Semiconductor Device Modelling and Simulation
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Lecture - 34
Semiclassical Transport

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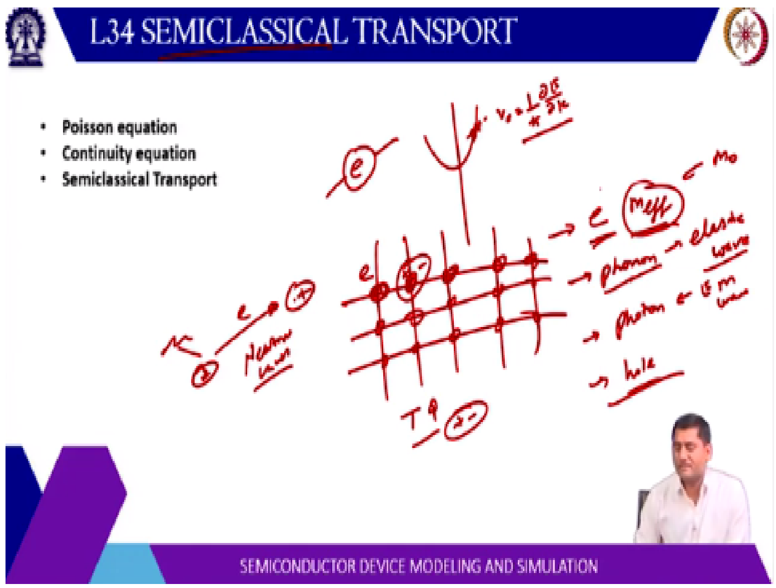

Hello welcome to lecture number 34. Today we will discuss a topic semi classical transport. As the name suggest in semi classical transport, we treat electrons as a particle. Now when we discussed about the band structure and then generally people discuss about the quantum mechanics there and the wave nature of these carriers come into the picture. But if you recollect this band diagram here and then we said that the group velocity is del E by del k times 1 over h bar.

So, this is some big packet here you can say each position can be represented by some ray packet with group velocity given by the band structure. So, the transport of these carriers they undergo a lot of interaction with the others particles. Now let us understand the concept of this particle. Let us say this is your silicon lattice unless these are the ions occupying these sides connected to these four nearest neighbours.

These electrons are moving around this one this crystal. So, some are bounded and those which are free they can move around. They are bounded by this crystal two and they are allowed to have certain wave vectors, and then under this condition what we do? We represent these electrons by a electron with mass M effective instead of the free space mass which is M 0. So, what we have done basically?

We have taken this electron which behaves as a wave in the crystal structure and we have represented it by a particle with different mass with some effective mass. So, that way we have taken care of the wave nature to treat it classically. Then at zero kelvin these atoms are fixed, these nucleuses are fixed. But as you increase the temperature this nucleus will vibrate and when this nucleus vibrate this vibration we also call it phonon.

So, this quantized vibration of this atoms on their lattice side again we represent it was some particle called phonon. So, this is basically comes from sound wave. So, the quantization is the so this elastic movement of this crystal atoms. So, this elastic wave in quantized form is called phonon. Similarly, when these atoms vibrate the electron cloud around it may go under distortion. So, this nucleus is positive, electron in the cloud is negative so this is a dipole.

So, this dipole may change the polarity. So, if dipole is oscillating it will do some give away some radiation. So, that will be electromagnetic wave and then active magnetic wave is represented by a photon in particle form. So, there is electron, phonon and photon and there is another particle which is the absence of electron and we call it hole. So, these two particles we have discussed in detail the electrons and holes.

But phonon you can understand it is basically tells you all the temperature of the crystal and it represents the elastic wave. So, what we do here in semi classical transport we monitor the behaviour of these carriers especially the electrons and phonons and we treat them particle between the collisions. So, let us say this wave pectate is interacting with some impurity or some phonon and then to get scattered and then again it interact with some other impurity of phonon.

So, in between these two collisions we can use the Newton's laws to monitor the movement of these carriers to model the flow of these carriers. So, that is semi classical transport. Why? Because we are using classical laws of Newton with some effective mass for the electron. So, this quantum part is basically taken in the form of effective mass and the corresponding band structure. So, now let us go at.

In today's lecture we will drive the Poisson equation, continuity equation and we will introduce the semi classical transport.

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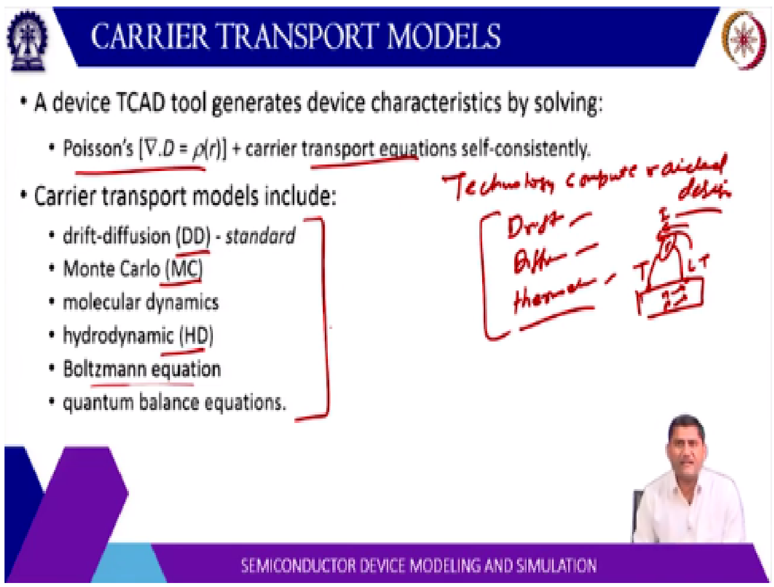

So, in case of technology CAD it is a branch of semiconductor device modelling. So, it is computer aided design. What we have to do? We have to solve for the carrier transport equations so that is a drift is one form of transport then there is a diffusion another form of transport then there is a thermoelectric current also. So, these two mechanisms we have already discussed. Thermoelectric is a missile another mechanism where due to change in the temperature.

So, let us say it is at this is a piece of semiconductor it has high temperature, this is at low temperature. So, then carriers will move both electron and hole will move from high temperature to low temperature. So, we can also find out from this one whether it is n type or p type. Because if you connect some meter here then this electron will move so this will give one direction of current if electrons are in majority here. If holes are majority, then holes will move like this.

So, I will be in this case along the hole and for n type current will be opposite to the movement of these electrons. So, the direction of current will be different. So, these are the basically carrier transport. Then the driving force for these carriers will be the electric field and that comes from the charge. So, we solve Poisson equation and the transport equation self consistently and there are various models that are available in the literature.

So, standard is a drift diffusion model and we have already discussed some part of it. In coming weeks, we will go in more detail about it. Then there is a Monte Carlo simulation which basically take care of the we follow the particle be through some set of you know few hundreds or thousands particles. We monitor them, we follow their path and then decide and calculate the observable quantity such as current and so on.

Then there are molecular dynamic simulation then the hydrodynamic models which are more advanced. Then of course we can directly solve the Boltzmann transport equation or we can solve the quantum balance equations. So, these are different models that are available. So, there are commercial tools for you for both of them but there is a physics bind it and if somebody is interested, they can they can write their own code and calculate these transport parameters.

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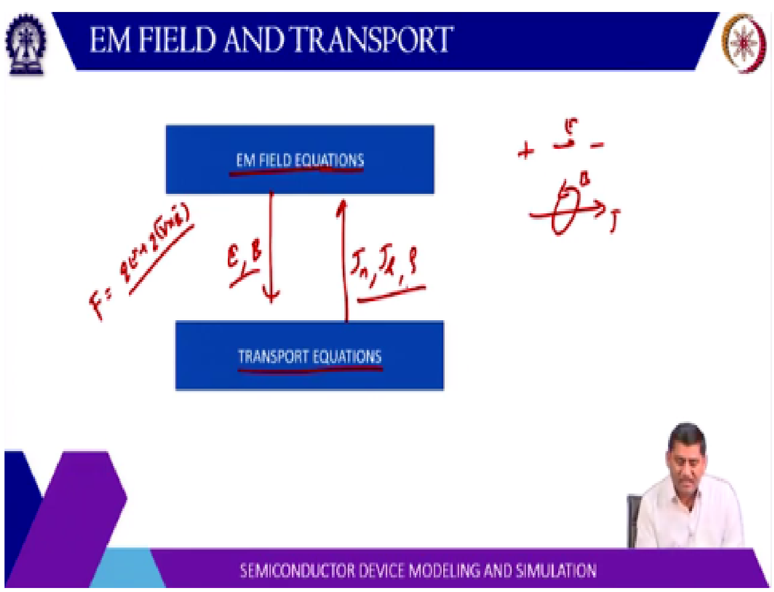

Now in case of solving for the semiconductor devices we require both the information. We solve for EM waves find out the EM fields and then this fields will basically cause the transport. So, what we do? We calculate the transport equations the current flow equations. So, those current flow equations will be like the current density of electrons the current density of holes. So, there will be the current density.

Then we can also find out when the current flows the charge distribution will also change so charge distribution. So, this will basically control the EM field basically. Then if you have certain charge here then this charge will inter modify the electric field. So, this charge will modify the electric field, the current will modify the magnetic field because if there is a charge here then this will give the electric field if there is a current flow then that will give a circulating magnetic field.

And the combination of this electric field and magnetic field will give the force. So, you remember this Lorentz force F = q times e. If q is the charge on the carrier, then forcefully q times E + q times V cross B if V is the velocity B is the magnetic field. So, this is the total force that will apply on a carrier of charge q. So, each of them affect so the transport out outcome of this transport equations which is the charge distribution and the current flow.

They control the parameters for the electric field and the magnetic field and this electric field when it will again affect the flow of the earth charge. Because this electric field will control the current flow. So, let us go through for this basic Maxwell equations.

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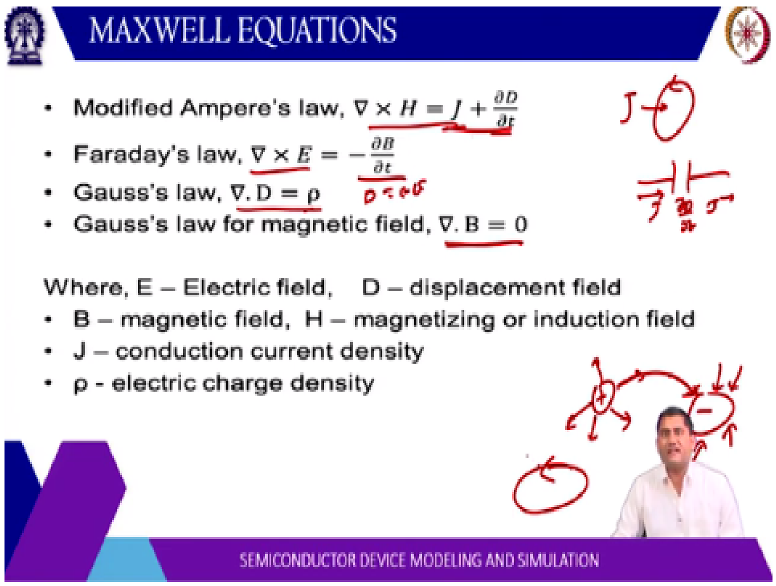

So, this Maxwell equations are one is modified Ampere law. So, all of you have learned in class 12th this Ampere circular law that a current J gives rise to circulating magnetic field. So, del cross H is J so this is the curl of H is given by the current density J. Now but Maxwell did he added another term to explain the current flow in a capacitor because in capacitor there is no conduction current so that current is called displacement current.

So, total current is conduction current plus displacement current. So, here it is J here it is del d by del t and again here is J. So, this total current give rise to the magnetic field or induction field and same is true for the time varying magnetic field. So, the time varying magnetic field give rise to the circulating electric field and thus a Faraday's law. Then Gauss's law says a charge will give rise to static electric field.

So, if there is a static charge it will give rise to static field because D = epsilon times E. So, these are displacement field is a electric field so this charge give rise to the so charge is related to the gradient of the electric field. So, if there is a positive charge here it will give the electric field moving away from this particle. If there is a negative charge then electric field will be pointing towards it.

So, that means these electric lines always start from the point of charge and they end at the negative charge and that is not the case in case of magnetic field. Magnetic field lines are always in a loop so that is why del dot B is zero. They are always in loop though they start at the same point at the end at the same point. So, there are no magnetic charges there is a physical significance. So, from these laws we can find out the Poisson equation and the continuity equation.

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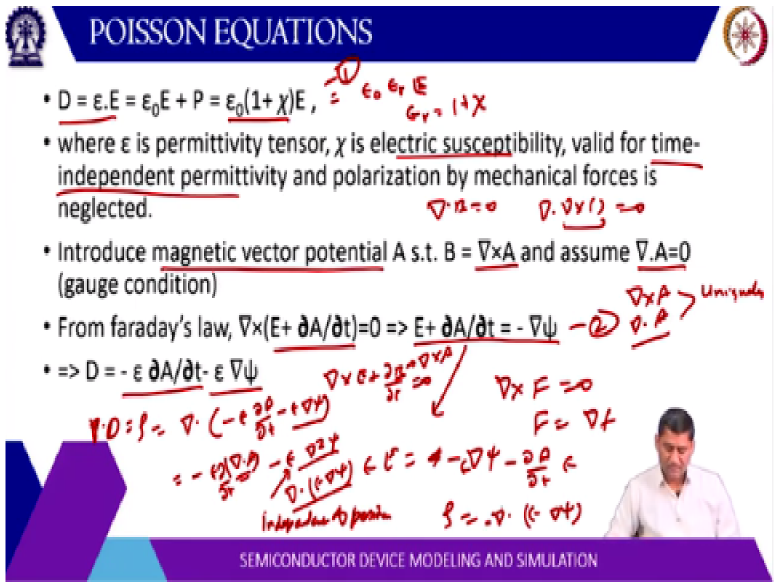

So, Poisson equation these are the constitutive relationship. So, D = epsilon E so epsilon can be done as epsilon 0 times 1 + chi or you can also write epsilon 0 times epsilon r times E. So, epsilon r is permittivity, relative permittivity is 1 + chi which is the electric susceptibility. So, now here if you pay attention here intrinsic assumption is that this permittivity is time independent.

So, it is possible in some scenario that permittivity may change as a function of time. But when D = epsilon E it is assuming that epsilon is time independent and polarization by mechanical forces neglected here. So, that we of course we will not encounter in this course. Then we know that del dot B = 0 and we know the relationship that del dot of and del cross of A vector is always zero.

So, this B can be represented by a del cross of A vector and we call it del cross A and A be defined as magnetic vector potential. And a vector is given if its dot product and cross product are given so if del cross A and del dot A are given then vector can be uniquely determined. So, because del dot A is not controlled by any of the Maxwell equation, we can assume that del dot A is 0 and that in phase we call it gauge condition.

Now when we substitute it to Faraday's law so Faraday law is del cross E = - del B by del t. So, del cross E + del B by del t is 0. Now B is del cross A so you can take del cross outside so it is become del cross E + del A by del D = 0. Now if del cross of something is zero so if del cross of some function is zero then that function can be written as a gradient of another function, so that is what is done here. So, E + del A by del t is written as - del psi.

Now this is equation two and this is equation one. So, D = epsilon E so here we can calculate E = - del psi - del A by del t. So, epsilon E will be epsilon times, epsilon times, epsilon times. So, D = - epsilon del psi - epsilon del A by del t. So, now we know that del dot D = rho. So, rho = del dot - epsilon del A by del t - epsilon del psi. Now this del dot can be taken inside so - epsilon del dot A del by del t - epsilon del square psi.

Now when we write like this so there are two B as we can write it. We can write del dot epsilon del psi or epsilon times del square psi. When we take epsilon out, we are assuming that epsilon is independent of position. So, if that is true then we can write like this. If epsilon is changing as a function of position, then we have to keep the epsilon inside the del dot operator only and del dot A is 0 by gauge condition. So, you can write rho = del dot epsilon del psi with - I. So, there is a Poisson equation.

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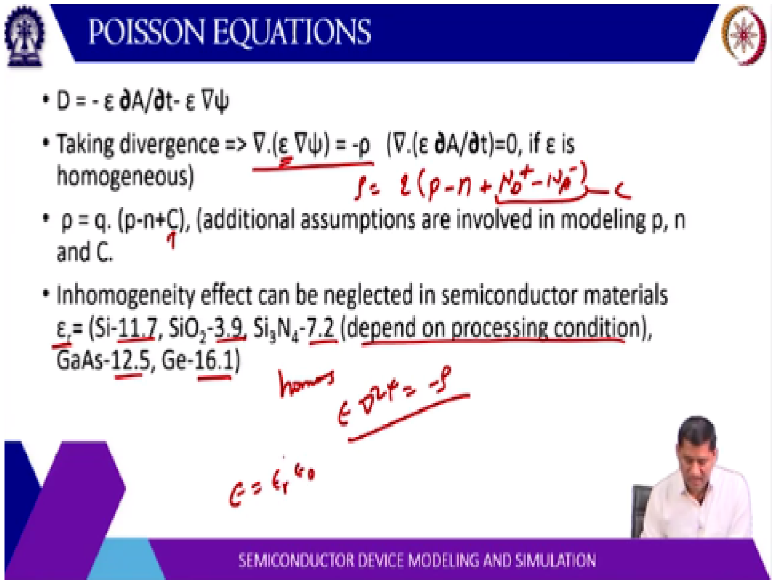

So, del dot epsilon del psi = - rho now rho is the charge density. So, rho can returns q times positive charges minus negative charges so positive charge is p negative charge is n. Now these are the mobile charges plus donor ions which are positive minus acceptor ions which are negative. So, this factor is C and of course when we run the expression for p and n then other assumptions are there whether the semiconductor is degenerate or nondegenerate or so on.

And then of course in semiconductor material if it is not homogeneous then this epsilon will be function of position. So, if it is homogeneous for homogeneous you can write epsilon times del square psi = - rho. And then for homogeneous materials for silicon is the relative dialectic constant around 11.7, for silicon dioxide 3.9, silicon nitride 7.2 and of course these values actually vary slightly depending on the processing condition.

So, for gallium arsenic at around 12.5, for germanium around 16.1. So, these are typical value of dielectric constant. So, here epsilon is epsilon r times epsilon 0, epsilon r is the dielectric constant or the relative permittivity and epsilon 0 is the permittivity of free space.

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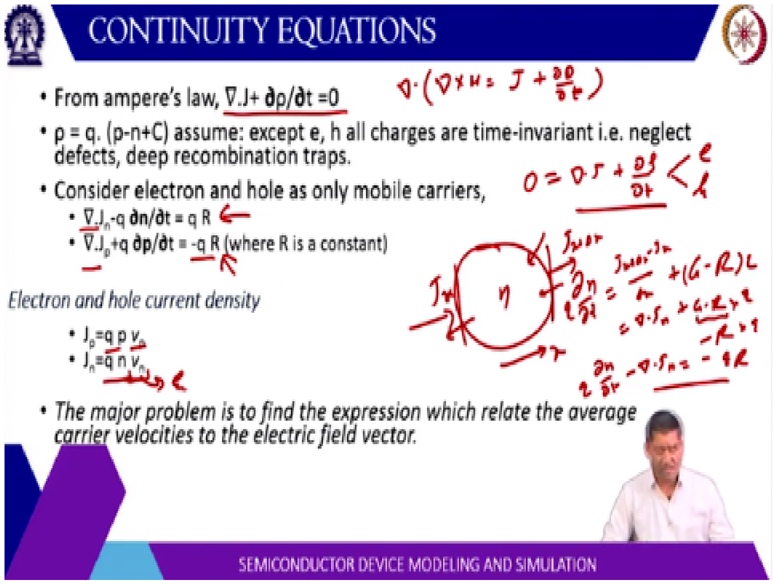

Now another equation that is that plays are all in semiconductor device simulation is the continuity equation. So, if you recall the Ampere law del cross H = J + del D by del t. So, if we take del dot of this whole equation then the left side will be zero because del dot del cross of a vector is zero. So, 0 = del dot J + del by del t of del dot D, del dot D 0. So, del dot J + 0 by d t = 0 this is what we get from Ampere law and of course rho = q times p - n + C.

And now this equation we can write for both electrons and holes. So, for electrons del dot J with subscript n. Now the charge on electron is - q so you can write minus q times d n by d t is equal to some constant. Similarly, for holes del dot J + q times d p by d t equal to some constant. Now this constant is basically related to the generation recombination. So, this is basically related to generation recombination.

So, you can visualize it like this. If you have this region and let us, say there is some electron concentration. So, you can write d n by d t is equal to electron entering plus generation minus recombination. Now what is electron entry? So, let us say this is let us assume this is in x direction. So, this is your x direction now J at x + delta x. So, let us say J is in x direction, so number of electron that are entering now this is the for electron.

So, electron means J x means these electrons are leaving and J x + delta x current leaving this electron are entering. So, this d n by d t will be J x + delta x - J x divided by delta x. So, this will be del dot J + generation - recombination. So, now this is basically containing charge here so you can have to multiply it by q. So, here also you have to multiply by q because this for the charge. So, q times d n by d t = delta J + generation - recombination or you can say net recombination.

So, if you take it to other side so del n by del t times q - del dot J n = - q times R, so this is the same as first equation, del dot J - q d n y d = q times R. Same way you can write for holes also. So, this continuity equation which is basically related to the conservation of these carriers can also be derived from Maxwell's equations. Now once we know these parameters, we can calculate the current. So, current is given by charge density times the velocity of these carriers.

So, for electrons q times n times V n so V n is a velocity of these electrons. Now we have to find out what is the velocity of these electrons. So, if we apply electric field if you apply a temperature some velocity will it will affect the velocity of these carriers and that velocity of the carries will affect the current flow. So, now the main target is basically we have to relate this velocity to the fields or the governing external potential or other physical condition.

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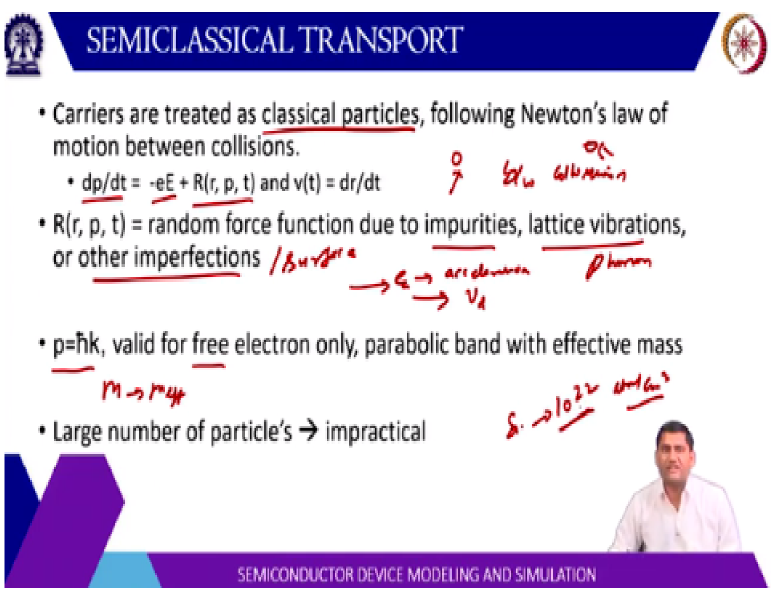

So, with this we come to the semi classical transport. Now semi classical transport carriers are at classical particles which follow the Newton's law of motion. Now these are classical particle only between the collisions so between collisions not during the collisions. So, you can write change rate of change in momentum d P by d t is the force. So, force due to electric field is q times E.

So, for electron you can write - E because q will be - E here and then some random force function due to other elements present in the lattice. So, these elements can be impurities can be lattice vibration so these are the phonons. So, we have phonon scattering, your impurity scattering or there will be crystal defects or line defects. So, different effects are there. So, they can also player on, it can be due to the surface scattering.

So, there are different mechanism which basically balance this force. So, that when you apply electric field, the velocity does not go on increasing rather what happens because this electric field gives the acceleration. So, acceleration means the velocity will keep on increasing. So, this random force function actually decelerated so that electric field effectively give some drift velocity or the terminal velocity.

Now P = h bar k the momentum can be written as now this is valid for free electron only. But we use it inside the crystal structure with little modification that mass of the electron is now M effective. So, that is basically taking care of the band effect. And of course, if you simulate this thing for large number of particle because if you see how many atoms are there in silicon crystal some order of 10 raised to power 22 atoms per cubic centimetre.

So, if you have one cubic centimetre piece of semiconductor there are 10 raised to 22 atoms and this will have some 14 plus electrons. So, there will be lot of electrons basically and you cannot track all those particles. Out of the let us say you know one electron per atom is movable still is 10 to 22. So, taking care or tracking all these electrons is impractical. So, what we do?

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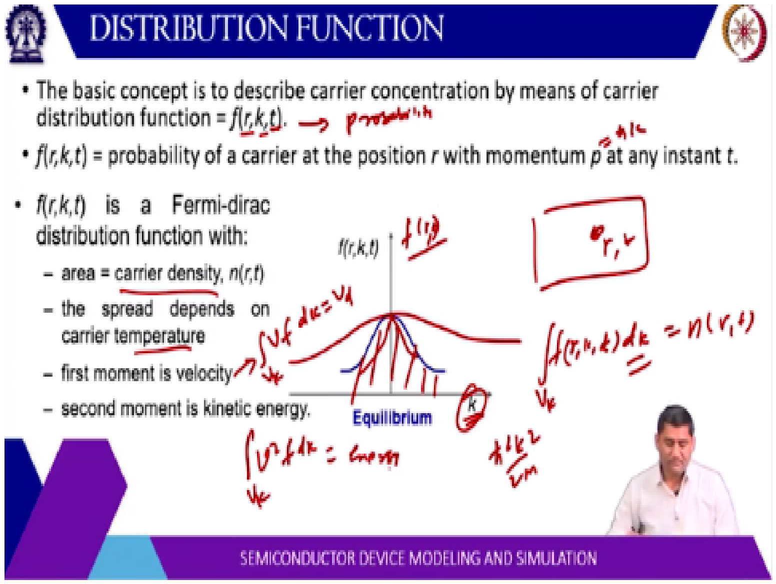

We describe or be introduce a constant of distribution function. So, what this distribution basically tells you is the probability of these carriers at position are with momentum h bar k so P = h bar k at a given time t so this is the probability. Now if you consider a piece of semiconductor at position r. Now in this position r at given time t so this will be r, t you can plot this f as a function of wave vector.

So, at given position there can be you know number of electrons with different momentum or different wave vectors. And if you integrate this f r k t over d k over a volume in k space you will get the carrier concentration at position r given time t. So, the area of this curve will give you the carrier density at position r at given time t then of course the spread will depend on the temperature.

So, if temperature is small this will be more narrow because this is basically the momentum. It is related to energy also h bar square k square by 2 M. So, if temperature is high then this will have a greater spread and if temperature is low then it will have a small spread. Then where is the peak of this function? So, if you integrate or you get the first moment so that is integral V times f d k over volume k you will get the drift velocity and the second momentum if you integrate V square f d k over the volume k you will get the energy.

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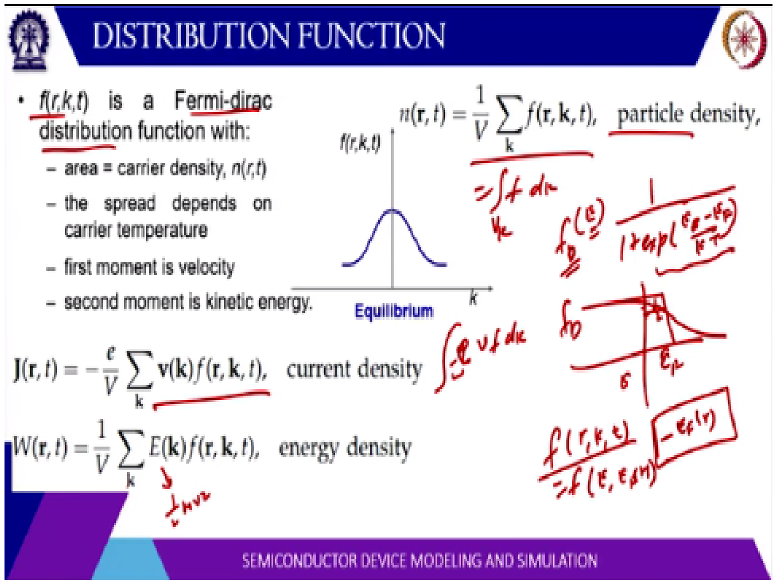

So, in the beginning we can think f as a Fermi Dirac distribution. So, all of you please recall, what is the Fermi Dirac distribution? f d = 1 over 1 + exponential E f - E by k t. So, at E = E f this is one so this f D is one, one by two this is one by two at t = F it is one by two. And if energy is less than E f so if E is less than E f then this is positive this would be E - E f. So, if energy is less than E f this is negative so this term will go to zero so this will be one only.

So, for energy less than E f so this is half here less than E f it is one and more than E f is zero so if t is small. If t is large then it goes like this. So, your Fermi Dirac distribution is basically is a function of energy and of course we have a concept of the fermi level. So, if there is a given fermi level then you can get the probability of electron with energy E as a function of energy. And how this is function of r, k, t?

Because when we define this parametric distribution, we applied it to whole of the semiconductor. So, if at a given position if E f is certain value so E f is a function of position so this is basically f is a function of E, E f which is a function of position and it changes with time also so its function of time also. So, that way this Fermi Dirac distribution is a function of r, k and t.

And then from the Fermi Dirac distribution we can calculate the particle density that is sigma f which is same as integral f d k over the volume for k. And the current density that is q times V times f d k, q is the minus negative, - E is the charge on electron. So, E V f integral so that is this thing. So, for discrete state if there are discrete state, we can use the summation and if there are continuous state, we can use the integration.

And for energy this is half M V square, kinetic energy times f d k so that will give you the energy density.

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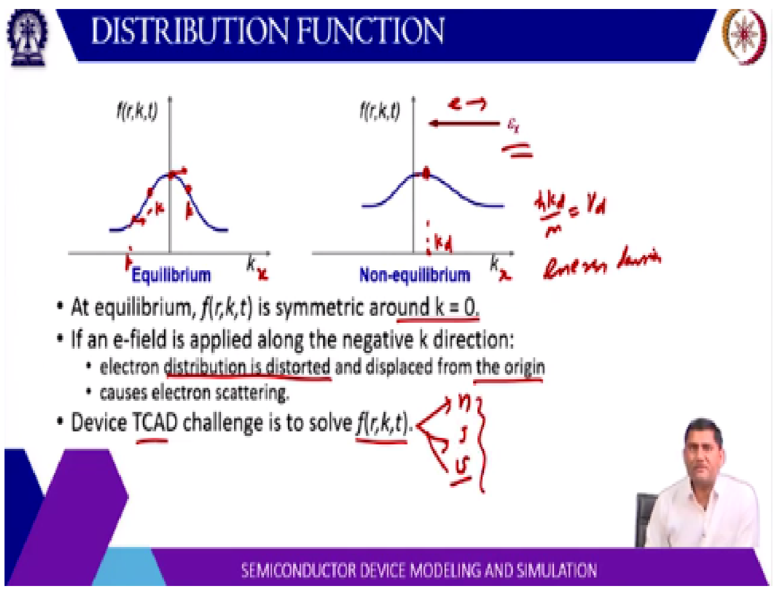

Now for the distribution function let us say you apply certain electric field in x direction. So, this is let us say k x. So, what will happen? These electrons will move in the direction opposite to the electric field so each of this electron is the value is let us say k it will become k minus some small value. So, what will happen? This peak will shift to somewhere here so that this average will come somewhere here and that will be the drift velocity.

So, this let us call this k d so h bar k d by m = P. So, that is h bar k is P so P by m so this will be drift velocity, h bar k d by m. So, at equilibrium this is symmetric around k = 0 because there is a particle with k and minus k and they cancel out so there is no net current flow. But at field now it is peak is shifted to somewhere here due to the electric field so it will have some average velocity or drift velocity.

So, when electric field is applied the distribution function is distorted, it is displaced from the origin and we can calculate the current density from this one. We can also calculate the energy density for this kind of function. So, in technology at what we do? We solve for this distribution function f either directly or indirectly. So, either we may solve for the f or we may solve for its moment like n or J or energy. So, either in terms of this parameter we solve it or we directly solve for this distribution function.

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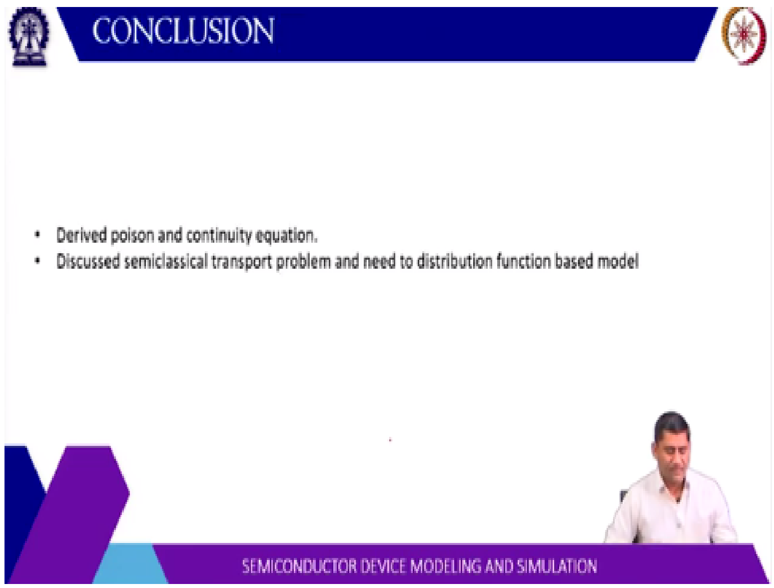

So, in this lecture we have derived the Poisson equation, continuity equation and we have discussed our semi classical transport problem and emphasized the need for distribution function. Thank you very much.