this is the equivalent effective mass DOS effective mass for silicon.

So, only for germanium there are 8 equivalent gamma L valleys, but you notice the number is 4 here, because, here the valley across at that John boundary that was just valley carried 2 cells outside cell, inside cell. So, effectively it becomes 1 / 2. So, this one is 4. So, that gives you around 0.56 m naught so, density of state effective mass for germanium.

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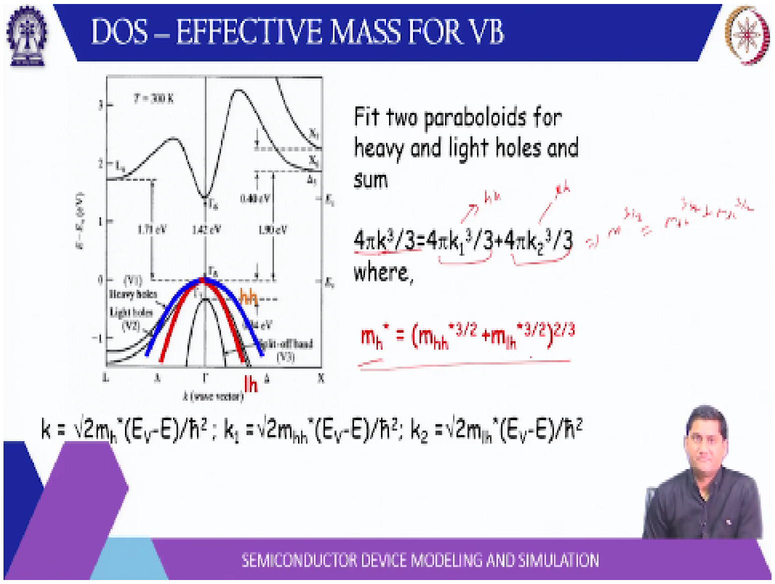

DOS – EFFECTIVE MASS FOR VB

Fit two paraboloids for heavy and light holes and sum

$4\pi k^3/3 = 4\pi k_1^3/3 + 4\pi k_2^3/3$ $\Rightarrow m^{3/2} = m_{hh}^{3/2} + m_{lh}^{3/2}$

where,

$m_h^* = (m_{hh}^{*3/2} + m_{lh}^{*3/2})^{2/3}$

$k = \sqrt{2m_h^*(E_V - E)/\hbar^2}$; $k_1 = \sqrt{2m_{hh}^*(E_V - E)/\hbar^2}$; $k_2 = \sqrt{2m_{lh}^*(E_V - E)/\hbar^2}$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

Then for the valence band also again we have 2 ellipsoids here heavy hole and light hole and we can add them. So, 4 / 3 pi k cube = 4 / 3 pi k 1 cube + 4 / 3 pi k 2 cube. So, k 1 corresponds to let us say heavy hole and k 2 correspond to less light hole. So, your m is basically you see this case proposer is square root of m. So, m to the power 3 / 2 so, you can write here m to the power 3 / 2 is equal to m heavy hole to the power 3 / 2 + m light hole to the power 3 / 2.

So, when you multiple take power 2 to the power 2 / 3 the effective whole effective device effective mass is m heavy hole to the power 3 / 2 + m light hole to the power 3 / 2 and total power 2 / 3 and because there are one such valleys you do not have to multiply this number a certain number.

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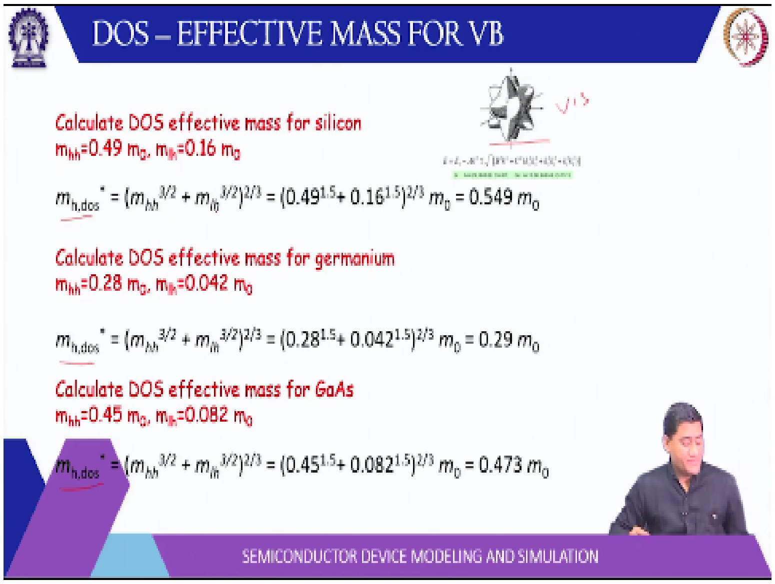

DOS – EFFECTIVE MASS FOR VB

Calculate DOS effective mass for silicon
$m_{hh}=0.49\ m_0,\ m_{lh}=0.16\ m_0$

$$m_{h,dos}^* = (m_{hh}^{3/2} + m_{lh}^{3/2})^{2/3} = (0.49^{1.5} + 0.16^{1.5})^{2/3}\ m_0 = 0.549\ m_0$$

Calculate DOS effective mass for germanium
$m_{hh}=0.28\ m_0,\ m_{lh}=0.042\ m_0$

$$m_{h,dos}^* = (m_{hh}^{3/2} + m_{lh}^{3/2})^{2/3} = (0.28^{1.5} + 0.042^{1.5})^{2/3}\ m_0 = 0.29\ m_0$$

Calculate DOS effective mass for GaAs
$m_{hh}=0.45\ m_0,\ m_{lh}=0.082\ m_0$

$$m_{h,dos}^* = (m_{hh}^{3/2} + m_{lh}^{3/2})^{2/3} = (0.45^{1.5} + 0.082^{1.5})^{2/3}\ m_0 = 0.473\ m_0$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

Send me an exercise here you can calculate the density of a state effective mass here it shows a picture of valence band constant energy surface for silicon and germanium it is quite complicated and inspired by the p orbitals and you can again calculate the density of effective mass for holes in case of silicon in case of germanium and in case of gallium arsenite. So, here there all 2 valence heavy hole and light hole bands, there is no periodicity. So, there is only one such sphere and you can calculate it.

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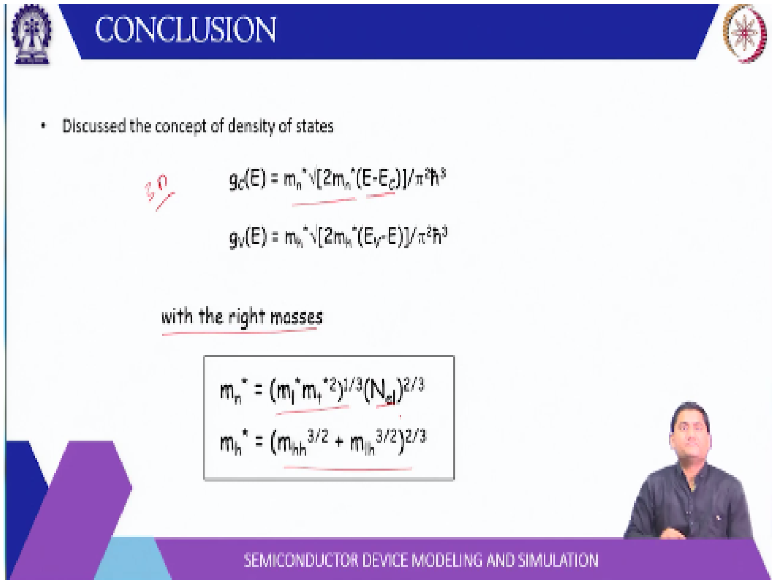

CONCLUSION

- Discussed the concept of density of states

3D

$$g_C(E) = m_n^*\sqrt{[2m_n^*(E-E_C)]}/\pi^2\hbar^3$$

$$g_V(E) = m_h^*\sqrt{[2m_h^*(E_V-E)]}/\pi^2\hbar^3$$

with the right masses

$$\boxed{\begin{aligned} m_n^* &= (m_l^* m_t^{*2})^{1/3}(N_{el})^{2/3} \\ m_h^* &= (m_{hh}^{3/2} + m_{lh}^{3/2})^{2/3} \end{aligned}}$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

So, in conclusion, we have discussed the concept of density of a states and for 3D semiconductors the density of a state is proportional to the m to the power 3 / 2 and a square root of E – E c and of course, when semiconductor does not have a spherical constant energy surface, then we can find out what is the nature of the surface and concentric surface and what is the how many ellipsoids are there. So, if N is the number of such ellipsoids, so, you can calculate effective mass by N to the power 2 / 3 times m 1 m 2 m 3 power 1 / 3 and for heavy hole you add like this. Thank you very much.