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Lecture – 40 Drift-Diffusion Model

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L40 DRIFT DIFFUSION MODEL	*
Drift-Diffusion Model derivation	
SEMICONDUCTOR DEVICE MODELING AND SIMULATION	

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RECALL BTE
• Assuming that all scattering processes are elastic and by neglecting all effects by degeneracy, the scattering integral can be approximated and the Boltzmann equation is reduced to a pure differential equation $\frac{\partial f}{\partial t} + \frac{1}{h} \nabla_k E \cdot \nabla_r f + \frac{\mathbf{F}_c}{h} \cdot \nabla_k f = -\frac{f - f_0}{r}$
• Suppose that at some moment of time t = 0 all external forces are switched off and f is homogeneous $\rightarrow \tau$ is relaxation time
$\vec{v}_{g} \cdot \nabla_{r} f + \frac{\mathbf{F}_{e}}{\hbar} \cdot \nabla_{k} f = 0 \qquad \qquad$
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Hello welcome to lecture number 40. Today we will discuss or begin a new topic called Drift-Diffusion Model. So, we will drag the drift-diffusion model. Now, let us recall the Boltzmann transport equation and there are terms the partial derivative with respect to time, with respect to position, with respect to vector k or momentum and f is a function of r k and t. Now, the next term which is basically taken care of a scattering.

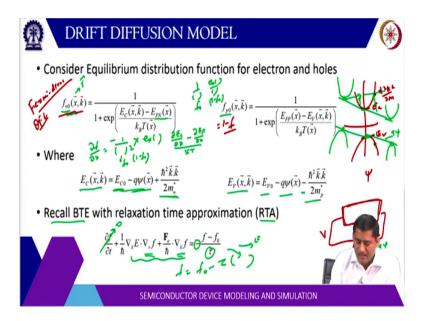
So, if we assume that all the scattering process are elastic and neglect the effect of degeneracy then this integral that is arising from the scattering processes can be approximated by f - f naught by tau. And it is significance we have already discussed that this tau is basically kind of restoring force. So, whenever distribution function f goes away from the equilibrium condition it try to bring it back.

So, your this f is basically E to the power – t by tau. So, this is the expression so, with this it actually, brings back to the f naught condition. So, if you write this as del f by del t is equal to this, if other forces are 0 then that expression we have already discussed. It is something like your RC circuit if you recall, where you have E to the power – t by r c. So, r c is a time constant, so, this voltage actually, approaches to this.

Certain value for this lecture charging of the capacity it reaches there basically. So, same way this tau is restoring a force due to internal scattering, so, it brings back to the equilibrium. Now, let us say at certain moment of time all the external forces are switched off and this f is now homogeneous. So, this, f is homogeneous means del F by del r is 0 and external forces are off.

That means del f by del k multiplied by extra force because this is del k by del t. So, this also goes to 0. So, you can write simply del f by del t is -f - f naught by tau. So, from this you can also understand that this tau is a relaxation time was a restoring force basically. Now, using this Boltzmann transport equation we can determine this or we can drive our model for drift-diffusion model.

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Now, let us consider a Fermi-Dirac distribution function, so, this is Fermi-Dirac we have already discussed two types of distribution function one is the Fermi-Dirac distribution other is displaced mixed valiant function. Now, we said the Fermi-Dirac distribution with quasi Fermi levels can be used for equilibrium cases. So, when the electric field is not very high or that means the electrons are in are near to the equilibrium or they are velocity arising from the electric field are much smaller than the thermal velocities.

So, your distribution function f can written as which is function of x, k is 1 over 1 + exponential E - a by kT. So, for electron. We can write E C - E FN. And for holes we can write E F - E V by kT. So, this f P is actually 1 - f because f is E - E F by kT. So, 1 - f is E f - E by kT. Now, why we have taken like this. If you look at the band structure below E C there is no energy, so, all the energies of the electron are above easy.

So, this is easy level. So, this is h bar square k square by 2m for parabolic band. So, energy of electron is E C + this kinetic energy. So, simply for the holes. This is E v, so, all the whole energies are below this 1. So that means a hole is here that means this? Energy is E v – h bar k square by 2m. So that will be whole energy and apart from this potential energy and kinetic energy, there may be some external potential applied.

So that is basically we call it psi, psi is the external potential. So, let us say if there is a piece of semiconductor and if you apply a voltage here V. So, this voltage will drop across this piece of semiconductor so, from high potential. This will go to 0, so, this difference will be 0

to v. Now, this is going from 0 to v so, corresponding energy will be minus let us say this is psi, psi varying from 0 to v inevitably -q psi.

So, energy will be varying opposite. So, let me use different colours here, so, this will be -q psi so, from this is -q v to 0. So, this will be 0. This will be -q v. So, this is how the energy is changing. Now, this energy changes for all the bands, so, if the energy is going up then E C and E v both will go up. If energy is going down then E C and E v both will go down. So, at different points you will have the band structures will be like this.

So, here energy is more, here energy is less. Here, energy is less here energy is more. So, when electron move from here to here, what happens is kinetic energy is now over here. See here it kinetic energy is almost 0. Here will be more here, it will be even more so, as it goes with the electric field is kinetic energy increases. So, this is just to help you to visualize. So, now, here E C is the energy of the electron in the conduction band E v is the energy of the hole in the balance band.

So, total energy is the band energy at the band edge then kinetic energy and the potential energy. Similarly, for the holes is the bandage energy – this + this potential energy and – h bar k square by 2m and we also know why this is minus sign here. Because here it is below this E v. So, the energy has to be less than E v. Now, we can substitute this distribution function into the Boltzmann transport equation with relaxation time approximation.

So, we can calculate del f by del r and del F by del K. Now, you note the terms which are dependent on k and know the term which are dependent on position. So, here this r is written X here so, X is a position vector basically. So, F naught is function of position r and the momentum h bar k or wave vector k. Where this Fermi level is a function of position only because Fermi level tells you the probability.

The energy level at which the probability of finding electron is half they are for semiconductors. They are usually in the middle or somewhere in the band gap only. So, Fermi level does not depend on the wave vector but the energy of this electron and hole. So, this E C naught is a basically property of the band structure and q psi is the potential which is change in these band edges.

So, this changes due to q psi. So, this depends on position and h bar k square by m depends on the wave vectors.

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DRIFT DIFFUSION MODEL
Let us calculate correction term to equilibrium $f_{v}(\vec{x}, \vec{k}) = \underbrace{f_{v0}(\vec{x}, \vec{k})}_{r,t} + \underbrace{f_{v1}(\vec{x}, \vec{k}, t)}_{r,t}$
For small perturbation from equilibrium $\left \frac{\partial f_v}{\partial t}\right \ll \left \frac{\mathbf{F}_{vv}}{\hbar} \cdot \nabla_k f + \vec{u}_v \cdot \nabla_r f_v\right \qquad 426 - f_1$
correction term f_{v1} to the equilibrium distribution $f_{v1} \cong -\tau_v \left(\frac{\mathbf{F}_{ve}}{\hbar} \cdot \nabla_k f_{ve} + \overline{u}_v \cdot \nabla_r f_{ve} \right)$
Gradient of the equilibrium distribution function wrt space and momentum $\nabla_{i} (h^{+}h)$
$\nabla_r f_{n0} = \underline{f_{n0} \cdot (1 - f_{n0})} \nabla_r \left(\frac{q \psi + E_{FN}}{k_g T} \right) \qquad $
$\nabla_k f_{v0} = -f_{v0} \cdot (1 - f_{v0}) \frac{\hbar^2 \vec{k}}{m_v^2 k_B T} - \mathbf{tr}$
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So, when we substitute here so, so, when we will substitute here, we will be able to calculate all these derivatives. Now, these are all equilibrium distribution function, f n naught and f p naught, so that is why they are written as f n naught and f p naught. When we apply a field this Fermi level distribution functions will slightly change. So, there will be some delta change, so, now, distribution function can be represented by equilibrium, value plus I small perturbation.

So, your this v can be n or P. So, f n = f n naught + f n1 which is a small perturbation. Similarly, distribution function for P is f P = f P naught the equilibrium distribution function plus f P 1. So, small perturbation. Now, for a small perturbation. This del f by del t is much less than these forces, so that means your f v1 can be approximated as here. So, this goes to 0 for a small perturbation and your f can be written as f naught.

This and tau goes to other side. So, F naught minus tau times this factor here, so, this is written here F = f naught – t time of this factor here. So, this is basically f v so, your f is basically f naught + f 1 and f 1 is – tau times, this term here which are derivative of wave vector k and the position r. Now, when we take this derivative because this derivative, actually that should come here is del k is total f and that is del k times f naught + f 1.

But now they are appearing as sum here so, we can approximate that this is almost same as f naught. And similarly, derivative with respect to r almost same as F naught. So that is what is done here. So, when we take the derivative of the distribution function, so, your distribution function, if you take the derivative, so, let us take the derivative here del f by del x so, x is position vector r here.

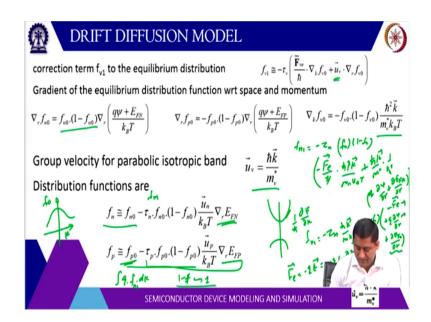
So, this will be denominator square minus times the derivative denominator. So, this will be exponential times del E c by del x – del E f by del x divided by kT. So, 1 over this factor is f so, this is f naught into 1 - f naught because 1 over factor times exponential by factor. So, this is f naught, this is 1 - F naught times this thing. So that is what is written here f naught into 1 - f naught times the derivative with respect to position and this is E C by E x and df by dx.

So, E C – E F by kT so, the derivative of E C – E F by kT. Now, if you look at E C the things here E C naught is not dependent position h bar k square by 2m is not dependent position. So, it is derivative will be 0, so only q side derivative will be there. So, it will be – q psi – E FN. So that is what is in here. This is q psi + E FN by kT so, minus sign is taken out. Similarly, derivative with respect to position we have taken similarly, we can write for holes.

So, there will be f P naught 1 or f P naught del r U psi + E fv by kT. So, in holes if you see here E fP – E v so, E v is – q psi. So, it is e fP + q psi here. So, it will have opposite sign to electric field, this electron distribution. So, there is a minus sign here and with respect to k E C naught and q psi are not dependent on k. Only the third term is dependent on k so, you will have again a f naught into 1 – F naught times 2 h bar square k by 2m.

So that will be h square k by m so, h square by k by m and of course, divided by kT. So, these are the derivative that will be used in estimating this distribution function. So, when we substitute these three equations 1, 2 for electron and 2 and 3 for holes.

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To f 1 what we get? f n = f n naught – f n 1, f n 1 is – tau n times del F k so, f naught into 1 1 f, f naught can be taken out. So, f naught into 1 – f naught can be taken out and then write f external by h bar times del f by del k. So, del f by del k as this factorial that is h bar square k by m kT. And there is a minus sign here. So, let us write a minus sign here then, with respect to position. So, this second term.

So, U is the group velocity, so, this is h bar k by m, for parabolic band the group velocity is same as the phase velocity. Just to tell you that just to remind you that group velocity is obtained from this derivative, so, del E by del k 1 over h bar. So because it is parabolic band so, del E by del k is h bar square k so that becomes h bar k by m times with respect to R. So, it is again, f naught 1 - f naught times the derivative.

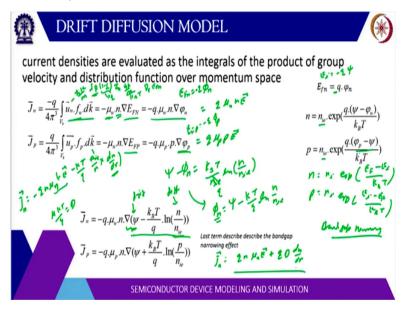
So, this is 1 over kT that is a (()) (15:58) 1 take constant times q del psi by del r + del E Fn by del r. Now, you notice here this is H bar k by m k t. So, this 1 h r will cancel here so, h bar k by m kT, h bar k by m k t that term is same here. So, again this can be taken out. So, your f n1 is – tau n h bar k by m kT times f naught 1 – f naught. Then, if you notice here, this is – Fe then + q del psi by del r and + del E FN by del r.

Now, you recall, del psi by del R is the electric field a minus of electric field. So, force 1 electron is -q times electric field and the electric field is - del psi by del r. So, this is q del psi by del r. So, this is Fe and this is - Fe, so, these two will cancel out. So, you will only have del E f by del r so that is what is remaining here del E f by del r. Similarly, for whole

also, it will be del f by del E p by del f Fermi level for holes derivative with respect to position.

And this expression I think we have also derived that when we consider the two component depth component and diffusion component, we get the current as a function of derivative of the Fermi energy level. So that is what is basically coming here. Rest of the terms are related to the equilibrium distribution function.

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Now, when we substitute it to the equation for current density. So, this is the expression here now, a expression for current density is basically let me write here only q times f dk. Now, f naught is equivalent distribution function, so, this is symmetrical f Naught is symmetrical. So that means, if you integrate, this is f naught k times f naught. So, it is a even function multiplied by the odd function it is integral will be 0.

So, only term that will remain is this small perturbation term. So, when we integrate q f dk we will have simply have q n1 dk. So it is q n1 dk. Now, n 1 is basically this tau p f p naught 1 is f p naught times u by kT times del r. Now, because if we consider non degenerate, semiconductor then 1 - f can be approximate as close as 1. So, what we will have here? So, we can only have f and here instead of f n into 1 - f n.

So, u n f n dk times u by kT times del e by del r. Now, del E by del R does not depend on the k vector. So, we can take it outside, so, this is will be outside and what you will have here? You have tau here and u which is h bar k by m times kT. So, this is basically this is h bar k by

m times, f 1 dk and f 1 is f naught into 1 - f naught times tau n times u n and the derivative are or E Fn. So, it can simply (()) (20:45) f naught can be approximated as 1.

So, this is h bar k by m transverse k by m by kT. So, it can be approximated integral f naught dk so which will be n here and rest of the component, will contribute to some effective parameter which is the mobility here. So, it can be written as q mu n times n del phi. Now, this phi is basically potential equivalent of the Fermi level. So, this Fermi level can be written as some potential phi times q and up to minus sign.

So, because Fermi energy is q times the Fermi potential. So, similarly, for holes also, we can write E fp = -q times pi p. So, this can also written as derivative or if derivative of phi p. So, this will be the expression for the electron current density and the whole current density. Now because this is the derivative of Fermi potential, so, negative of this potential derivative is the electric field. So, this is basically your u times mu p times P times, electric field.

This is q times mu n times n times electric field and for non-degenerate semiconductor. If you recall, the expression n = n i exponential E F - E i by kT. So, your E F is -q phi E i is -q psi. So, the sign will basically change here because E i is -q times i E F is -q times phi. So, this will be q psi -q phi by kT and similarly for p = n i exponential E i -E F by kT. So, it will be q phi -q psi, so, the sign has become like this.

Now here it is n ie this is basically this effective intrinsic carry concentration that will basically takes care of band gap narrowing. So, because due to the change in the band gap, this intensive carry concentration, does change so that takes care of the band gap nearing effect and when we substitute here this phi p in terms of p and phi n in terms of n. We can substitute here so, this, let us say, phi n = kT by n ie log of n by n ie log of this times kT = vector by q is psi – phi n.

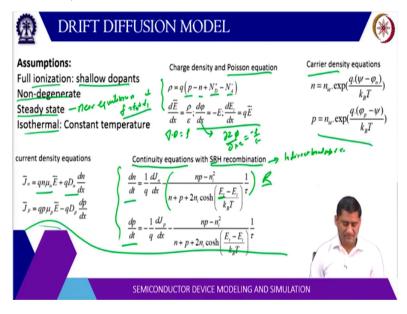
So, if you take derivative of this thing, so, it will be phi n will be psi - kT by q log of n by n ie. So, derivative i n is derivative of psi - kT by log, n by n i derivative of that thing, so, this is what is written here. Now, if you see here, there are two component derivative of psi. That is a potential and derivative of this carrier concentration. So, this basically gives you the drift component because this electric field and derivative n this gives you diffusion component.

So, we can further simplify this one. Let me write it here, so, J n - q n mu n times del psi so, del psi is nothing but the electric field divided by q. So, this is del psi E i by q so, this will be electric field, so, this will be minus of electric field. Then -kT by q times log of n by n ie. So, if you take the derivative of this thing, so, this will be n ie by n times dn by dr times 1 by n i. So, this will cancel it will be 1 by n log dn by dr.

Then this is mu is the drift velocity and then mu times kT by q is the diffusion coefficient. So, it will be different, coefficient times, dn by dr. So, these are two components that we are getting so, we can write J n = q n times mu n times electric field. And + k T by q times mu is d. Then n will cancel out so, q times d times, dn by dr. So that is why the name of this model is drift-diffusion model.

Because in this model the current component that weight that we get consists of two terms, one is a dr term that is coming from the change in the potential, so that is electric field. Another diffusion term that is coming from the change in the carrier concentration.

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Now to summarize the drift division model we have already assumed that is a non-degenerate semiconductor, and also temperature gradient is not taken into account, so, it is isothermal. That means constant temperature and dopants are fully ionized. So that is possible when they are shallow depend and at sufficient high temperature or room temperature. And then it is a steady state or near equilibrium.

It is valid near equilibrium because we have assumed that f = f naught + f 1. So, this f 1 is very small compared to f naught and we have used the Quasi Fermi-Dirac distribution function which itself implies that it is valid only when you are near equilibrium. Then we have only drive the equation for the charge density and the Poisson equation, so that is, rho is equal to q times positive charges, p + N D + - negative charges, N - N A -.

And of course, from the Gauss law del dot d = rho so or del dot = rho by epsilon, so, dE by dx is rho by epsilon and E can written as psi by dx or d phi by dx or it can also written as electric field is 1 over q dE i by dx. So, these are different forms of this Poisson equation that you may encounter. They have different names also, so, you can write it as dE by dx or you can write d 2 psi. Because this is d by dx and E is d psi by dx.

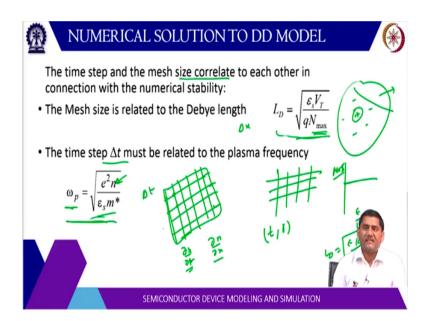
So, you can write d2 psi by phi by dx square = rho by epsilon, – rho by epsilon because E is – d phi by dx. Then this is the carrier density equation that also I have discussed. Then current density is basically two component drift component and the diffusion component. And the calculated equation we have derived where this term was simply written as net recombination or recombination minus generation.

So, dn by dt is gradient of the current density plus some net recombination term or there can be generation due to other means like optical and so on. So that also has to be included. So, net is plus generation minus recombination. Now, here we have chosen a specific model for recombination called SRH recombination which is dominant in indirect band gap semiconductors.

So, that is SRH Shockley read Hall recombination which basically assumes that there are trap energy levels in the band gap at energy curl E t and they initially assessed the recombination of these carriers. So, you can write this continued equation for both the carriers for electrons, as well as holes. And by solving this set of equations. So, if you see there are 1 Poisson equation and then two continuity equation.

So, these three many questions are there and supporting equations are the current density and the carrier density equations.

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One can fully solve the drift diffusion model to get the parameters now when we solve it. Generally, we discretize just to just make an making a note here that we will discuss this numerical procedure in coming lectures, as well as generational recombination of models also will be discussed in coming lectures. So, because this drift diffusion model as derivative with respect to time and with respect to position.

So, there are two parameters, t and r or x. Now, the derivative with respect to time has to be discretized with respect to plasma frequency. So that means the time step must be small enough to take care of this plasma frequency and the mesh size in terms of space discretization. The delta x and this is delta t. So, delta x should be smaller than this debye length.

Now, debye length we have already discussed now d by length is basically if there is a some charge here so, up to what distance this charge will be screened out. So, basically, what happens? This positive charge attracts some negative charge around it and then this charge get discrete. Software is some distance, it is field will be very much weak. So, this is called charge screening and this is basically debye length and we have also discussed this debye length in case of flat band.

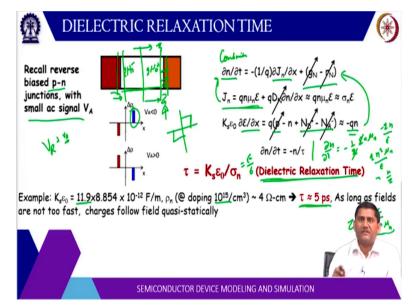
So, when in moss, while discussing the moss, we said that when this flat band. The capacitance for this semiconductor part is epsilon by L D. And L D is epsilon KT by q square times the doping, let us say, N A or N D and square root of this thing and KT by q is actually, thermal voltage vT. So, this is basically the debye length now in metal. The debye length is

even very small, so, the field does not actually penetrate but in semiconductor this length is significant.

And it actually, length reduces if you increase the doping. So that means when the doping is high, this screening is even higher and plus of frequency is basically it is related to the property of the material and that is given by e square n by epsilon m. You can understand it in terms of if you take a piece of semiconductor and if you apply electric field. This plasma can be generated with certain oscillation frequencies and each material has a specific plasma frequency and in case of semiconductor.

If you, if n is the carrier concentration then it can return as e square n by epsilon m. So, when the carry concentration is i, it can oscillate at higher plasma frequency. So, what will happen when you are discretizing dn by dt. So, if the time step is more than this plasma frequency or if you dn by dx if this distance more than debye length. Then this fine variations will not be accounted.

So, they will be bypassed because when you make some these simulations in using numerical methods. We do not have the values of the variable at continuous coordinates and as a function of continuous time. We have them at discrete positions and discrete times. So, these positions and times have to be sufficiently small to capture the variation in the physical properties or the carrier consultation here.



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Now, there is another concept of dielectric relaxation time. So, if you recall the reverse, biased, p-n junction let us say this p n junction is reverse biased. So that means this is a depletion region here. Let us say this is some N A - q times N A - this is q times N D + some point to charge here some negative charge here and let us say we apply a small signal here, over this reverse bias DC.

So, this is basically some V reverse bias + small ac signal. So, when ac signal is has the same sign as the reverse bias sign then this depletion which actually, increases. And when this is opposite, sign this depletion which actually, decreases. So, this is the variation with respect to this V A sinusoidal variation. Now, this charge is actually, added at this position here. So, what we can do?

We can write the continuity equation for this case and continuation. dn by dt is gradient of current density plus generation minus recombination. So, let us assume here that generation recombination is negligible and let us say let us say the doping is also uniform. So, in the depletion region, you can just say that current is due to the drift of this carriers. So, very small number of carries are coming here so which is somewhere here.

They will be attracted to this year this junction here and they drifted along this field here. So, if you substitute here so, you can write. dn by dt is dJ by dx and dJ by dx is this and mu n times d by dx. Now, this d by dx using Poisson equation, can be related to the carriers here. So, if you consider, let us say on the N side, so, in this region, this many carries are there, rest is neutral. So, for a given background, this is the change in the charge.

So, there is no p doping here. So, p goes to 0 and N D +n a is basically balanced for neutral region. So, this is a neutral region here and when charge this electron comes here, this is neutral. When electron leave this region then the we are assuming of course here this abrupt depletion here. So, if it is abrupt then the change is basically q times n only. So, d by dx here is q times n and if you substitute to the first equation so, J is sigma i.

So, d by dx here, so, what you will get? You will get del n by del tau t = 1 over q dJ by dx and dJ by dx is q and mu n times d by dx and d by dx is -q n by epsilon. So, this q will cancel here so, n square. So, q times n square mu n by epsilon. So, if you write this as n by

tau, so, if you compare this thing, tau you will get is epsilon by q n times mu n. So, q n times mu n is basically the conductivity of this because sigma = n mu.

So, your tau is simply epsilon by conductivity and this is basically called the relaxation time. So, it is the indicative of a speed at which the majority carrier respond in case of semiconductor. And if you make a rough calculation, let us say doping is tensor fifteen and dielectric constant is 11.9 for silicon. So, if you substitute you get around 5 picosecond. So, this is actually, pretty fast and if you compare this time constant with the magnetic area lifetime, it is quite small.

So that is why in solving the semiconductor device equations, we are more concerned about the minority carrier lifetime. We are not so much worried about the majority carrier lifetime, so, they have this some lifetime but there is quite quite small basically and we characterize the response of this majority carrier by this time called the dielectric relaxation time.

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So, in this lecture we have discussed and drive the governing equation for drift-diffusion model. Thank you very much.