Semiconductor Device Modelling and Simulation
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Lecture - 14
Semiconductor Statistics

Hello, welcome to lecture number 14, we will discuss about semiconductor statistic. Since we have already discussed about density of a states we calculated them for different band structures, parabolic band structures, we calculated for 1D, 2D and 3D materials for 0 dimensional materials.

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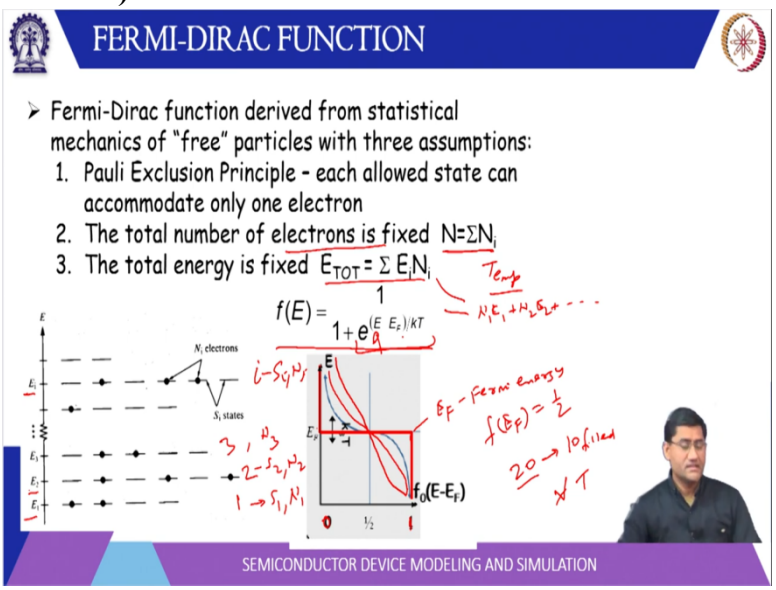

Now, in this lecture, we will learn how do the states are filled by electrons as we know electrons are fermions and therefore, they follow this function called Fermi Dirac distribution function. So, this is basically derived from a statistical mechanics of free particle with the following assumptions. We have this Pauli Exclusion Principle which actually allows that each state can accommodate only 1 electron and if second electron is there, it must have an opposite spin.

So, we can distribute these electrons under different states and each state will have 1 electron and of course, for a given scenario, total number of electron is fixed. So, let us say there are n number of state. So, this is energy level 1, level 2, level 3, this is ith level and the energy corresponding to each level is shown in the y axis E 1, E 2, E 3, E i. So, E i is the energy for ith level and each level has certain number of a states.

So, first level will have S 1 number of state this will have S 2 number of states and this will have S i number of states and total number of electron is N and they can distribute among these N number of states. So, N 1 N 2 N 3 that say these are the number of electrons in the each states N 1 N 2 N 3 and N i. So, summation of N i is total number of electron because that is fixed for a given piece of semiconductor material and at a given temperature we can say that energy is fixed.

So, E total energy is summation of all the energies. So, E 1 electron with energy N 1 electron with E 1 energy N 2 number of electron with E 2 energy. So, total energy will be N 1 E 1 + N 2 E 2. So, this is basically sigma N i E i so, N 1 E 1 + N 2 E 2 and so on. So, these are the 2 questions and third principle and when we use these 3 principles, we get a distribution function which we call Fermi Dirac distribution function.

So, it tells you the probability of finding electron in a state with energy E and that is given by 1 over 1 + exponential E - E i / kT where E F is called Fermi energy and this by definition is the energy level at which the probability of finding electron is half that means, if there are 20 states at this energy level, that means 10 of them will be filled and so on. So, whatever number of states are there half of them will be filled.

Now, this is true for any temperature. So, for any or for every temperature this is true. Now, if you follow this equation at 0 kelvin, this exponential term goes to infinity it becomes very large. So, that means, when E is more than E F this will be very large and if E is less than E F this will be very small. So, basically below E = E F this probability is 1 and above E = E F probability is 0. So, this is the probability 1 this is a probability 0 if you increase the temperature.

Then it gets basically some slope and as you increase the temperature, this slope further increases. So, all these curves they are for different temperatures they become more, they have greater slope for high temperature now how do we get this equation?

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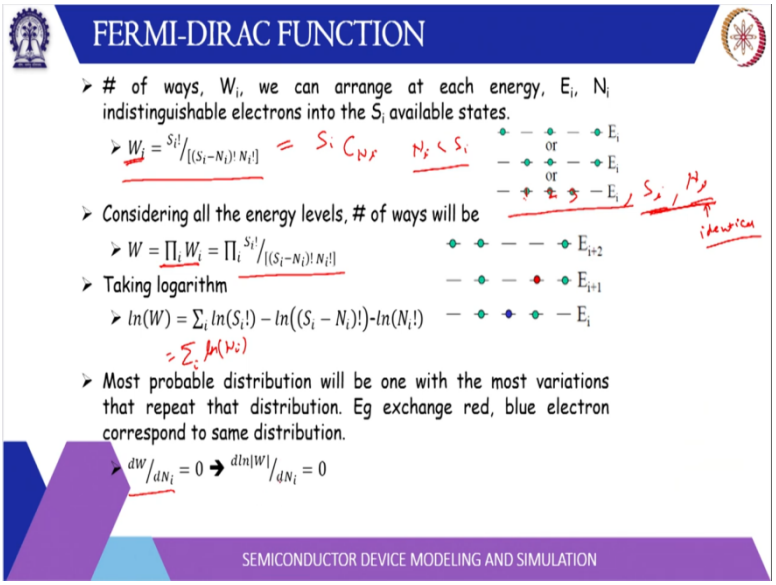

We can drag this straight from the statistical mechanics. So let us consider a state with energy E i. So let us say there is a state with energy E i and it has S i number of states, so, there are S i number of states with energy E i and let us say N i number of electrons are filling this state. Now, if you want to fill these S i state with N i number of electrons, because these electrons are identical so, whether let us say this is electron 1, this is electron 2, this is electron 3.

So, whether you have configuration 123, 312 or 321, they both are all are basically same. Therefore, what we will use the number of possible combinations will be S i C Ni. So of course, for a given a state you cannot have electrons more than the number of state, so, your N i has to be less than S i. So, this number of possible ways is S combinatorial N and that is basically given is S i factorial / S i - N i factorial times N factorial.

Now, this is the case for all the energy levels i = 1, 2, 3 and so on. So, total number of ways will be the product of number of ways for individual energy level. So, for i this is W i number of ways for 1 it will be W 1 for number 2 it will be W 2 and so on. So, total number of ways will be a product of W i so W 1 W 2 W 3 and so on and of course, if you take the logarithm of this then product becomes addition.

So, log of W becomes log of sigma log of W i, so, W i is log of S i - log of S i - N i factorial - log of N i factorial, we want to maximise this function. So, that means when this is maximum the derivative with respect to N i should be 0. So, d of W / d of N i should be 0 and that also translates to d of log W i dN i should be 0. So, this log of factorial can be approximated using a Stirling approximation.

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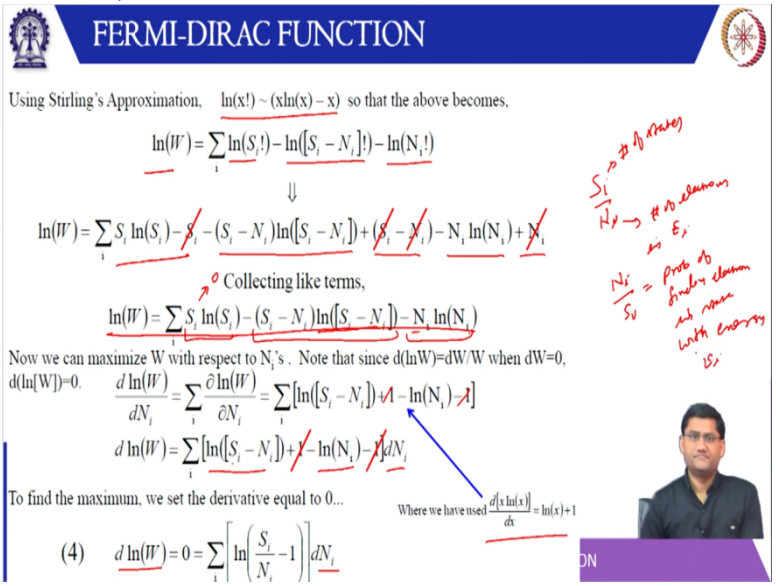

So, log of x factorial is x log x - x and then of course, log of W will become summation over i log S i factorial log of S i - N i factorial log of N i factorial and then of course, if you expand this term, so, this will be S log S - S S - N log S - N S - N - N - N log N minus becomes plus, plus N i and then these terms basically cancel out you only are left with a logarithmic terms this expression for log of W then what we can do let us take the derivative and equate that to 0.

So derivative of log W / dN i that will be so, individual term this is first term is independent of N. So, this derivative S derivative will be 0 second and third both are dependent on N i. So, they are derivatively finite and here we can use again this relation derivative of x log x is log x + 1. So, this will be log of S - N + 1 and this is log of N + 1 with minus sign. So, this 1 and 1 will cancel out.

So, what do you have eventually d / dN of log W is basically log of S - N - log of N and then you can write log of S / N i - 1 and multiply by dN i if you take dN i to the right side. So, this is the expression now, if you look at this term S i / N i, S i is the number of states and N i is the number of electrons in states with energy E i. So, basically inverse of this that N i S i is the probability of finding electron in state with energy E i. So remember this expression right now.

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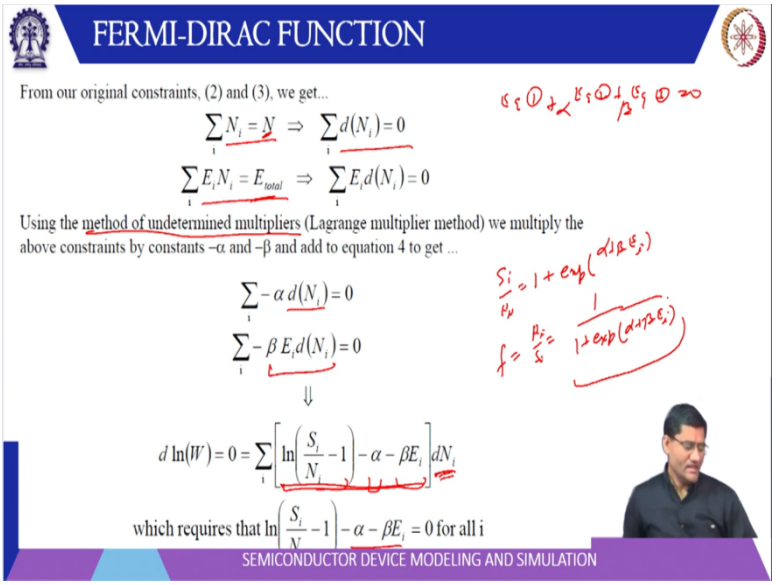

Then we can use other 2 constant that sigma N i = N there is a total number of electrons that is conserved and sigma E i N i is the total energy and of course, if you differentiate with respect to dN i, so, this is sigma dN i will be 0 because, N is fixed so, dN is 0 energy is also fixed, so, d total is also 0. So, sigma E dN i is also 0. Now, when we use these 3 equations and that method is called method of undetermined multipliers.

So, if there are 3 equations, equation 1, equation 2 and equation 3. So, we can basically say equation 1 + alpha times equation 2 + beta times equation 3 = 0, because these 3 equations are individually equal to 0 with the method of undetermined multiplier, we can write these 3 and equate it to 0. So, we can say 0 is equal to equation 1, equation 2 which is dN i is alpha times dN i and equation 3 is beta E i times dN i and that is equal to 0.

So, because dN i is the change in the N i, so, for a given configurations, where this is 0, if dN i is not 0, then this term in the bracket has to be 0, and if you rearrange this term, S i / N i - 1 will be exponential alpha + beta E i. So, you can write from here S i / N i will be 1 + exponential alpha + beta E i and then of course, probability is N i / S i that is 1 over 1 + exponential alpha + beta E i. So, this is the format of Fermi Dirac distribution function.

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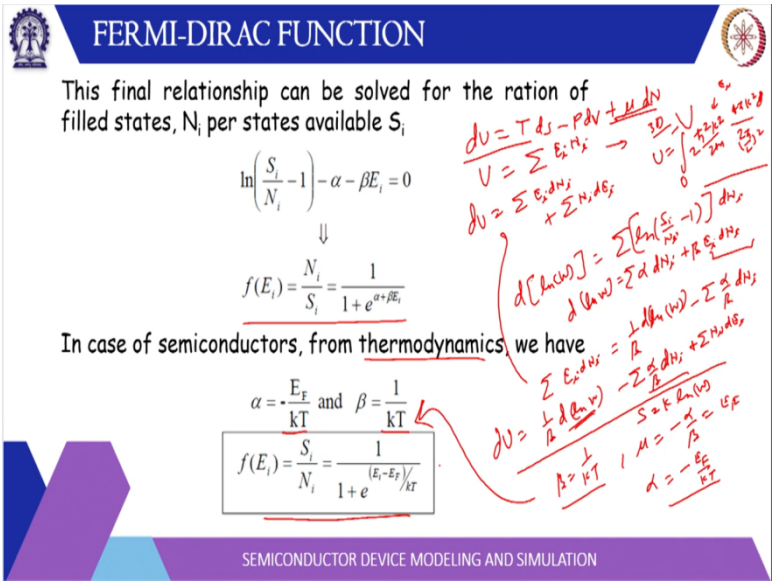

And using the thermodynamics, we can evaluate these coefficients which are alpha and beta this is the Fermi Dirac distribution function with some coefficient alpha and beta and from thermodynamics we find that alpha comes out to around minus E F i kT and beta comes around to be 1 / kT and when you substitute you get this expression. So, let me elaborate about these thermodynamics, what we can say that change in the internal energy is equal to Tds T is the temperature, s is the entropy minus Pdv.

Where P is the pressure v is the volume plus mu times dN and dN eventually change the number of carriers and mu is some kind of internal energy with some of relate to the Fermi energy. So, this is the expression in terms of thermodynamic parameters and if we write this equation in terms of this number of carriers here, what we can see your internal energy is equal to sigma E i times N i.

This we have already used this expression in our one of the problem previous problems session I think problem number 2 where we calculated that for 3D with a parabolic band structure. We said the internal energy was energy of individual electron that we said h bar square square k square / 2m. So, that was E i times number of states with this energy and that we calculated using the volume.

So, 4pi k square dk that was the volume and divide by the volume of individual state that was 2pi / N whole square and this state has 2 electrons. So, we already multiply by 2 and then we integrate it from k = 0 to a certain energy level and that gave us the total internal energy. So,

same thing we are using here. So, U = sigma E i times N i and dU will be of course, sigma E i times dN i + sigma N i times dE i again we can find this term sigma E i times dN i.

And for that we have to use these 2 expressions you recall d of log W = sigma log of S i / N i - 1 times dN i and another expression from the previous slide we can use this d of log W = alpha times dN i + beta times E i dN i. So, from this we can find out E i dN i. So, E i dN i is equal to this is sigma here so, divide this term with beta so, 1 over beta that is log of W - sigma alpha / beta dN i, this is d of log tau.

So, if you substitute this thing here and the expression for dU internal energy change is equal to 1 over beta d of log of W - alpha / beta d of N i + sigma N i dE i. So, this equation we can compare with the third thermodynamic equation. So, this log W is basically telling us about some of the entropy. So, your S = k times log of W. So, by comparing these 2 we can find out that Tds = 1 / beta log W and that tells you that beta kT = 1 / beta.

So, beta = 1 / kT and mu dN is this term here. So, that tells you mu = - alpha / beta. So, mu is basically is your Fermi level so if you rearrange it and some substitute beta = 1 / kT you get alpha = - beta E F so, E F times beta is 1 / kT. So, you get these 2 terms, which you can substitute here to get the expression for Fermi distribution function.

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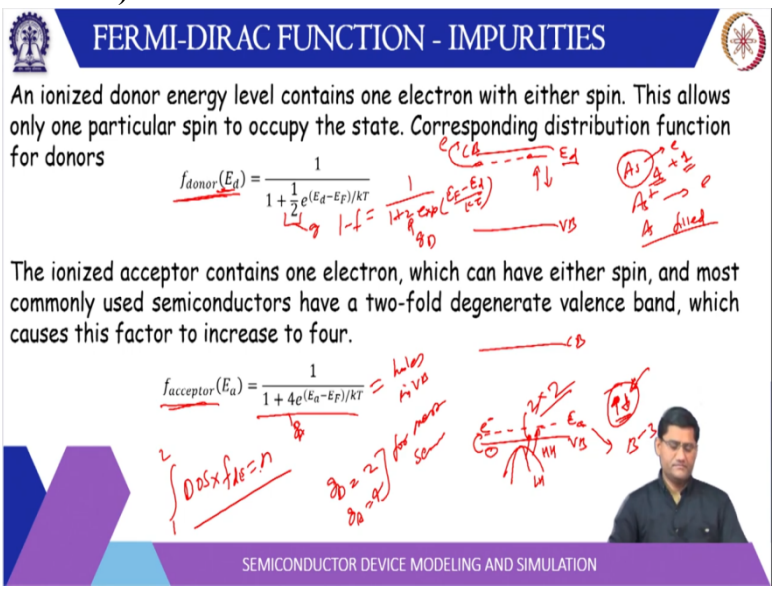

In case of the donor and acceptor level as we have already discussed about the doping. So, let us say this is your band structure and when we dope it with a donor, its energy level come somewhere here and we call it E d a donor energy level, when we dope it with acceptor, the

energy level comes somewhere here near the valance band, and we call it acceptor energy level and of course, this is valance band, this is conduction band, this is valance band, this is conduction band.

Now, this donor is basically an atom with 5 electrons with for group 4 host, a group 5 atom will act as a donor so, this has 1 extra electron. So, let us consider some atom let us say arsenic, and this gives away 1 electron. So, its outer orbital will now have 4 + 1, which is imitate. So, what are the ways that it can take that electron or give that electron, so, this Fermi distribution basically tells you the number of ways that a state can be filled.

So, this Fermi distribution function for a donor will tell you the probability that this donor level is occupied with electron. So that means it will not become negative, but it become may become neutral, because when it is positive, when arsenic is positive, it is giving away 1 electron and when it is neutral, it is filled basically. So, it can be either be filled or it can be a donor, if it gives away 2 electrons.

Then of course, energy level will change, then that energy level will not be this E d that will be different energy level. So, now what is happening because the 4 electrons are already there, the fifth electron will come to a new orbital, where it can have either a spin up or it can have a spin down. So, the electron that can come has 2 options, either a spin up or spin down. So, this allowed that only 1 of the spin can occupy the state 2 occupations are not possible, because that will change the energy. So, we have this factor of half there.

So the probability of this donor level being filled is 1 over 1 plus a factor which we call degeneracy factor, let us say g exponential E - E F / kT and of course, we are calculating this as donor energy level E d so E becomes E d here. Similarly for the acceptor, acceptor is the atom which takes 1 electron. So it takes 1 electron from the valence band and becomes negatively charged. Now, what it is doing? It is completing its octave.

So, that means it already has 1 electron with certain spin. So, the second electron that has to come has to follow the spin. So it does not have option to choose a spin it has to have an opposite to spin to the existing electron, that electron here let us consider this atom is let us say boron. So boron orbital has 3 electrons and it can accept 1 more electron, this electron has to come from the valence band.

So, now this valance band is 2 fold degenerate, so there is a heavy hole and light hole. So, either electron can come from heavy hole or electron come from light hole also, this gives you a factor of 2, another factor of 2 comes from this existing electron spin. So it can either be up or it can be either down. So there is 2 fold degenerate from here. So the incoming electron has to follow this 1. So it is spin basically is dependent on the existing electron.

So there is a degeneracy factor of 4 here for the valence band and therefore, we can write for the acceptor case f, the Fermi Dirac distribution function, the probability of occupation is 1 over 1 + 4 which is a factor times exponential E - E f / kT. Now, in case of acceptor this function will tell you the probability that this level is filled, the acceptor level is filled. So when acceptor level is filled, that means it has electron it has a hole here.

So, this will tell you the number of holes in valence band. So this will be g only but in case of donor, this f is the probability of donor level will be filled, but a filled donor level is not useful it has to give away the electron to the conduction band and it has to be empty. So, empty means 1 - f so, 1 minus probability of being filled is the probability of empty and that if you see calculate what you will get? You will get 1 over 1 + 2 exponential E f - E d / kT.

So, this is called degeneracy factor for donor and this is called degeneracy factor for acceptor. So, g D = 2 and g A = 4 for most semiconductors. So, now, next lecture, we will calculate the carrier concentration using these 2 non-functions. So, the density of a state when multiplied by the probability of filling the state and integrate over energy, we will get the if you integrate over energy from certain level 1 to level 2, you will find the number of electrons in particular band or within that energy level. So, thank you.