Semiconductor Device Modelling and Simulation

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Lecture - 13
Problem Session - 2

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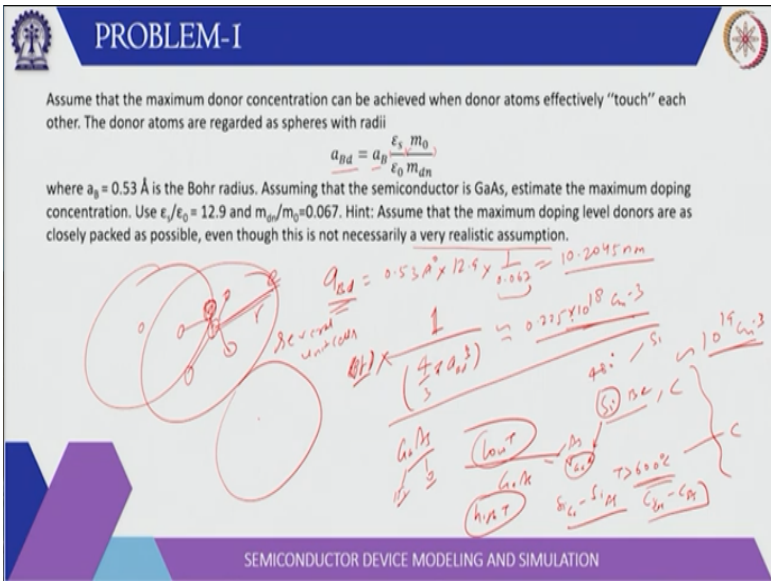

PROBLEM-I

Assume that the maximum donor concentration can be achieved when donor atoms effectively "touch" each other. The donor atoms are regarded as spheres with radii

$$a_{Bd} = a_B \frac{\varepsilon_s}{\varepsilon_0} \frac{m_0}{m_{dn}}$$

where a_B = 0.53 Å is the Bohr radius. Assuming that the semiconductor is GaAs, estimate the maximum doping concentration. Use $\varepsilon_s/\varepsilon_0$ = 12.9 and m_{dn}/m_0=0.067. Hint: Assume that the maximum doping level donors are as closely packed as possible, even though this is not necessarily a very realistic assumption.

$a_{Bd} = 0.53\,Å \times 12.9 \times \frac{1}{0.067} = 10.2045$ nm

$\frac{1}{\left(\frac{4}{3}\pi a_{Bd}^3\right)} \simeq 0.225\times10^{18}$ cm^{-3}

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

Hello, welcome to problems session 2 so, in this lecture, we will discuss the problems related to whatever we have discussed in this week. So, let us consider problem number 1 it says assume that the maximum donor consultation can be achieved when donor atoms effectively touch each other donor atoms regarded as the spheres with radii some a Bd or Bohr radius for donor atom which is given by the Bohr radius of hydrogen atom times dielectric constant times m 0 y m effective mass of n gallium arsenide.

So, let us estimate the maximum doping concentration let us understand the concept first. This will give you a rough idea it will not give you because it is not a very realistic assumption. Let us say this is your zinc blende structure these are the 4 neighbour atoms when an impurity occupies the site so that is a there is impurity here either it gives the electron number that means it has a free electron extra electron or it has a vacancy.

So let us consider it as a some electron here. And then the electron is free or loosely bound. Now, this electron because this electron is loosely bound, the radius of this electron will be much larger that you can calculate. So, a Bd so, Bohr radius for the dope point is a B which is

0.53 angstrom times dielectric constant that is 12.9 for gallium arsenide times m 0 y m dn that is one over 0.067 so, this mass is quite small here.

So, that was this radius will be quite large, then if you calculate, you get around 10.2045 nanometers you compare this thing with the dielectric constant so, this is much larger than the unit cell that is this free electron spends several unit cells. Now, if we assume that dopants are well spaced and they do not interact with each other, that will give you some idea of the doping concentration, but it is possible that you can insert more dopants.

And this is actually intersect. So, but of course, then some of them will basically kind of may not be active and then effective consultation will be less than the number of dopants, but if we just assume that this is a sphere corresponding to the radius of this a Bd the Bohr radius of the document and its volume is 4 / 3 pi a cube. So, the density will be 1 by the volume of the sphere and that if you calculate comes around 0.225 10 is to power 18 per cubic centimeter. So, it is kind of rough estimate.

But if you compare this thing with doping and gallium arsenide, so, gallium arsenide as you know it has group 3 atom and group 5 atom occupying the adjacent lattice site. So, if you grow this gallium arsenide at low temperature using MB or so, what you will get this surface will be arsenic covered. So, that was inside there will be vacancy for gallium, so, gallium vacancies will be there.

And that is the silicone or if you insert beryllium, they will occupy this site and that will be incorporated on the gallium site and they will act as n type dopant. Silicon will act as a n type dopant if you do it at high temperature then generally what will happen the silicon at gallium site and silicon at arsenic site they will form some kind of pair especially for the temperature is more than 600 degree centigrade.

And they will achieve higher concentration in case of other dopants such as carbon. So, carbon can also appear at gallium site and arsenic site. So, their doping concentration roughly as reported in literature gets order of 10 is to power 19 per cubic centimeter that is the highest. So, and of course, this peak set high temperature more than 6 around 600 for carbon and it peaks around 480 for silicon.

So, the value will get around 10 is to power 19 per cubic centimeter and if you consider these non-interacting spheres for the electron contributed by the impurity, you get around 10 is to power 18 per cubic centimeter. So, it gives you the rough estimate and of course, here you are assuming that you know that this is 1 / 4 / 3 pi a cube then if you consider that these are the hardest spheres, then some of the probability that what is a packing fraction is also to include it so, that will give you a smaller value.

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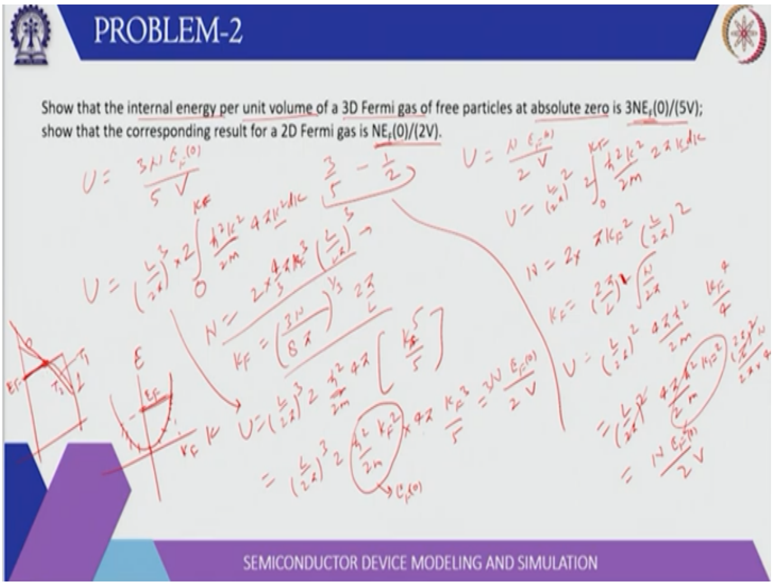

PROBLEM-2

Show that the internal energy per unit volume of a 3D Fermi gas of free particles at absolute zero is $3NE_f(0)/(5V)$; show that the corresponding result for a 2D Fermi gas is $NE_f(0)/(2V)$.

$$U = \frac{3N\,\varepsilon_F(0)}{5V}$$

$$U = \left(\frac{L}{2\pi}\right)^3 \times 2 \int_0^{k_F} \frac{\hbar^2 k^2}{2m} 4\pi k^2 dk$$

$$N = 2 \times \frac{4}{3}\pi k_F^3 \left(\frac{L}{2\pi}\right)^3$$

$$k_F = \left(\frac{3N}{8\pi}\right)^{1/3} \frac{2\pi}{L}$$

$$U = \left(\frac{L}{2\pi}\right)^3 2 \frac{\hbar^2}{2m} 4\pi \left[\frac{k_F^5}{5}\right]$$

$$= \left(\frac{L}{2\pi}\right)^3 2 \underbrace{\frac{\hbar^2 k_F^2}{2m}}_{\varepsilon_F(0)} \times 4\pi \frac{k_F^3}{5} = \frac{3N\,\varepsilon_F(0)}{2V}$$

$$\frac{3}{5} - \frac{1}{2}$$

$$U = \frac{N\,\varepsilon_F(0)}{2V}$$

$$U = \left(\frac{L}{2\pi}\right)^2 2 \int_0^{k_F} \frac{\hbar^2 k^2}{2m} 2\pi k\, dk$$

$$N = 2 \times \pi k_F^2 \left(\frac{L}{2\pi}\right)^2$$

$$k_F = \left(\frac{2\pi}{L}\right) \sqrt{\frac{N}{2\pi}}$$

$$U = \left(\frac{L}{2\pi}\right)^2 \frac{4\pi\hbar^2}{2m} \frac{k_F^4}{4}$$

$$= \left(\frac{L}{2\pi}\right)^2 4\pi \frac{\hbar^2 k_F^2}{2m}$$

$$= \frac{N\,\varepsilon_F(0)}{2V}$$

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So, let us go to the next problem. Now, let us consider it says so, that the internal energy per unit volume of a 3D Fermi gas of free particles at absolute 0 is 3. So, the U internal is 3 times n is the number of particles, then E F is the Fermi energy at 0 kelvin divided by 5 times volume. So, this is our internal energy per unit volume. And for 2D this internal energy is around n times number of particles times Fermi energy at 0 Kelvin evaluate 2 times volume.

So, Fermi energy or if you want to calculate the internal energy of a system energy is given by let us consider 3D case. So, energy is given by in the energy of individual electron is h bar square K square / 2m and again you have to integrate over volume in 3D. So, again we can consider a sphere 4pi K square dK and this is at 0 Kelvin. So, that means up to Fermi energy is basically an energy level where the probability of finding electron is half.

So, at 0 Kelvin up to Fermi energy all the states are filled and above Fermi energy all the states are empty. So, what we have to do? We have to integrate from 0 to let us say km. So, if you consider the EK diagram, this is E versus k. So, let us say this is the fermi energy E F.

So, corresponding K F will be this. So, all these states are filled up to this point. So, the energy is h bar square K square / 2m times 2pi K square dK.

And 0 to K F that is the energy of electron then of course, you have to multiply because there are 2 state each state will have 2 electrons and the again you have to multiply the volume so, that is divided by the volume, so, density L / 2pi to the power cube. So, that will be the internal energy. So, but K we have to find out so, K we can find out in terms of the carriers. So, we can also find out the carriers.

So, number of carriers will be n is given by we have to calculate volume. So, 4 / 3 pi K cube for each state there are 2 electrons because of spin and then you have to multiply or divide by 2 pi / L so, so, multiply by 2pi / L whole cube. So, this is the volume of 1 state. So, that will give you the n. Now, this is up to K F, so, you can write K F here because this is 0 Kelvin. So, occupation probability is 1 up to E F so, the occupation probability 1 is 0 n.

So, you do not have to worry about that distribution function. So, from this you can find K F = 3N / 8 pi and then power 1 / 3 times 2pi / L and when you substitute here U you will get L / 2pi cube times 2 h bar square / 2m 4pi. So, K square K square K 4 so, it becomes K 5 / pi K to the power 5 K power 5 / 5 and K 5 K to the power 5 is there we can write L / 2 pi power cube 2 into h bar square / 2m you can take K F square here and 4pi K F cube / 5 here.

So, this is h bar K square / 2m is E F 0 and then when you simplify that will come around n times E F 0 / 2 times V, V is a volume and you can get from here K F cube here from K F cube we can get n so, 4 pi KF cube / 3 this is 3 we will come here same way we can do for 2D. So, 2D the internal energy is this first 1 to n, n = 2 times 2n spin per state then in a this pi K squared times L / 2pi square is the area divided by 2pi whole square.

So, that tells you find K F = 2pi over L square times n over 2pi square and this goes to 1 then U is the internal energy that again we can find for 2D then integrate x bar square K square / 2m again here we will have area. So, 2pi K dK 0 to K F and again 2 times L / 2 pi square. So, U = 1 / 2 pi square times 4pi h bar square / 2m K cube is there 2 + 1 K cube this is K F 4 / 4. So K you can substitute here L / 2pi square times 4pi h bar square / 2n K F square / 2 here and K F square / 4.

So, K F square can be written as 2pi / L square n / 2pi times 4, so, L / 2pi will cancel here and this is energy this is 4pi 1 / 2, this is N times E F 0 / 2 N times h bar K square E F 4pi, 4pi will cancel 2 is in the bottom. So, this is per unit volume so, from this basically exercise we can realize that internal energy is proportional to the number of electrons multiplied by the Fermi energy and of course, per unit volume with some multiplication factor in case of 3D the multiplication factor is 3 / 5 in case of.

So, in case of 3D multiplication factor is 3 / 5 in case of a 2D the multiplication factor is 1 / 2 similarly, you can do for 1D also and that will tell you about the energy that is there now, this energy distribution will be helpful when we do the calculation for, when we will discuss the semiconductor statistics that time this energy distribution we will look into it that what is the probability of occupation of different energy states.

So, of course at 0 temperature 0 Kelvin the probability is 1 up to Fermi level and beyond Fermi level the probability is 0, but if you go to high temperature, this probability actually decreased this changes the configuration changes. So, at E F the probability is basically half below that it is more than half above E F the probability is less than half and increase the temperature this becomes the slope actually increases.

So, let us say this is a T 1 and then this T 2. So, this at higher temperature this becomes was more sloppy. So, that means, more and more electron can have higher energies.

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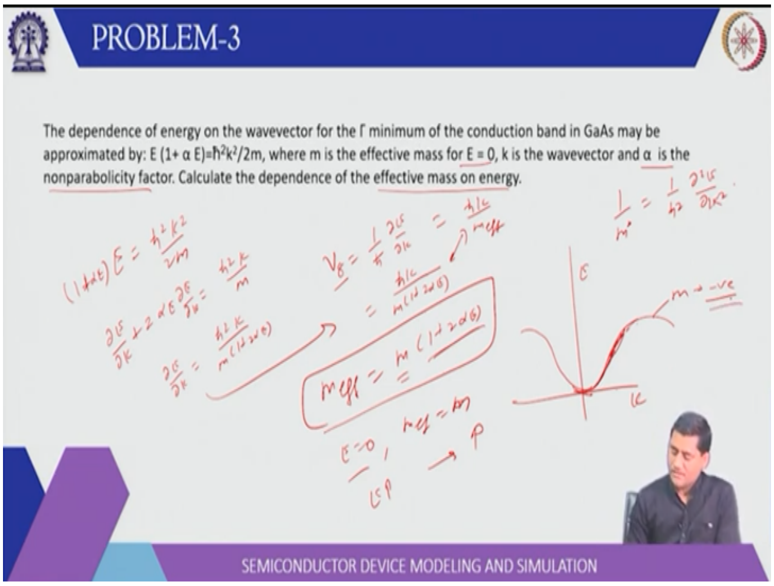

PROBLEM-3

The dependence of energy on the wavevector for the Γ minimum of the conduction band in GaAs may be approximated by: E (1+ α E)=$\hbar^2k^2/2m$, where m is the effective mass for E = 0, k is the wavevector and α is the nonparabolicity factor. Calculate the dependence of the effective mass on energy.

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Let us consider the third problem. So, far we have discussed that bands are parabolic. So, E = h bar square K square / 2m however, real bands may not be parabolic and they may be approximated by a function 1 + alpha e times e = h bar k square / 2m where m is the effective mass for e = 0, where it is parabolic and alpha is the non-parabolicity factor. Now, can you find out what is the effective mass and how does it depend on energy it will be a function of energy.

So, we can differentiate this with respect to K. So, on left side what we get dE / dK + 2 times alpha E dE / dK = h bar square K / m. So, we can say dE / dK = h bar square K / m times 1 + 2 alpha E. Now, let us get this in the format for group velocity. If you recall what is the group velocity? It is 1 over h bar del E / del K. So, if you get the expression from here 1 / h bar del E / del K is h bar K / m into 1 + 2 alpha E.

And this is h bar K / m effective, because it is a group velocity, so h bar K / m effective. So, we are comparing these 2 expressions, we can say that m effective = m times 1 + 2 alpha E. So, that is your effective mass of course, at E = 0 effective mass is m. So at E = 0, m effective is m and as the E increases, your effective mass actually increases 1 + 2 alpha E times m. Now, why it increases? If you see here, it is non parabolic, then, this basically mass is what?

If you recall mass is 80 to the curvature. So, here curvature is this here curvature is slightly broadened due to the non-parabola setup. So, the mass has actually increased and if curvature goes like somewhere, then here mass will become negative. So, what we can do? We can calculate the double derivative at different positions as a function of K and we can assign the mass is there.

So, that is another way we can calculate the effective mass. So, that is 1 over h bar square d2E / dK square, if you recall, 1 over m effective is 1 over h bar square d2E / dK square. That we also we can calculate to the effective mass.

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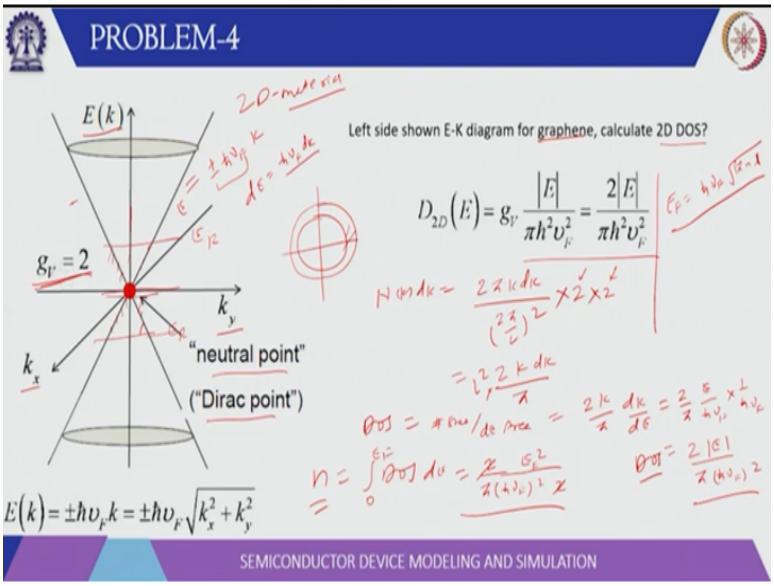

PROBLEM-4

Left side shown E-K diagram for graphene, calculate 2D DOS?

$$D_{2D}(E) = g_V \frac{|E|}{\pi\hbar^2 v_F^2} = \frac{2|E|}{\pi\hbar^2 v_F^2}$$

$E_F = \hbar v_F \sqrt{\pi n}$

$N(k)dk = \frac{2\pi k\,dk}{\left(\frac{2\pi}{L}\right)^2} \times 2 \times 2$

$= L^2 \frac{2k\,dk}{\pi}$

$DOS = \#\text{ states}/dE\ \text{Area} = \frac{2k}{\pi}\frac{dk}{dE} = \frac{2}{\pi}\frac{E}{\hbar v_F} \times \frac{1}{\hbar v_F}$

$n = \int_0^{E_F} DOS\, dE = \frac{\pi E_F^2}{\pi(\hbar v_F)^2 \pi}$

$DOS = \frac{2|E|}{\pi(\hbar v_F)^2}$

$E(k) = \pm\hbar v_F k = \pm\hbar v_F\sqrt{k_x^2 + k_y^2}$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

Now, let us consider one last problem. Here, you see the EK diagram for graphene, graphene is a 2D material. So y axis is E x axis is k so k x and k y is a 2D material. Now g v = 2 means, it is doubly E degenerate. So, there are 2 such band structures, there are 2 such bands. So, at this point, where k is 0, we call it Dirac point or neutral point and this EK is a linear basically.

So, your EK is plus minus this is plus and this for minus so plus minus h bar nu f times k. So, it's a constant of proportionality h nu times k. So, now, we have to calculate the density of a state is a 2D material. So, the density of a state will also be 2D density of a state here I have given the expression. So, let us find out how do we calculate it. Now, let us find out Nk dk, that is a number of states, number of states Nk dk is basically again you can calculate.

You recall the way we calculate the density of a state for 2D we consider one annular region then we find out the area that is 2 pi k dk. So there is a whole area divided by the area of Fermi state that is 2 pi / L whole square times each state can have 2 electrons so for 2D spin, there is a degeneracy of 2 and this you have to there are 2 such bands basically. So we have to then multiply by 2.

So, 1 for that is spin that is Pauli Exclusion Principle and 2 for degeneracy and that comes out to be 2 to 4 to 8, so, that is 2 this is k dk. So, 2k dk / pi and then L square now, if you see this is E. So, we have to convert this into dE. So, dE = h bar nu F dk. So, DOS is number of a state per unit dE and per unit area in case of 2D. So, divided by L square and divided by dE. So, that comes out to be 2k / pi times dk / dE. So, dk / dE is basically 1 over x nu that comes out to be 2 / pi k is E / h nu.

And dk / dE is 1 over x nu x bar nu that comes out to around 2E / pi x bar nu F square. So, that will be the density of states. Now, density of each state has to be positive and energy can be you know it can be above the 0 level. So, we will put a bar here so, 2E / 5 x nu F x bar nu F square so, that will be the density of a state. Now, let us go one step further we can find out also the carrier concentration.

So, the Fermi level can be somewhere here at the Dirac point Fermi level can be somewhere here above the Dirac point Fermi level can be somewhere here. So, E F is above that means it has some extra electrons here, if Fermi level is below, then it means it has some holes basically. So, in either way, we can calculate the DOS we can integrate the DOS So, if you integrate the DOS 0 to E F over dE that will tell you the number of electron concentration.

So, remember this is for 0 Kelvin at high temperature of course, you have to multiply this thing by the occupation probability because for 0 Kelvin up to here the probability of occupation is 1 so, you can just simply integrate that DOS and that comes out to be around 2 / pi h bar nu F square times E dE. So, it will be E square / 2. So, this will be E square / 2. So, this is up to 0 to E F, so, this will be E F square - 0.

So, that is E F square / 2 and from this you can also find out the Fermi level in terms of N. So, this 2 will cancel here. So, you can find out the Fermi level at 0 Kelvin, we will be x nu F times pi N. So, if you take a square root, so, this is curve will become 1 and this will be 1 / 2 so square root of pi N. So, this of course, because m can be electron or hole we just take the mod here.

So, that will tell you the Fermi level so, that was an example for 2D material and if you are given any arbitrary band structure, you should be able to find out the density of the state and the carrier concentration at 0 Kelvin for a given band structure. Thank you very much.