Semiconductor Device Modelling and Simulation
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Lecture – 43
Drift Diffusion Model (Continued)

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Hello, welcome to lecture number 43. So, in this lecture we will discuss about the scaling and the discretization method for drift diffusion model. In the discretizing this Scharfetter Gummal discretization is very important because that ensures that when you do the simulation it actually converges. And we will also discuss the problem with normal discretization of the continuity equation.

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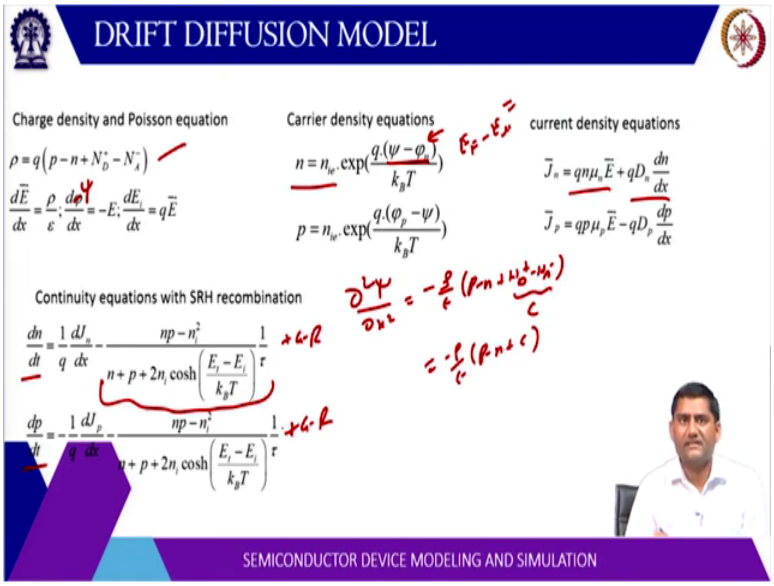

Now, let us recall the drift diffusion model, so, there is a charge density and the Poisson equation. So, generally, the poisson equation is written like this d 2 psi by dx square. So, here, psi of potential is equal to minus rho by epsilon times p – n + N D + – N A –. Now, these are fixed charge, so, they can return as c. So, this is – rho by epsilon times p – n + some C. And n can be written as n i exponential q psi – phi by kT.

So, this is related to Fermi potential, so, here it should be actually psi. Then your n is written as basically, n i exponential q psi – phi by kT. Now, the difference between this potential psi and phi or you can write E F – E i is actually q times V the potency difference potential applied potential V. Because with respect to the applied potential the Fermi potential follows applied potential with respect to the internal potential.

So, the difference is basically the applied voltage. Then you have this current density equation where you have a drift current plus diffusion current. And then of course, the continuity equation. So, this is written for SRH but you can write a general expression which is + G – R or + G – R where G is the generation rate and R is the recombination rate. Because generation rate tend to increase the carriers, so, it is plus recombination tend to decrease it, so, it is minus.

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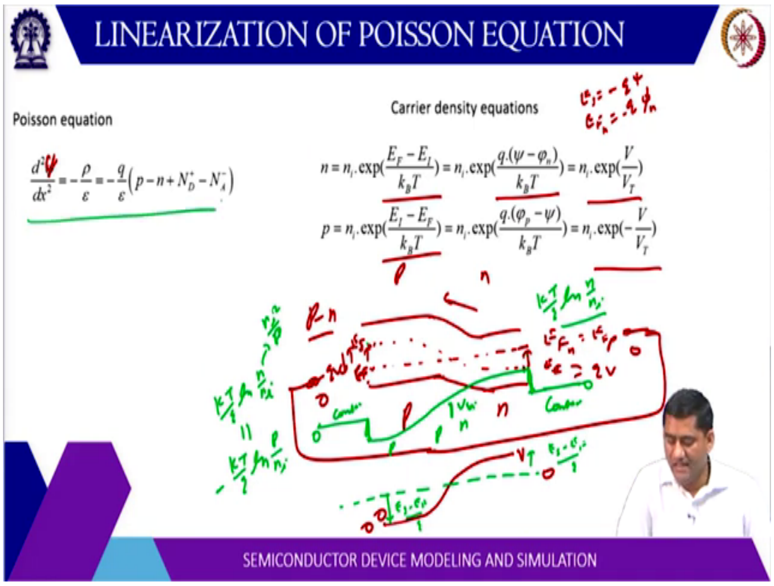

Now, linearization of the Poisson equation. So, this is d 2 psi by dx square is equal to minus rho by epsilon. So, this is –q by p – n + N D + – N A by this is the equation. And then the carrier density equation you have seen different forms E F – E I by kT then that is also written as q psi – phi n by kT where E = –q psi and E F = –q phi, so, n becomes phi N and p become phi p. So, this basically get reverse.

So, this is E is basically E i the internal potential, is same as the potential. So, if you look at the band diagram of let us say p n junction, if you recall the p n junction, so, this is p type. So, in p type, the Fermi level is somewhere here and in n type Fermi level is close to the conduction vent. So, this is your E F. Now, here E F n = E F p in equilibrium. And then if you look at the internal potential which is E I so, this is E I.

Now, for n, n = ni exponential E F – E I so, this difference. So, this is basically your q times V. And here, if you see this is E I – E F so, for a p type, it is E I – E F so that is phi p – pi. So, if you see here, E f is below E I is above so, this will be – q times V the energy. So, you see here, for p type or for the whole concentration exponential – V by V T for electron it is exponential V by V T.

So, V is as far as the band diagram is concerned, is the difference between the Fermi level and the intrinsic level, so that difference is q times V so, applied potential. So, if you apply a potential here and let us say this potential is 0 then potential is 0 here, potential is 0 here. Now, what is happening? So, on the p sat on the n the inside, so, your E I is above E F is now you notice here that E F is aligned with the potential throughout the E F is 0.

But then how the potential is changing inside this device? So, you can see here E I is above. So that means there is some positive potential and here E I is below so, this energy is – q V. So, there is negative potential energy here. Now, if you will plot their band diagram, the potential diagram, so that energy is increasing. So that means potential is decreasing. So, potential will increase like this, so, this will be 0, this will be V.

So that potential is increasing. But if you see here it is 0 potential, it is 0 potential here. So, how do we understand this thing? That inside the potential is increasing when you go from p to n side but outside that the terminals this is also 0 potential, this is also 0 potential. So that has to be understood in terms of the intrinsic energy level. So, this is aligned with the Fermi level. So, this side, intrinsic energy level is up you see.

Here intrinsic energy level is down so, here basically, what you see? You see some positive energy. So, positive energy means that means different colour here positive energy means the potential is down here. So, this is your 0 potential inside there is a potential change and that is the difference between E I – E F. So, this is E I – E F by q. And here also, this is also E I – E F by q.

So, here E I – E F by q is positive and here E I – E F by q is negative. So that means potential is up here potential is down here. So, what it does see here? Potential goes inside it sees a jump here then inside it actually increases and at this boundary **(()) (08:03)** here and this 0 so, potential is like this basically. This is how the potential diagram inside the p n junction will look like. So, at this terminal potential 0 and at this terminal potential is 0.

So now, you notice here there are three built-in potentials. One is at the p n meteorological junction that is V B i then at the this contact and p type region, this potential which is negative and then at the N type and the contact and this is positive potential here. So, what is the value? If you take it is E I – E F so, this will be kT by q log of p by n i. Because this is so, p type, so, whole is large but this is negative, so, this – kT by q log p by n i here it is positive.

So, the potential is kT by q log of here see that difference E F – E I which is n by n i. So, this can also be written as kT by q log of n by n i. Because here n is n i square by n i or p so, this both are same basically. So, the potential with respect to the contact and the semiconductor is kT by q log of n by n i. So, if electrons are more than the potential inside is more or that means the energy is actually low.

So, this basically explains that with respect to the boundary condition, how the potential is varying inside a piece of semiconductor? So, once we understood this point here. Now, we can discretize this Poisson equation.

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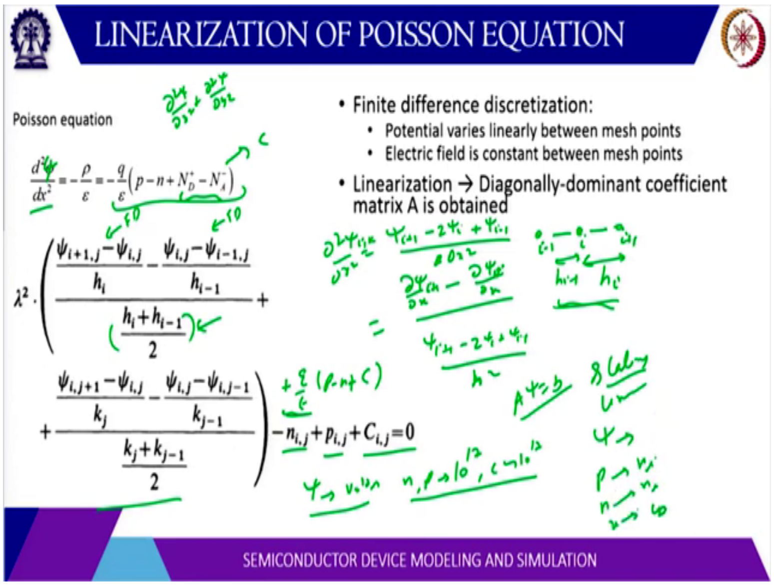

So, this we have already seen that d 2 psi by dx square is now, this is I have written for 1 dimension but for 2 dimension it will be d 2 psi by dx square + d 2 psi by dy square. Now, d 2 psi by dx square, we wrote that d 2 psi by dx square is psi at point i, K psi i + 1 – 2 psi i + psi i – 1 divided by 2 delta x square. Now, here it is shown for non uniform grid. So, this can also be written as d 2 psi by d axis.

So, can also be written as d psi by dx – d psi by dx at 2 neighbouring points, so, this is at let us says we take at i + 1 and we take at i and divide by your the gap between the 2 basically. So, if you consider these two points here, let us say this is i this is i + 1. This is i – 1 so, psi i + 1 the derivative, so, i + 1 – i divided by delta x then psi i derivative, i – i – 1 divided by h i – 1. So, this is simply, you can identify. What is this one?

This is forward difference, this is also forward difference. Then we are taking the derivative at i + 1 and i. Then this is the difference basically. So, what we do here? Because this distance and this distance, so, this we call h i this we call h i – 1. So, we are basically having derivative in these two regions, so, we are dividing this thing by the average of these two because we have taken the double derivative here at middle point.

So, divide by this average of h i + h i – 1 by 2 so, this can also be done but if you consider that h i = h i – 1. What you will get? This h i into h i – so, this will become h i so, this is h i by 2 so, 2 h i by 2 becomes h i square. So, this is basically psi i + 1 – 2 psi i + psi i – 1 divided by h square, so, actually delta h square. So, for uniform grid you will have just h square at the in the denominator.

Similarly, for y derivative along y so, this is d 2 psi by dx square then this is right side we can take to other side that is –q by psi becomes positive here. So, + q by psi, p – n + + N D + – N A C. So, let us call it C. Now, you notice here if you, when you are going to solve the equation, the change in potential is order of few volt. So, your psi is order of few volts. Then you have this n and p which is order of 10 is to power 17, 18 and so on.

And then again C is also of same order 10 is to power 17 or 16 the doping. You notice here this is few volt this is 10 is to power 17. So, the difference is quite big. So, when you try will make the matrix to solve this, you will get A psi = b. This will be very much is skewed. That means you will have number some number visually small and then there will be some number 10 is to power 17.

So, it will be difficult to solve this kind of equation. So, what is done here? We linearize it and we scale it. So, there is a process called scaling and then linearizing it. So, linearizing is done through the writing these difference equations and converting to algebraic equation. And scaling is so that we make it the values are such that they are of the same order. So, how do we scale it? What we do? We can take q by epsilon from here.

And this is of course constant if epsilon is constant, this can be taken out and it can be merged with some constant. Then instead of writing psi we write this equation in terms of scaled potential. So, we scale psi with some scaling potential then p with some value. Let us say you can scale with n i and so on. N can also be scaled with n i and position x can also be scaled with respect to debye length. So that we have done.

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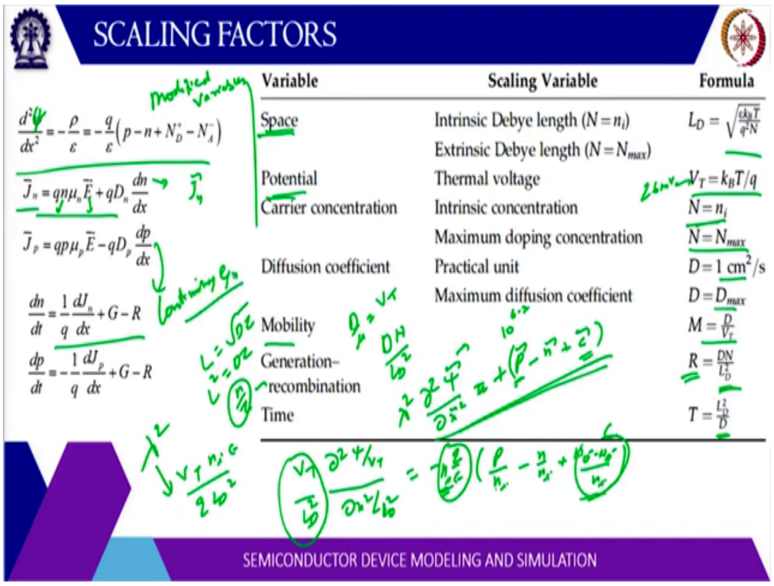

So, these are the different scaling things. Now, let us apply this to Poisson equation d 2 psi by dx square. So, here, if you write d 2 sin a dx square, so, d 2 psi. Now, psi we have to scale the potential is to scale with V T. So, what we can do? V can divide by V T and V can multiply by V T then dx square. Now, dx square, it will be divided by length and the length will be your space there is a debye length.

So, you can divide by L D and you can multiply by L D for this x square. So, to L D square by L D square then is equal to – q by epsilon. Now, you have p so, p can be scaled by intrinsic carrier concentration or the doping level. So, there are two ways basically, you can scale with n i or you can scale with the **(()) (16:32)** scale with n i. So, p by n i then multiply by n i then – n by n i and multiply by n i then + N D + – N A – divided by n i and multiply by n i.

Now, what we do? V T by L D square and n i times q by epsilon, we can put them together. So, V T times n i epsilon by q L D square, so, this becomes your lambda. So now, you have all these are scaled variables. So, we can write d 2 psi let us say tilde by d x tilde square is equal to or if you take the right left side that becomes p tilde, so, p by n is p tilde and this is your lambda square or lambda whatever this if it is lambda square.

Then –n tilde + this we call C so, this is C tilde, so, we are basically solving in terms of tilde. Now, all these x tilde, p tilde, n tilde, c tilde these are scaled values. Now, if you see the change, this psi will change let us say if your scaling volt is 26 millivolt and you have a range between some 0 to 5 volt. So, it will be some 0 to 5 by 26 millivolt. So, better than of 0 to

100 then p, let us say it is 10 is to power varying from 10 is to power 16, 15, 17 to 10 is to power 10.

So now, instead of varying having the variation of 10 is to power 17. Now, the variation is over order of 10 is to power 6 or 7. And this is of course and if you reduce the variation then you can scale instead of n i we can scale with some maximum doping also that can be done. But then you have to select whether you are dealing with the multi carriers. So, if you have to consider multi carriers, it is better to scale with respect to n i.

And if you are not dealing with multi carrier, it is better to scale with respect to the maximum doping. So that the idea is that the variation should be small and then the whatever algebraic question we wrote, we can write this algebraic equation for this modified variables. So, what we do through the scaling? We get modified variables. Similarly, for current density J is q and mu time C.

So, n will be scaled and mu D here n you can be scaled and electric field. So, potential can be scaled, so, the electric field will also be scaled according to the potential and the space. So, this is for the space and then for potential is the thermal voltage at room temperature is around 26 millivolt then carrier concentration with respect to n i or the maximum doping.

Diffusion coefficient usually scaled with respect to one or it can also be scaled with respect to the maximum value that is in the device that mobility. Mobility we know that D by mu is kT by E so that is V T. So, if D is 1 then M will be 1 by V T if D is D max then M by D max by V T. So, accordingly, the mobility will also be scaled and then generation recombination is a recombination rate, so that is related to the tau.

So, you remember D is a diffusion coefficient n is the carrier concentration divided by length square. So that is basically because this diffusion length is equal to root of D tau, so, diffusion length square is equal to D tau, so, tau is L square by D. So, this is what done here L square by D. So, 1 by tau and then generation recombination is basically is proportional to n by tau. So, it is scale with respect to D N by L D square.

Then time of course L D square with respect this tau. So, this is L D square by D. So, all these points are covered. A space potential carrier, concentration, mobility, time generation, recombination, all these are scaled. And instead of using the original variables scaled variables are used. So, here the range is basically, the range of variation of these parameters is actually reduce.

So, instead of J n you will have some tilde J n the modified current density and here also. So, these are is used in the continuity equation.

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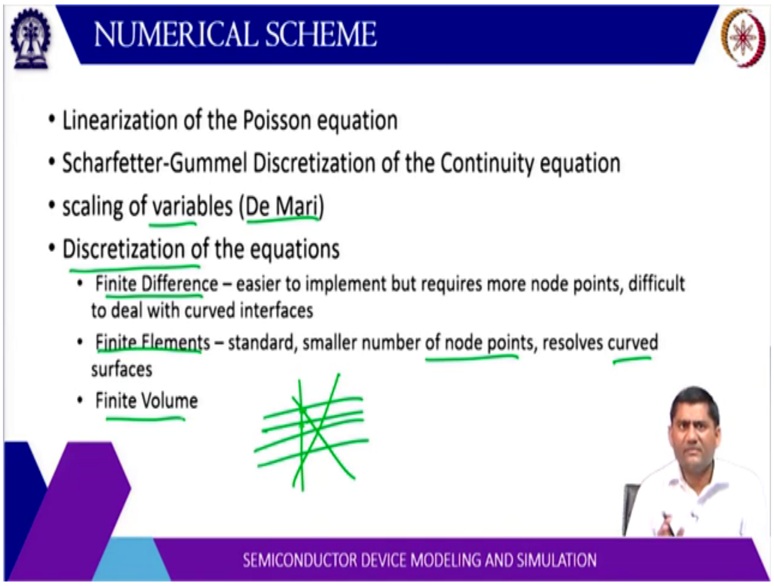

Now, numerical scheme so, once we scale and linearize then we use a discretization. So, for Poisson equation the discretization is normal finite difference, discretization and that is with respect to the potential. And scaling of the variable is attributed to De Mari a scientist introduce this technique. Then of course, this discretization that we have discussed, is at some level basically. Because there are different methods of discretizing it.

So, the different ways of discretizing so, it could be finite difference that we have discussed it could be finite element. So, in finite element, what is done? Instead of taking a point some elements are chosen basically. And here you can have more irregular geometries. So, this some triangles are formed and around that triangle you actually do the through variational approach.

You integrate this region and modify the equation accordingly. So, this is a finite element which is good for non standard geometries or curved geometries but and it has a small number of node points and it can easily resolve the curved surfaces. Then there are other method like finite volume then there are other spectral methods are also there. Boundary element, matters are there. So, there are different methods to discretize and solve these equations.

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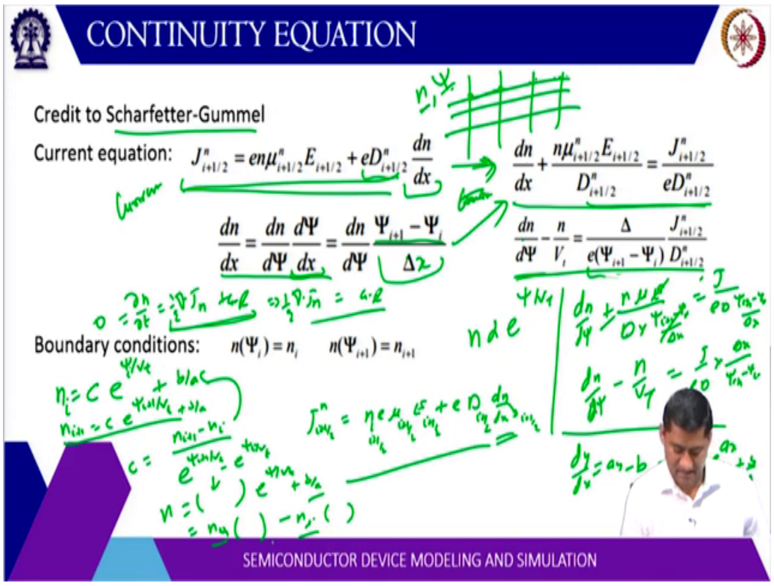

Now, the continuity equation this is attributed to Scharfetter Gummel scientist to introduce this method, what happens? If you consider simple, let us say this is your grid point. Now, if you discretize along this grid point. So, let us say we are discrete as in the potential. So, when we discretize potential, we make some assumption that potential is linearly varying. Then we will also discretize this for carrier concentration.

So, if we discretize and then we say that carrier concentration is legally varying which will not be correct. Because your carrier concentration is proportional to exponential psi by V T so, it is a exponential function. So that means, if your psi linearly varying the potential is linearly varying across grid point then your carrier concentration cannot vary linearly. It has to vary exponentially.

So, in this method what is done for the carrier concentration? A different technique is used. So, let us look how it is done basically? Now, let us look at the current equation. This is the equation for current and we look at the continuity equation This is the continuity equation is dn by dt this del dot J n 1 by q + generation minus recombination. So, in case of steady state dn by dt will be 0. So, this continuity equation will reduce to del dot J n will be some generation minus recombination 1 by q with some sign.

So, this will be your continuity equation. So, continuity equation basically uses the current density equation. Now, you look at the current density equation, so, what is done here? These are the grid points. So, you cannot define current at 1 node. The current has to flow between the nodes. So, let us consider i and this is i + 1. So, what is the current between these two nodes?

So, what we do actually? We take the middle where there is no node and let us call it i + half. So, J between node i and i+ 1 is written as J at i + half now we know that J = n e mu, so, n E mu times electric field + e times D times dn by dx. Now, this all has to be elevated at i and half so, n also need to evaluate i n half. E is constant mu also need to i n half E also at i and half electric field D also at i n half and this n also at i and half.

Now, since we cannot use that n i and n i + 1 so, this we cannot write that in the middle, this will be n i + n i + 1 by 2. So, this we cannot write because your current, the carrier concentration vary exponentially with respect to potential. So, it does not vary linearly between two node points. Of course, if you take node points very small, even then the variation can be significant and there may be convergence issues.

So, the another possibility is to make the spacing very small but that will be impractical and lot of grid points will come into the picture. So now, what we do? Instead of discretizing the n we discretize only the potential psi. So, we can rearrange this equation and from this we can get dn by dx and we express in terms of current. Now, current can be assumed constant between these two nodes.

So, your dn by dx is you divide by e D so, n mu e by e D so, e cancel out, is equal to J by e D. So, this equation directly coming from the current density equation. Now, dn by d psi we are not discretizing n with respect to x. So, we write dn by dx as dn by d side times d psi by dx. So, N is a function of potential psi and then this is d psi by dx. Now, psi we assume is linearly varying.

So, if psi is linearly varying then psi d side x can be written as psi i + 1 – psi i by delta x + m so, this will be times dn by d psi. Now, we substitute this into the equation here, so, we can write dn by d psi and we divide by this term here. So, let me write here dn by d psi, this + n mu E by D times psi i + 1 – psi i by delta x = J by e D times i, i + 1 – psi I, by delta x. Now, this E and d psi x are same with a sign, so, we will write a minus sign here and cancel these two.

So, d by mu is V T, so, this can be written as dn by d psi – n by V T because d by mu is V T = J by E D times delta x by psi i + 1 – psi i. So, this is the written equation written here. Now, if you look at this equation, this is a linear equation. So, if you recall this in mathematics, dy dx = a by – b. So, what is the solution for this equation? Y = e to the power ax + b by a. So, some coefficient times c times e to the power ax + b by a.

And then so, here also you can write for the n. So, your n can be written, as n is equal to some coefficient times e to the power ax. Now, a is 1 by V T, so, it can be written as psi by V T then + b by a so, this is let us say b. So, let us say, b by a. Now, this is subjected to two boundary conditions. So, n at point i will be exponential psi i V T and n at i + 1 will be c times e to the power psi i + 1 by V T + b by a.

So, from this you can get c, c will be you take the difference n i + 1 – n i divided by e to the power psi i + 1 by V T – e to the power psi i by V T. So, this will be coefficient and then you substitute back here, so, your n will be this C here times e to the power psi by V T + b by a. Now, b by a is this J by e D times psi V T so, this we already know. Now, if you notice here, it will have some coefficient of n i + 1.

It will have some coefficient of n i so, n i + 1 will have e to the power psi by V T by denominator and this will have some also –e to the power psi by V T and then this denominator here. This domain can be multiplied by e to the power psi by psi i by V T.

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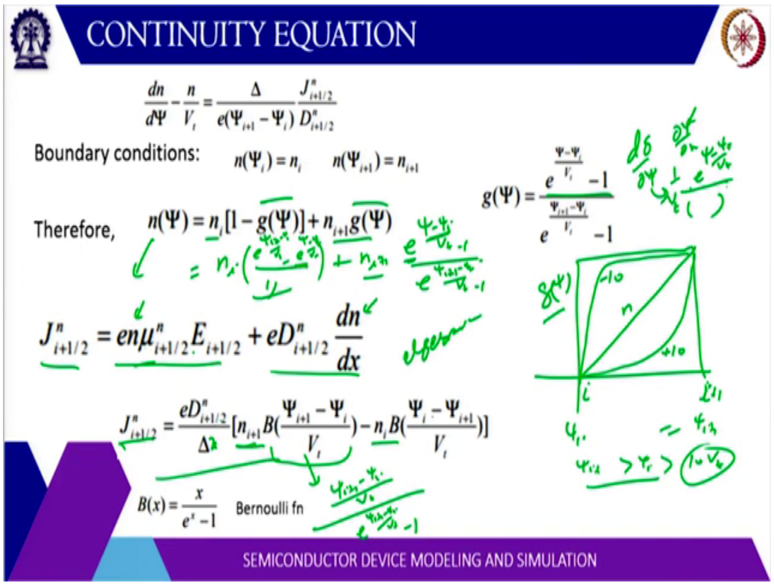

So, what you will have basically? you will have basically this is n i then this is n i + 1 e to the power psi – psi i by V T –1 e to the power psi i + 1 – psi i, i by V T – 1 and this is 1 – this thing, so, this will be denominator will be same as this 1 and e to the power psi i + 1 – i, i by V T – a to the power psi – psi i by V T. So, e to the power psi V T for n i + 1 coefficient is positive for n i the coefficient is negative that you can easily see here.

For n i + 1 the population positive for n i coefficient is negative. So, to write it compact we replace this function by g psi so, this is your g psi. So, your n is simply written as n i times 1 – D psi + n i + 1 times g psi. Now, if you look at the g let us say g psi. So, if you see a reason here, let us say this is point i this is point g i + 1. Now, the field is varying linearly, so, your psi varying linearly but your n will vary exponentially.

So, if your psi – psi i by V T if it this is 0, let us say psi i = psi i + 1 so that is, potential is 0, so, there is no change. So that means your this will be linear, basically because this coefficient is 0 this coefficient is also 0. So, your n will vary linear here if psi i + 1 is more than psi i so, it is plus a few 10 of V T because let us say this is 10 times V T so, psi i it is some 10. So then it will increase actually exponentially.

So, your it will be something like this and as you increase it so, at higher voltage, it is actually have more slope basically. And if it is minus then it will basically look like this. So, this is–10, this is +10, so, this is how it is changing. So, your n is not changing linearly, so that is what you have done and when psi is changing linearly. Then of course we can substitute this n into the current density equation which has e n mu times e + E 10 times dn by dx.

Now, here you have n here you have dn by dx, so, n means this g psi is there dn by dx means, if you take the derivative of dg by dx or that will be dg by d psi times d psi by dx. So, dg by d psi times d psi by dx which is electric field, so, electric field has come here and mu and d are related by V T. So, dg by d psi you can find from here. This will be same denominator is same. It is not varying because psi i and psi i + 1 are the node values.

So, with respect to psi, if you take, it will be 1 over V T times e to the power psi – psi i by V T by this denominator. So, here you have e to the power this psi i – i V T and times 1 by V T. Then when you substitute and by it there is some algebra is there but you can do it so, by algebraic simplification. J i for J n can be represented as e D by delta x times n i + 1 times a function called Bernoulli function which is B x is x by e to the power x – 1.

So, this will be basically psi i + 1 – psi i by V T divided by e to the power psi i + 1 – psi i by V T –1. So, you see here for n you have g psi for dn by dx you have this function. So, when you rearrange it basically, so, it will have some coefficient for positive for n i + 1 and so, n i + 1 has positive g psi n i is – g psi so, again this signs are followed here. And the current is expressed in terms of psi, so, it is not in terms of n i + 1 – n i by delta no.

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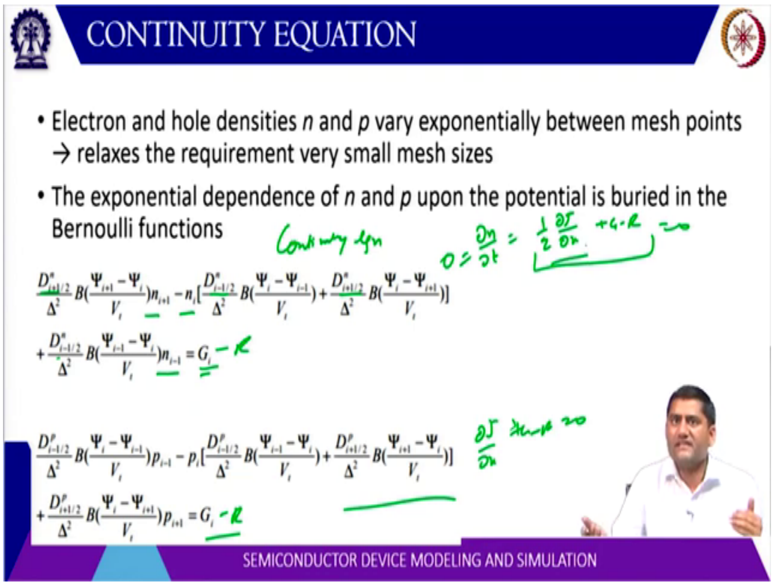

It is in terms of psi only and then this is the basically equation and then you substitute to this the continuity equation, so which is basically dn by dt and so on. So, if you see here this is basically n i + 1 – n i and this is the coefficient of n i – 1. So, a double derivative of, if you see dn by dt = 1 over q del J by del x + generation minus recombination. So, for steady state let us assuming state is a dn by dt 0. So then this becomes 0.

So, this is dJ by dx. So, instead of writing in terms of n this J expression that we dragged here is used here, basically so, J of n + half and J of n – half. So, what is done here? See J of n + half D i + half times these Bernoulli functions. So, D i + half i – half and D i + half times Bernoulli and this is d i + half this is d i – half d i + half and d i – half is equal to net generation minus recombination.

Similarly, the expression is written for the wholes, also dJ by dx + generation minus recombination is equal to 0. So, you get this kind of equation. Now, this is in you can write an x, you can write in y for 3-D also, you can also write it because more and more complicated. So, idea is that for the drift diffusion model when we discretize these governing equation, governing equations are the Poisson equation.

Then continuity equation and continuity equation is basically expressed in terms of the current density. So, we have to discretize the current density equation, using the Scharfetter Gummel method.

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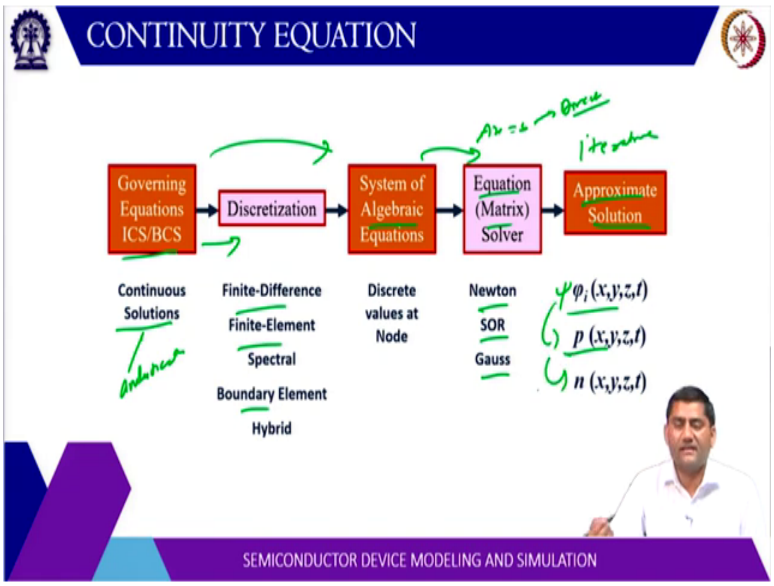

So, finally, what we do? So, this governing equations, of course, when solved analytically, we have continuous solution. So, where we discretize them so, using finite difference, finite element, boundary element and so on. Then what it does basically discretizing does it convert the differential equation into algebraic equations. And then algebraic equation we get some Ax = b. So then of course, we have to solve for the matrix.

And there are different methods Newton method, successive over relaxation method, Gummel method, Gauss method and so on. And through iterative solutions, iterative solvers, we get the approximate solutions which are close enough to the accurate solution. And of course, if you directly solve it then you will get exact solution but direct method is difficult and it takes and impractical especially for the large size of the problems.

And then you get these variables the potentials, the psi and then from psi you can calculate the p and n.

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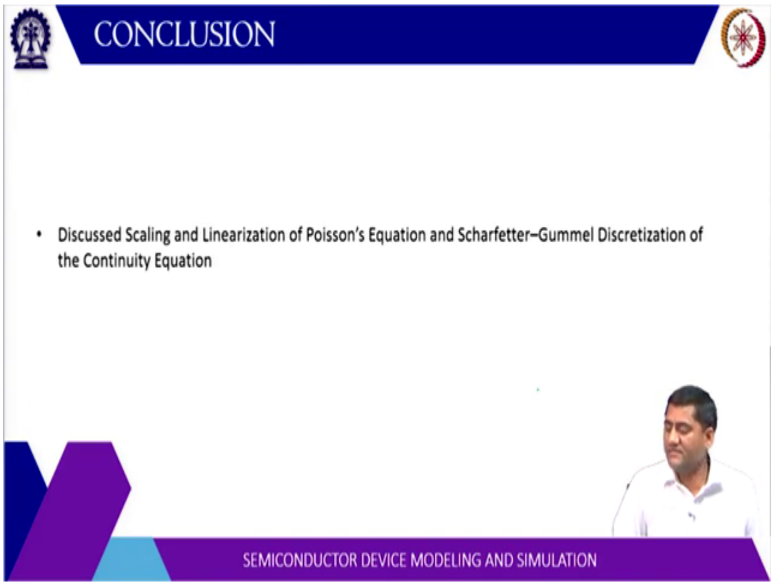

So, in this lecture we have discussed the scaling and the linearization of Poisson equation and the Scharfetter Gummel method for the continuity equation. Thank you very much.