**Semiconductor Device Modeling and Simulation**
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**Lecture - 46**
**Solving DD Equations**

Hello, welcome to lecture number 46.

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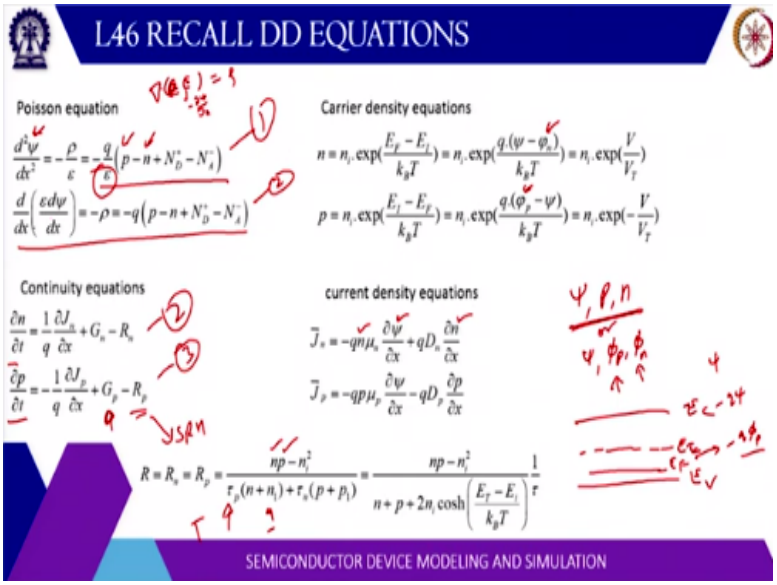


So today we will discuss how to solve the drip diffusion equations. So let us recall the drip diffusion equations. So there is a one Poisson equation. Now please note what are the unknowns here. If you are given a piece of semiconductor, then doping and the properties such as diffusion coefficient, the mobility, those things we will know a priori or we need to know them beforehand.

So in Poisson equation the unknown is the potential psi. Then p n, now p n they are function of psi. So they are also unknown. Apart from function of psi they are function of this phi n or phi p. So what we can set, we can set this psi as one unknown, p as one unknown or n as one unknown or another set that is used by people is psi, then instead of p we can use this phi p or phi n.

So these are three unknowns here, rest are known in Poisson equation. Then in continuity equation dn by dt, so n is unknown which is already included. Then there is a dJ by dx. So dJ by dx is the current density. So if you see the expression for current

density n is again unknown, psi is again unknown and it is again d, q, mu these are knowns, the constant. Similarly continuity equation for holes.

Then there is a generation recombination term. So generation can be due to certain source. So or whatever is the mechanism and in general if there is no such source then we can write just R there when its value is positive then it is generation or recombination when it is negative then it is generation. Then if you see this R value for SRH recombination, which is typically so in case of silicon; np minus n i square.

So n is unknown, p is unknown. Then tau is the property of the semiconductor depending on what is the doping, but at the level of number of traps there, trap density times cross section of those traps times the thermal velocity. So it is again a function of temperature. So which we also know a priori. Then n, n 1; n 1 is again computed from this. So this is also known.

Then, so if you see here, there are only three unknowns, the potential, hole concentration or electron concentration. And what we are actually solving, we are solving two equations, equation 1, equation 2 and equation 3. Now we have not considered the heat flow equation. But if you go for higher order models or if you operate your device at high temperature or high fields, then this heat flow will also come into the picture.

So heat flow is nothing but the phonon transport basically, so that equation can also be included. But as far as solution technique is concerned, we are focusing on the these three equations, how to solve them simultaneously. So these three equations are simultaneous differential equations with three unknowns psi, p, n. And because p and n is basically the concentration of the carriers, so which basically varies a lot and even if you scale it, still the variation is quite high.

So people what people do, they also have another choice for the variables. So they use psi p, phi p and phi n, which is nothing but the Fermi potential for electron and holes. So if you recall this band diagram, let us say this is E v, this is E c. And let us say this is some Fermi level here E F and let us say this is the intensity level E I. So when the potential is varied as a function of position, then these bands basically change.

So if the potential is let us say psi, then these bands will shift by minus q psi. And E F is nothing but the Fermi energy level. So this is related to minus q times phi. So it can be if it is for holes then phi p. For electrons we write q phi n. So this is the concept of Quasi Fermi level. So this is basically solved for these three variables. So to simplify the expressions, we will stick with psi p n in this lecture.

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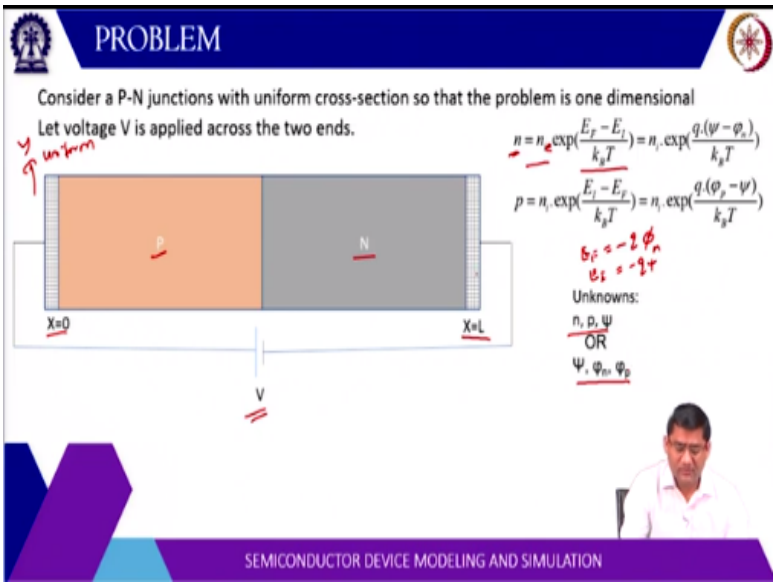


Now let us consider a simple problem. So if you can approach this simple problem, then similar way other complicated problems can also be approached. So let us see there is a p type region here, there is a n type region here. Then there is a metallurgical junction in between and some voltage V is applied. And then this is basically boundary X = 0, this is X = L. In y direction, let us assume it is uniform.

So there is no variation. So the problem is basically one dimensional problem. So now recall the expression for n is n i exponential E F minus E I by kT. Sometimes it is written as n i e. So n i it basically takes into account the bandgap narrowing effect. So if bandgap is changing then this n i effect will basically change, times E F minus E I by k T. And E F can be written as, so this is for n. So they may have different Fermi level.

They may have same Fermi level. So for n E F is minus q times Fermi potential, so this is phi n. And energy level E I is minus q times psi. So this can be written as q times psi minus phi n. This can be written as q times phi p minus psi by K T. And let

us say np psi or psi phi and phi p these are the unknowns. Now when we approach it, we have to look at the boundaries first.

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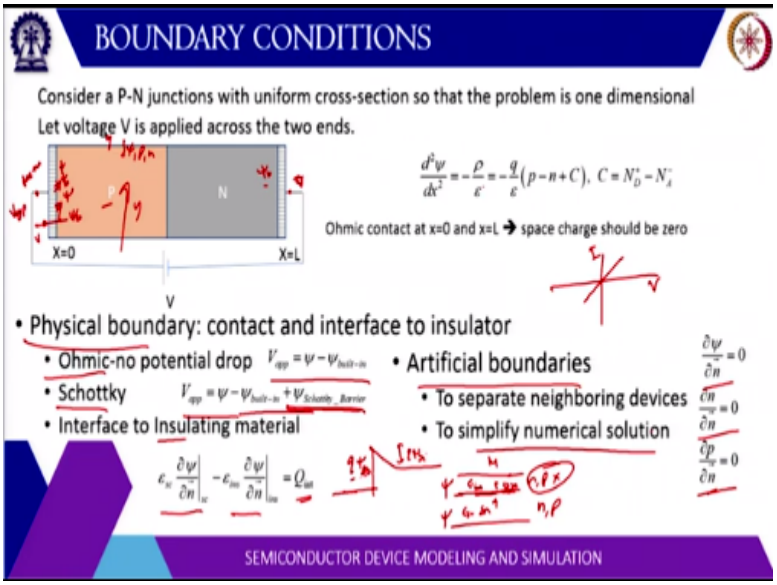


So at the boundary condition, there are different types of contacts. One is Ohmic contact. Ohmic contacts are those contact for which it does not discriminate whether you apply a positive potential or you apply a negative potential. So this v I relation is linear. That means, at the junction itself there is no drop. So here is basically p type semiconductor and there is a metal contact here.

And we are assuming there is a Ohmic junction, Ohmic contact, so there is no potential drop. So what does it mean? That the voltage applied is here is V applied and inside the potential psi they should be continuous. That means the psi and V applied this will be related by, this V applied should be equal to psi plus if there is any built in potential here, let us say psi b. So V applied should be psi minus psi built in.

Now how is that possible? So you can say, let us say this is the interface here. So this is voltage here. Then if you move inside and there is some built in potential b. So this potential will be basically jumped by this amount. So the potential inside, just inside will be this outside potential plus this built-in potential. And similarly at this junction. Here the potential is let us say some V potential or you can take it as a difference.

So it can be zero potential. Then here will be psi built-in potential. So V applied is equal to psi built in here. Now for Schottky, there is a definite barrier there and that is

called Schottky barrier. So we also have to include that Schottky barrier. So if you recall that for metals, we had this Schottky barrier. So this was this height wise q psi Schottky barrier. And then there was this built-in potential.

So the net difference is this Schottky barrier minus q v v i, so we will call it psi v i. So Schottky barrier minus built in. So there is a net difference. So this much discontinuity in the potential is there. Now in this case, we are assuming ohmic contact, so we can derive the expression for potential at these two end contacts. In some scenarios, let us say if you consider a MOS structure, there is a metal, there is a oxide, there is a semiconductor.

So here is the interface to the insulating region. So now silicon is interfacing with the oxide. So in oxide region there is no n there is no p. So np is not there. This is only there in silicon region. But psi is there in both of the region, oxide region as well as the silicon region.

So at this interface, this is basically you can say there are two dielectric here, this is epsilon insulator and this is epsilon semiconductor and if you recall those Maxwell's equations or Gauss law that del dot d equal to rho by, del dot d equal to rho. So by that relationship we can say the field that is perpendicular to this one. So that is d psi by d n. So d will be epsilon d psi by d n.

So the difference, they should be continuous if there is no charge. And if there is a interface charge, then there should be a difference between two derivative of displacement flux, derivative with respect to the normal direction. So this condition can be used if you encounter the oxide and silicon or insulator interface. Then apart from these real boundaries or the physical boundaries, there are some artificial boundaries.

For example in this structure, you can see nothing is connected on the top side or nothing is specified there. So what kind of boundary we can take. So one obvious way to take the boundary in this region if we assume it is uniform, so uniform is the derivative of the psi p or n in y direction or in this normal direction, so it will be zero

because there is no variation in y direction you can assume it is large enough in y direction and there is no variation.

So it can be assumed uniform and then we can apply this Neumann boundary condition that d psi by dn, dn by dn and dp by dn is 0 where this n with vector is the normal direction. So these are the artificial boundaries. So they are used either to separate the neighboring devices or to simplify the numerical solution. Now let us consider this equation the Poisson's equation.

Okay, here actually I forgot to mention, this is the Poisson equation we are using, but in this case there is the assumption that this epsilon or dielectric constant is constant throughout the piece of semiconductor. But in case it happens to be the function of position then we cannot take it outside the derivative because if you recall del dot D, D is epsilon times E is equal to rho.

So this there is a derivative on this epsilon also. So D by dx of epsilon now this is minus D psi by dx. So if epsilon is function of position then you have to use the expression below it, okay. So these two expression are similar. The only difference is that the expression two takes care of the non-uniformity of dielectric constant. okay.

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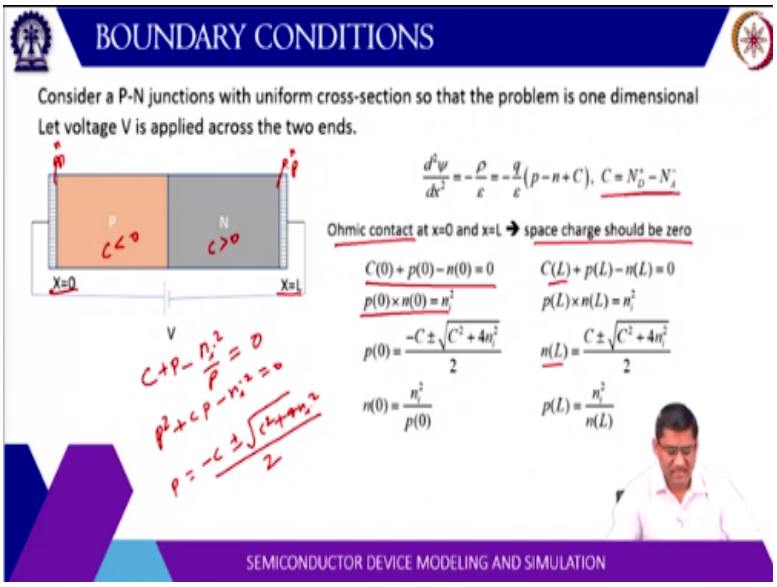


So now let us apply the boundary condition to this P-N junction device. Here at the two ends, so let us say the length of this device is L, this is X = 0, this is X = L. So at X = 0, at X = L, we are assuming the contact to be ohmic. So ohmic charge means,

there is no space charge, so space charge should be 0. Then of course, you can write this expression that charge neutrality.

So the charge neutral neutrality should hold basically. So that means p minus n plus nd plus minus na should be zero. And then nd plus minus na minus is represented by a value c which is a constant in a given region of space. So we can say C + P – n = 0. And it also obeys this law of mass action. So pn product is n i square. So from this we can estimate what are the values of p and n.

So maybe what you can write C + P – n. So n can be written as n i square divided by P equal to 0. So if you write it as it can be written as p square plus c p minus n i square equal to zero. So it is a quadratic equation in terms of P. So P is minus b plus minus root of b square minus 4ac divided by 2a. So this is the expression for P. And of course, n can be obtained by n i square by P.

And same thing we can do for at X = L where we obtain this n equal to in terms of this C because n is basically this is C is more than zero here. C is less than zero here. So that is why if you see, it is minus C is coming here then plus minus this is square term. And you notice one more thing here. This is actually minus C will be positive. Then this is plus.

So it may be slightly more than C basically okay and P can be obtained as n i square by n L that is P L. So this is the value of the carrier concentration. So this is the boundary condition. So now we have found what is the value of N, what is the value of P, what is the value of N, what is the value of P at these two ends. Now third unknown is psi. So let us estimate the relation for the psi.

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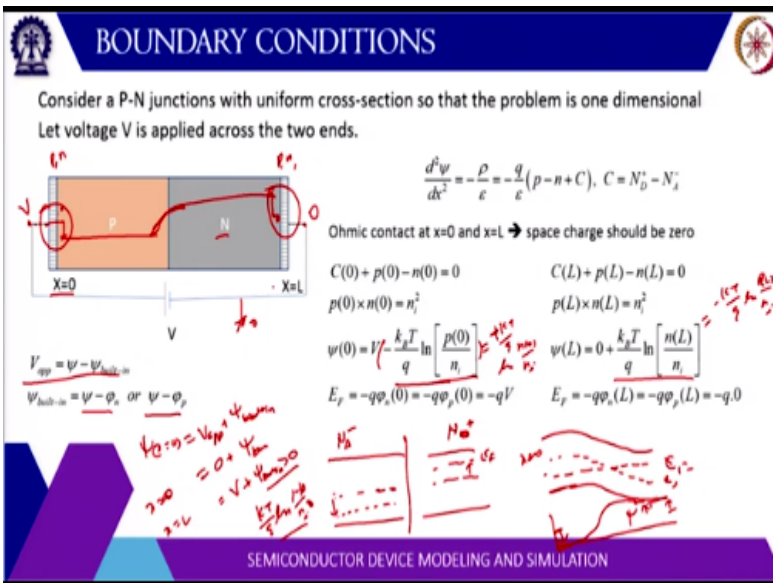


So we already know what is the p here what is n here what is p here what is n here. Now let us find the psi. So psi of course, we can find out that V applied is equal to psi minus psi built in. That means the psi here is V applied plus built in. So you can write that psi at x equal to zero is V applied plus psi built in. So if you see here now as far as voltage is concerned, we do not consider absolute voltage.

We only consider the relative voltages. So somewhere we have to take a reference. So let us say this is your reference. This is a ground zero volt we can define. So this potential is zero now and this potential will be V. So at x equal to L the potential inside the semiconductor will be zero plus psi built in. Similarly, at x equal, this is at x equal to zero. At x equal to L the potential will be V plus psi built in.

Now what is the psi built in? Psi built in is basically the difference between the intrinsic energy level and the Fermi level. So that means when the intrinsic energy level and Fermi level, so that is also the Fermi level for undoped semiconductor. So in that case there is no built in potential. When you dope it, let us say we dope it with let us say p type.

So let us say now the charges are N A minus and this side is doped with donors. So the charges are positive here. So when you dope with acceptors here, the Fermi level actually goes down. So this means, the energy level has gone down. That means potential has gone up. So for p site the built in potential will be positive and the value

will be this difference that will be K T by q log of N A by n i square or N A is equal to p at zero.

So you can also write K T by q log P 0 by n i, sorry P 0 by n i. So this is at, this is at x equal to 0. Similarly for x equal to this is at x equal to zero this is N. I think I wrote it other way around. No it is correct. x equal to zero is p type okay. So this potential is V here. Then K T by u log p by n i okay. Then at x equal to L it is n type. So the built in potential will be this is the intrinsic level, Fermi level will be here.

So now energy has gone up. So the built in potential will be you can basically draw the energy diagram her. Let us draw the band diagram first to illustrate it further. This is your let us say the Fermi level, okay. Let us say no voltage is applied and let us say V equal to zero. So this is P site the valence band is here and conduction band is here and this is n site okay.

Now if you notice here the potential will look like this. Potential will this E I is going down, this is E I and the potential going will go up like this. So this will be the nature of psi. So at this point the potential is going down, at this point potential is going up. So at x equal to zero the psi will be minus K T by q log p by n i. On P site, this potential will be KT by q log of n by n i.

Or we can use this expression on either side, because this is same as plus this thing, is same as plus K T by q log of n at zero by n i. This expression is same. So whether you use a log n by n i or log p by n i, you do not have to worry about the sign basically. So it is positive if you use n here and it is negative if you use p here. And this is same as minus K T by q log of p at L by n i.

So this takes care of the built in potential. So there is a built in potential here. Then there is a built in potential here and there is a built in potential here, like this. So this also explains that why there is no conduction of current when you connect P-N junction to simply a wire without any source outside. Because this built in potential inside the P-N junction is canceled by the built in potential at the two interfaces.

So overall, there is no potential basically. This can be written as psi minus phi n, psi minus phi p. So when this built in potential is positive, then psi is more than phi n. That means E F is more above this E I. So the built in potential is negative on P site and positive on N site.

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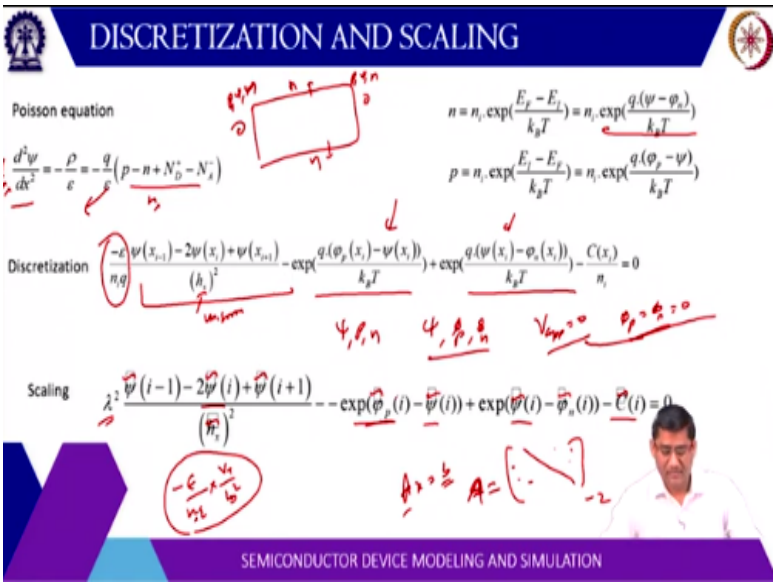


Now the Poisson equation. Once we have identified the, so what we have done here? We got the boundary condition for p, n and psi for all the three components at the, these two edges. So we now know the value. So we have basically kind of Drichlet boundaries here, where the values are gone. And along this upper boundary and lower boundary, we have Neumann boundary.

So d by dn perpendicular or d by dy is zero for all three unknowns p and n psi. So now for this reason, we know both the boundary conditions for x, y and for all the three unknowns. Now once we calculated the boundary conditions, so you see the Poisson equation here, now we have already determined what are the boundary conditions here. You look at the Poisson equation here.

Now we have already determined what are the boundary conditions. So there are Drichlet boundaries here, there are Neumann boundaries here. And here, we know the value of p, psi and n, we know the value of p, psi and n. And here we know the derivative r equal to zero here. So we know the boundary. Now we can discretize it.

Discretize all of you know that d 2 psi by dx square is written as psi at i minus 1, -2 psi at i, plus psi at i plus 1 divided by h x square. And of course we are writing h x square because we are assuming uniform spacing. Then this epsilon by q can be taken to this side, so minus epsilon by n i q. And this side is divided by n i. So you have 1 over n i here. So this basically, now we have expression only epsilon psi minus phi n.

So you can write these two equations or you can simply write p minus n. And then, now we have this equation, it can be basically solved. Now if you see here, there are three unknowns psi, p, n or if you write this equation, then unknowns are psi, phi p, phi n. Now if you consider a simpler case, let us say your V applied equal to zero. So if V applied is equal to zero, then in that case, your phi p equal to phi n is equal to zero.

So for V applied equal to zero you can directly solve the Poisson equation without solving any other equation. So that can be homework for you, you just write a code and solve it accordingly. So in that case, this potential itself will determine what the value of p and n at the junction. So this can easily be done. Then what we do, we can scale it also. So this thing and then scaling parameters.

So this should be actually the scaled parameters, okay? They are not showing properly here, okay. So size is scaled with respect to V T. So this is basically divided by V T and multiplied by V T. Then H x is scaled with respect to L d. Then phi with respect to V T and C with respect to n i. So this is represented like this and this is already there. K T by q is V T. So these are the scaled parameters already.

And then here x axis is scaled so divided by L D multiplied by L D. So this is basically lambda square becomes minus epsilon by n i q times V T divided by L D square. So this becomes your parameter for scaling. So now you have all the values which are small basically. If you see here, the variation will be small.

So if you take care of the scaling parameter, the variation will be small, and then you can discretize it over and solve for the, get basically this expression A x equal to b, where x are unknowns and A will be a matrix. And if you notice here, only three

consecutive unknowns are there in each equation. So A will be most likely a kind of tridiagonal matrix with one few elements here and there.

So that is what you will get. This will be your matrix A and b will be the forcing function, which is on right side. These are especially for the special case phi n phi p equal to zero. You can substitute here. You have this exponential here, exponential here, and C here. So C will be unknown. So C will come at b here and the psi will somehow again come back to this A only and this exponential will add up here.

So your diagonal will be basically of the form minus 2 here psi i. Another coefficient is exponential psi i. So that will also come into the picture. Now this is still not linear, because you have exponential term here. So this has to be solved basically iteratively. So it has to be solved iteratively.

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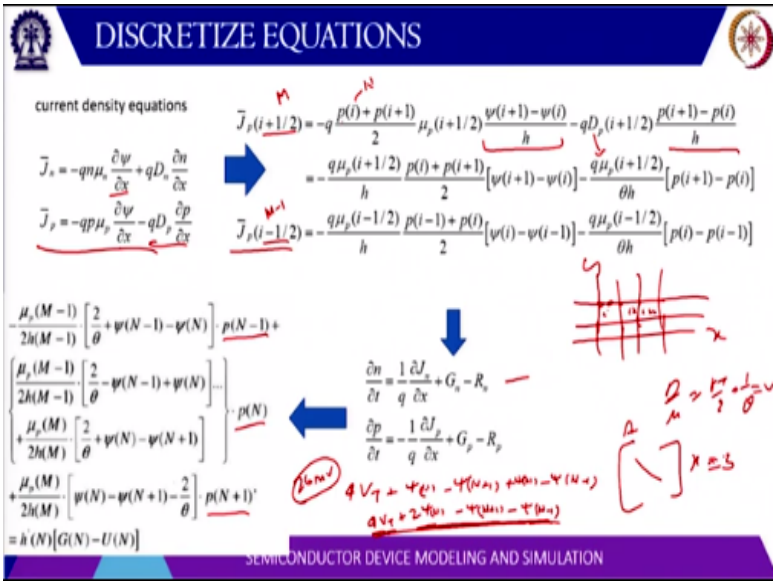


Now similarly for the discretization for the current density equation. So one way we tempt it to discretize that d psi by dx can be written as psi i plus 1 minus psi i by h. Nowthis is i these currents are calculated at the middle of this region. Let us say this is your, let us say this is your x axis, this is the y axis. So if you consider 1-D case now this is i this is i plus 1, this is i plus 2 and so on.

So the current at i and i plus 1 this calculate here at the middle point. So at the middle point, we have to estimate what are the value of n. So n or this is gp actually. So

middle point is p i plus p i plus half by two. Then mu p times q and then d psi by dx psi i plus 1 and psi i by h. Then q dp, dp by dx, p i plus 1 minus p i by r.

Then if you rearrange it further and substitute that d by mu is equal to K T by q, which is denoted by theta here. So your d is mu by theta. So this d is replaced by mu by theta here. And similarly, you get write current density at i minus half point. So this is called m this is called m minus 1. So m are the middle points basically and these are basically n here. Then what we have to do basically?

This current density expression it has to be substituted, it has to be substituted in the continuity equation. Then we have some expression like this, where the coefficient of p n minus 1, p n and p n plus 1. So the diagonal event will be this thing. So if you check here the diagonal event will be 2 by theta plus 2 by theta, so 4 by theta. So this is 4 V T because 1 by theta is V T. So 4 V T.

Then if you see here plus psi n minus psi n plus 1 plus psi n minus psi n minus 1. So this is basically 2 psi n minus psi n plus 1 minus psi n minus 1 plus 4 V T. Now if you notice here there is a general rule that if you want to solve for A x equal to b, then this A should be diagonally dominant. That we say this diagonal should be big enough. Now if you notice here, this is 4 V T plus 2 psi minus psi n plus 1.

So this actually requires that your this term because 4 V T square is small and these are the potentials here. So your potential step should be order of this V T and V T is how much? V T is 26 millivolt at room temperature. So this will basically require a very fine mass. Otherwise, this system of equation A x equal to b will become unstable, and it may not actually converge. So to overcome this effect, Scharfetter-Gummel discretization is used basically.

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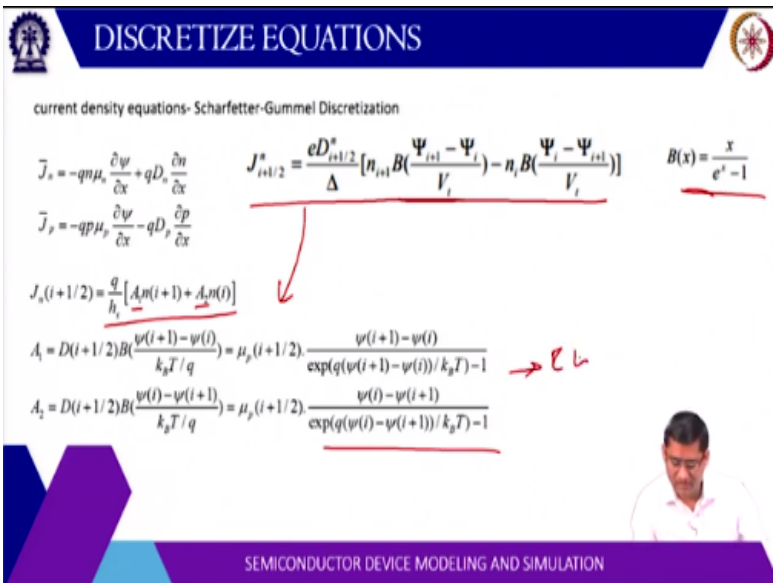


So that we have already discussed that using the Scharfetter-Gummel discretization J is given by this function of B and where B is the Bernoulli function x by e to the power x minus 1. And then if you substitute this into the expression for the continuity equation. So this is the expression for, simplified expression for J, where A 1, A 2 are the coefficient evaluated from this Bernoulli expression.

So that simplifies to psi i plus 1 minus psi i by q psi i plus 1 minus psi i q i K T minus 1 and so on.

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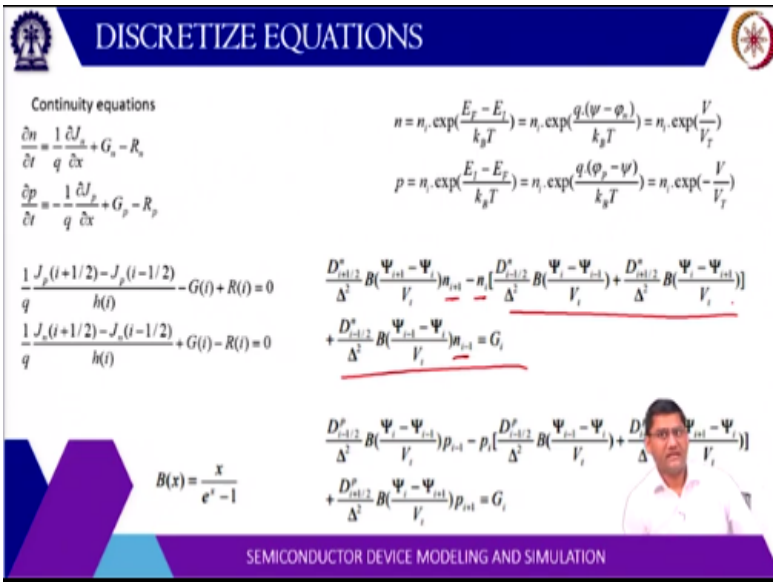


Then if you substitute this to continuity equation you get some equation like this. And if you see the coefficients here that for n i for n i plus 1 and n i minus 1, this will be diagonally dominant regardless of the or for a broader range of step size. So generally

this kind of discretization is used. So we have already discretized the Poisson equation. We have discretized the two continuity equations. So there are total three equations. Now what we have to do?

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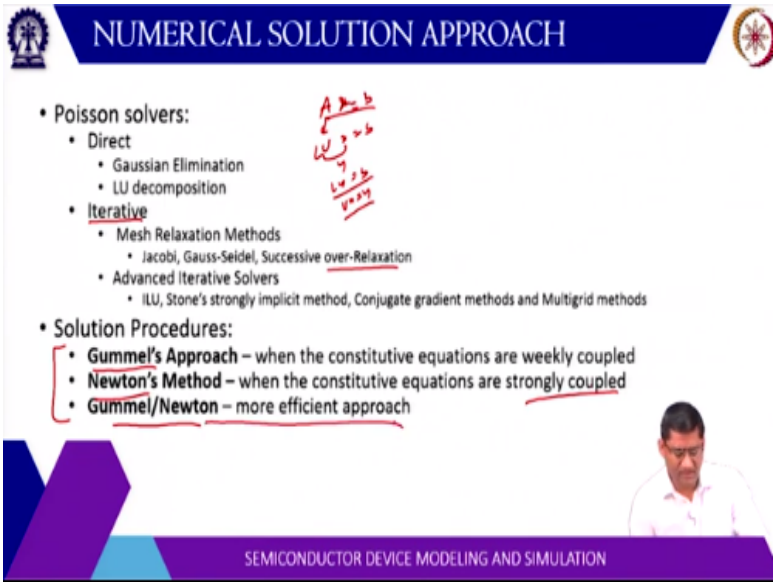


We have to solve them. So how to solve them? So for solving them, there are various methods. One is the direct solution. So if you have A x equal to b and the method is called Gauss elimination. So Gaussian elimination what it does? We solve for you know one unknown at a time by eliminating all other unknowns from that equation. LU decomposition  this A is converted to LU x equal to b.

So then U x is let us say y. So L y equal to be it can be easily solved. Then once you know the y then U x equal to y, then this can also be easily solved because now it is lower triangular and upper triangular matrix. So it is straightforward. Then of course, there are iterative methods. So the mesh relaxation Jacobi, Gauss-Seidel over-relaxation successive over-relaxation and some advanced techniques are there.

Now in commercial tools generally they use this Gummel's approach, Newton's approach or rather mixed approach. So Gummel is usually slow, but it has higher chance of convergence. And Newton method is of course, is good for coupled equations and it converges fast. But you of course need a very good initial guess, which should be nearby only. And then for general case, they can be combined together and used in efficient ways.

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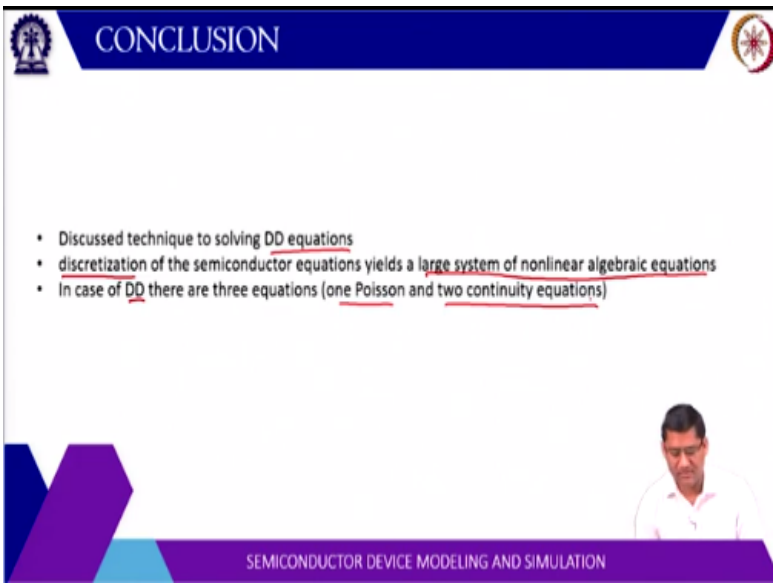


So in this lecture, we have discussed the technique to solve the drift diffusion equation. Then we have also discussed the discretization of continuity equation, Poisson equation to yield a large system of nonlinear algebraic equations. And of course, in case of drift diffusion, there are three equation, one Poisson and two continuity equation, which is for isothermal case temperature at you know some fixed temperature. So thank you very much.