Semiconductor Device Modelling and Simulations
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Lecture - 61
Simulating Junctions

Hello welcome to lecture number 61. In this lecture we will further continue our discussion on device simulation software and Silvaco and how do we simulate some devices such as PN junction or metal semiconductor junction.

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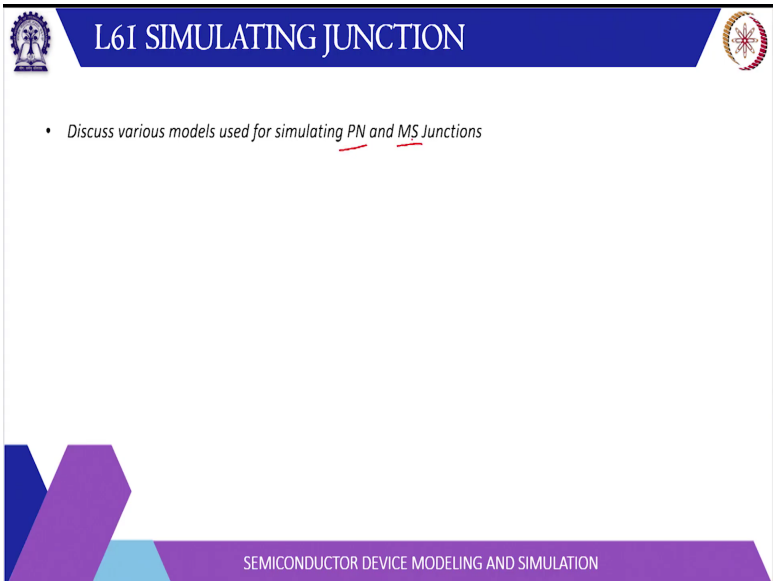

So, specifically the PN junction and metal semiconductor junctions.

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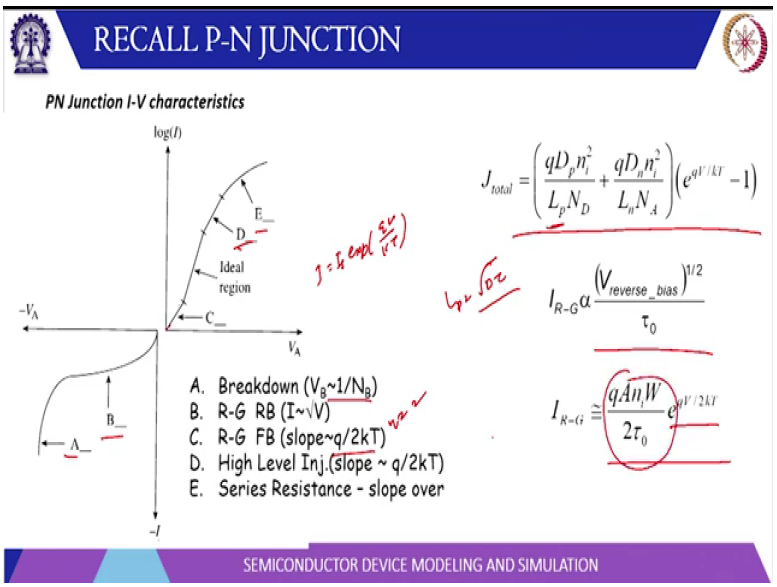

Now if you look at the PN junction IV characteristic you can recall from the discussion we had earlier. The IV character looks something like this and you can classify that into different regions. So, this is basically region where this is bred down and this is proportional to the inverse clipper version to the doping density. Then there is another region which is generation current, so it is a depletion region basically and which is bad enough.

In this region as the voltage increases this region becomes white, more generation of carrier takes place. Therefore, current slightly increases although not as large as the forward bias junction but significant current flow. Then there is a ideal region where it follows this relationship I = I s exponential qv by kT. Then blow this the for a small voltage there is another region where the bias is small.

Therefore, now this recombination current actually dominates in this region and the slope becomes q by 2 kT, so you can say the non ideality factor is two basically. Then if you go for further high voltage then of course in D you have high level injection and E is basically the current is so high that series resistance plays at all. Now you can also recall that we got this expression for the diode current density J so which is qD p n i square by L p times N D.

Of course, this L p is there for a long diode where the length of the p side and N side is much larger than the L p, L p is basically a square root of D tau. So, D is a diffusion coefficient. Now is the light carry lifetime so this L p we can see a diffusion length per whole and the electron respectively and in B region, this is square root of B by Tau because this contribution is mainly coming from the generation date.

And of course, in lower voltage forward wise it is again exponential qV by 2 kT multiplied by q An i by Tau 0 which is basically coming from the recombination part.

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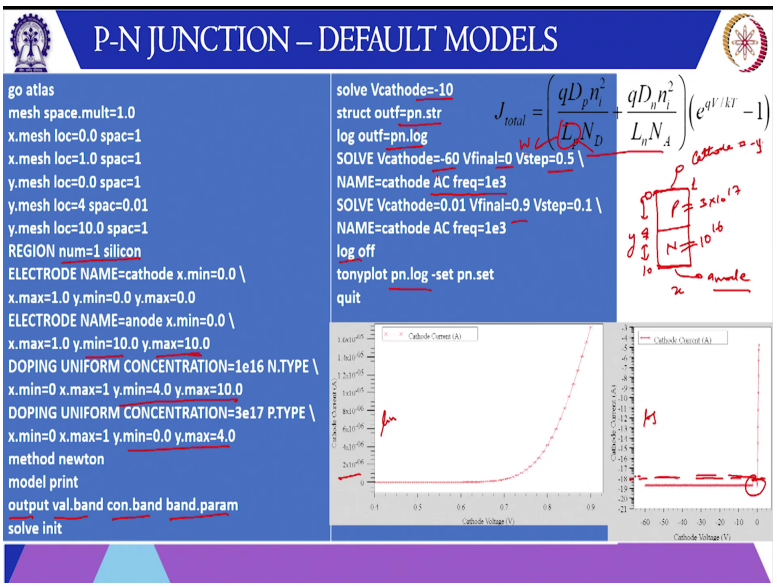

Now let us begin and write a simple code for a PN junction in Silvaco Atlas. So, what I have done here? I have chosen one small PN junction diode, so from y = 0 to x mesh location 0 to 1, so this is x axis this is y axis. In Silvaco y axis actually goes top to down, so top is 0 and as you go down it increases, then it is up to 4 and 10. So, this is 4 here this is 10, so 0 to 4 if you see the electrode, electrode is X min 0 and X max is 1 so that means x is 0 to 1 y is 0.

So, this is basically your electron name cathode then there is a syntax on region number one so that means whole thing is silicon basically because we have to define the region as discussed in the previous class. Then there is a Y min is 0 Y max Y - 10 Y max is 10 so that is anode, so this is your anode. Then there is a doping uniform N type doping from Y min 4 2 by max 10, so this is basically your N type and the value is 10 raised to power 16.

Then from 0 to 4 y that is P type and the doping is three into 10 raised to power 17. Then method Newton is default model print basically prints all the parameters that are used by the simulation. Then if you want to have some other specific output which has not available at default that you can write in the output command. So, here I am writing the valence band conduction band and then parameter is output.

So, they will appear along with the structure file if you have any structure file. Now solve unit sets the cathode voltage to be zero energy voltage to be 0 and solves for the internalized structure you know what are the different parameters, how the potential profile carry concentration profile will look like. So, this is basically solving for all the voltage set to 0 solving it, then you can directly jump to solution of V cathode - 10.

So, when is V equal forward is set to - 10 that means this is reverse biased. So, we say V cathode is - 10 and V anode is unchanged we have not respected any value, so it carries the previous value which is 0. And which is set by solve in it. Then at this point we have saved one structure file. So, that will tell you the internal state of the device at V cathode - 10 volt reverse bias.

Then you can solve for different voltage and get the terminal characteristic in the log file. So, this is a log file out F = PN dot log. Then we are solving this V cathode from - 60 to 0 in the step of 0.5 and you can also have the AC parameter along with it, if you have to just specify the AC and the frequency. So, you have to mention this this parameter AC and then mention the frequency, then solve we gathered from 0.012.9 in the step of 0.1.

Now I have broken it because in the reverse bias you can take a bigger step. So, it will easily converge because there is not much change but in four wires you know there is significant change. So, you cannot do the same step, so otherwise it will take lot of backtrack and take lot of time. So, you can always split your command like this, so this way it will cover all the range from - 60 to 0.9 volt and then of course you can log off.

Then you can Tony plot the log file, you can tony plot the structure file. So, at the bottom of the window you can see the IV characteristic. So, you remember in this program we have not included you know the regeneration recombination model. So, any models we have not included, it is a default model simple different model. So, default model we basically assume the mobility will be some constant and the **(()) (07:39)** will be finite and it will not use the specific models basically.

So, it is simply the conduction and you can see that it captures the IV characteristic it does not capture the known idealities. So, you see here this is in linear scale, this is in log scale. Now here see you see some kind of bump here which you can observe here. This is basically already below the limit of the convergence. So, if you see anything below 10 raised to power - 17 or 18 unless you specifically set it in the solid statement it is or basically error thing.

So, it does not make does not have physical meaning because this is the tolerance limit for the solution. Another thing you can notice here although we can use this equation to compare

with the current but if you notice here the length of the device is only 4 Micron here and 6 Micron here. And if you calculate the L p, it will be actually larger than this. So, you can use only um length of the device here instead of using the diffusion length.

So, that means if you change the geometry of this device if you change the language instead of 0 to 4 and 4 to 10 you make it 0 to 10 and 10 to 20. Then this IV curve will change basically the current will actually probably reduced because now the slope is less because that now this W here which was the width of the noise is more because we have not included any specific models here as such.

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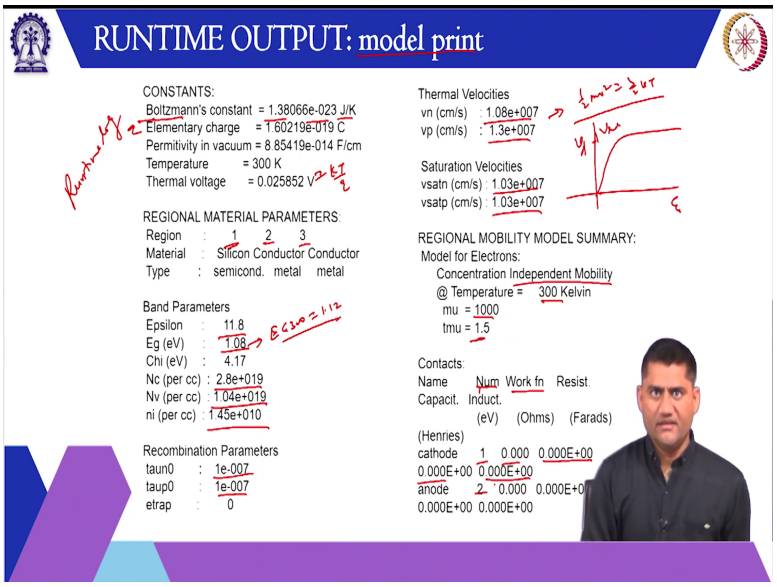

Now in the runtime output due to this statement model print, it prints all the values it prints a constants that it has used like Boltzmann constant is 1.38 10 raised to the power - 23 Joule per Kelvin. Then electron charge q, then permuted in vacuum temperature thermal voltage that is k T by q, then you have defined the region. So, we have only defined one region and two electrodes, so electrodes are also assumed to be region.

So, region two and three are the electrode, so for one region one there is a silicon material and its epsilon is 11.8 the directory constant, the band gap is 1.08 you can set this band gap using E g 300 = 1.12 so that will set the band gap. So, you can under the parameters you can change this to the actual or the band gap that you want to set. Then N c is basically number of effective density of states in the conduction band effective density of states in the valence band.

This is the intrinsic carrier consultation. So, these values are required when you make analytical evaluations, so these are all listed in the run time log this is listed in the runtime log. Then the recombination parameters we have not set the model but it uses some default parameter Tau n and Tau p is 10 raised to the power - 7 seconds. Then the saturated thermal velocities v n and v p, saturation velocity.

So, you what is the difference between thermal velocity and saturation velocity? Saturation velocity some kind of you know if you recall that due to field you know electric field this V's drift velocity source this kind of nature, so this is the V set saturation velocity. Thermal velocity correspond to the half m v square = 3 by 2 kT. So, due to the temperature what is the maximum velocity that can be attained.

So, these two are different parameters, then of course if you see the models that is using so it is using mobility model. So, it is a consultation independent mobility that means mobility is constant and it is 1000 at 300 Kelvin. Then of course it is variation with respective temperature is taken as some minus the T to the power - 3 by 2 or something. Then this is power, so this 3 by 2 is 1.5, then for different contacts you can have contact number, contact number 1 contact number 2.

The work function is zero resistance attached to that contact is 0, **(()) (12:10)** is 0, inductance is 0. So, that means we have not defined any inductance capacitance or resistance attached to the contact and work function is zero which is the Omega contact basically because we have not mentioned any other property of the contact. So, at default it will assume the contact to be ohmic.

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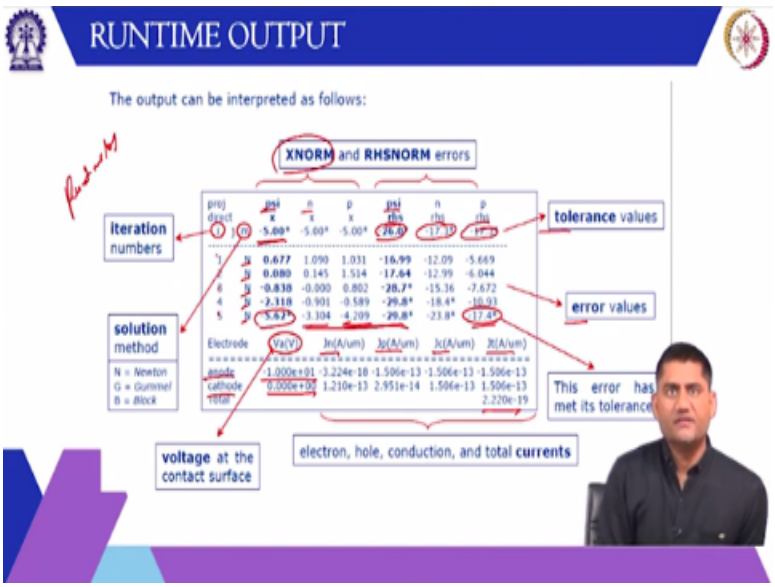

Now another portion of the code will look something like this where it actually solves for different voltages. So, let us say solve for anode equal to let us say here is a - 10 volt, cathode is 0, so when it solves it is a simple on this thing solution from the runtime this is also from runtime log. So, it is basically iteration number so 1 2 3 4 5 and then it is a method basically so we have mentioned Newton method, so it is the Newton method here.

It can be block method, it can be Gummel method then the G or B will appear there. And these are the voltages this is a cathode this anode and then this is the current densities due to electron due to hole, this is a current conduction current density, this is a total current density and for each iteration these errors are updated basically. So, for example this is a potential psi, then the convergence criteria is 10 raised to the power - 5.

So, if for successive iteration is less than 10 is 1 is 5, then we say it as converge. So, you see star appears here that means it has converged so for electron concentration, this is no star is there so that is potential is converged then we stopped it. So, only for whole concentration, then this is this equation containing these parameters. So, the left hand side equal to right hand side, so what is their difference.

So, that error the conventionally 10 is to **(()) (14:03)** is 26 for potential times 1 is 17 for electron concentration 10 is 1 is 17 for whole concentration. So, once they reach certain value, they satisfy the convergence criteria then we stop the simulation. So, these error values, so we commensurate with the tolerance value and once they meet certain criteria then the simulation is stopped and we have this solution then it go to the next solve statement.

So, this left side is called X norm you can set this parameter by setting the X norm you can change this value instead of **(()) (14:47)** - 5 you can change the value and this is called RHS norm, so this also parameter you can change.

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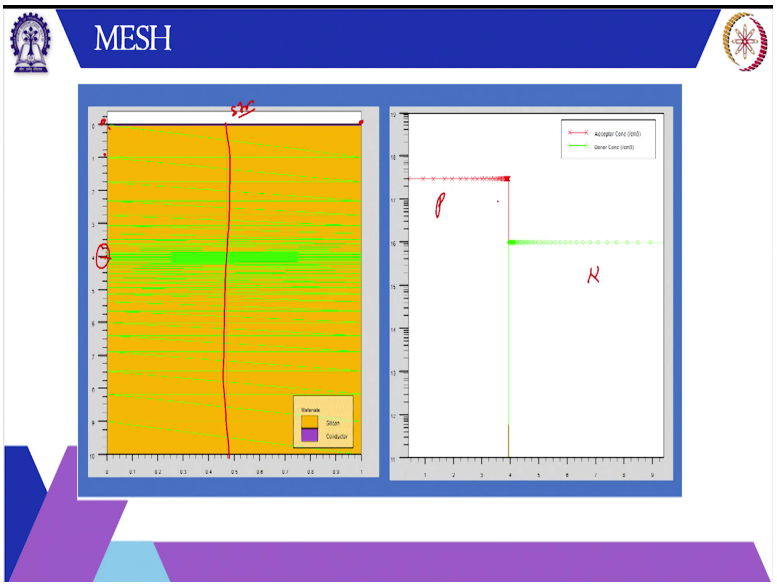

Then you see this eye structure file that we saved, so if you look at the mesh you can go to the code here see this is location 0, X is spacing 1 location 1 specific 1 so that means there is spacing of one. Then for Y location 0 space in 1 Y location 4 spacing is 0.01. So, that means it goes from spacing 1 to 0.01 and then to 1 so that you can see here in x axis it is spacing is 1. So, there are actually only two grid points here but in Y direction it is starting with 1 and goes to 0.01 here.

So, it is very small here, so it gradually move to that spacing. Now why have we have chosen this grid? Because we will have a junction here at the junction these parameters change you know drastically. So, we have to have a fine mesh here other reasons where mesh is not critical you can have a you know broader mesh. Now on the right side is basically a cut line it is a vertical cut line like this.

And it basically plots by default it plots the net doping here we have plotted the acceptor concentration and the donor concentration. So, because this region is P type this region is N type so it shows receptor concentration it shows the donor concentration, you can plot other parameters that are available also.

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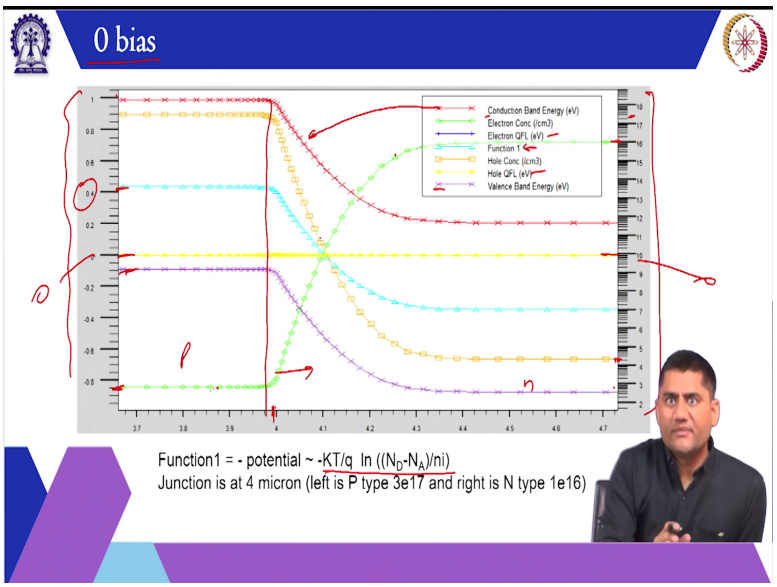

So, this is for 0 bias, we can save this structure file after the solve in it then this is a corresponding parameters from the cut line. So, because we have all mentioned in the output the conduction band the valence band the band parameter you can find out this is a conduction when energy the red line. So, this is the conduction band energy and for this you see this left side, so it is at one year and the valance band energy is this curve.

So, this is a valance band energy. So, this gap will be 1.08 because this is the band gap we have defined, so everywhere it will be 1.08, then you have this electron concentration. Now electron concentration unit is different from the band energy unit. So, this is shown on the right side, so you see here this electron concern is a green curve. So, it is you know very small like 10 is to power 3 or something here because this is p dot or end of it is 10 raised to power 16.

So, only the whole concentration is the yellow 1. So, you can see here this region the whole concentration tends to cover four something and here it is 10 raised to power 3 into 17. So, this is P type, this is N type. Then you can see the fermi levels whole fermi level and the electron quasi fermi level they are actually coinciding. So, this is the fermi level so because we have not applied any bias, so this fermi level are 0.

So, you have applied 0 volt here you applied 0 volt here. So, this formula is constant throughout but the internal energy level is different internal energy level is roughly in the middle. So, this line actually is roughly in the middle. So, this is basically the potential so this is basically - q times the potential so potentially because this is an electron volt. So,

potentially - 4 volt here and then this will be around plus 0.4 volt here, so minus 0.42 plus 0.4 volt it will change.

So, this you can actually using kT by q log N D - N A by N A. So, that also you can plot, so this is as function one. So, not only the available parameter but their operations also can be plotted in the structure file. So, you have to just select function and write the expression corresponding expression there and junction is at 4 Micron. So, this is a junction and you can see in this region the change is quite small but here is quite gradual.

That is because the doping is small here. So, most of the depletion region actually falls to the right side. So, it is basically kind of gradual.

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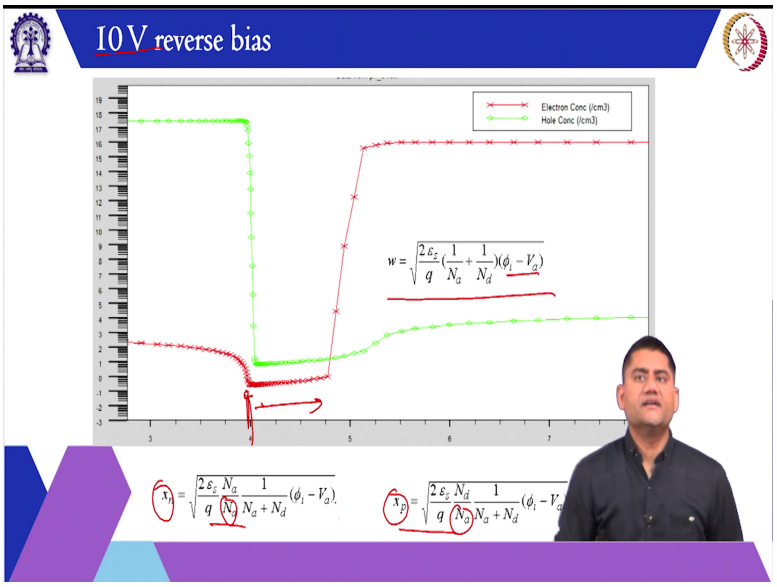

Then you can see this for 10-volt reverse bias, so for 10 volt reverse bias you see here this is the junction year 4. So, you see most of the devolution region is on the right side, on left side is very small because it is proportional to the carrier concentration and then if you recall the expression for the depletion weight 2 epsilon by q 1 by N a + 1 y N d times phi i - V a phi i is basically the built in voltage and V a is the applied voltage reverse applied voltage and then for x n side is this for x p side is this.

So, whichever doping is more let us say x and doping is more so that is N d is more then x n will be small, if N a is more then x p will be small and so on. So, this thing you can compare with the analytical calculation also.

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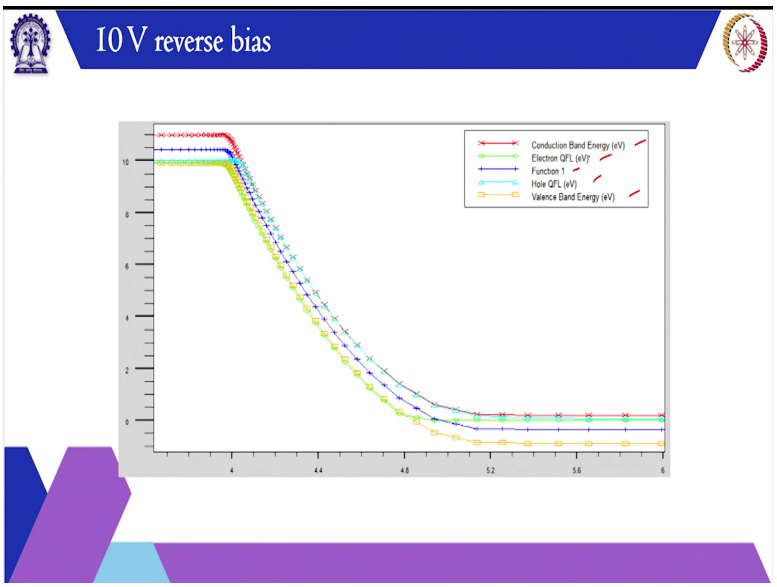

Then at the 10 volt you can see same thing the conduction energy the Fermi levels and the balance band energy and that function that specified.

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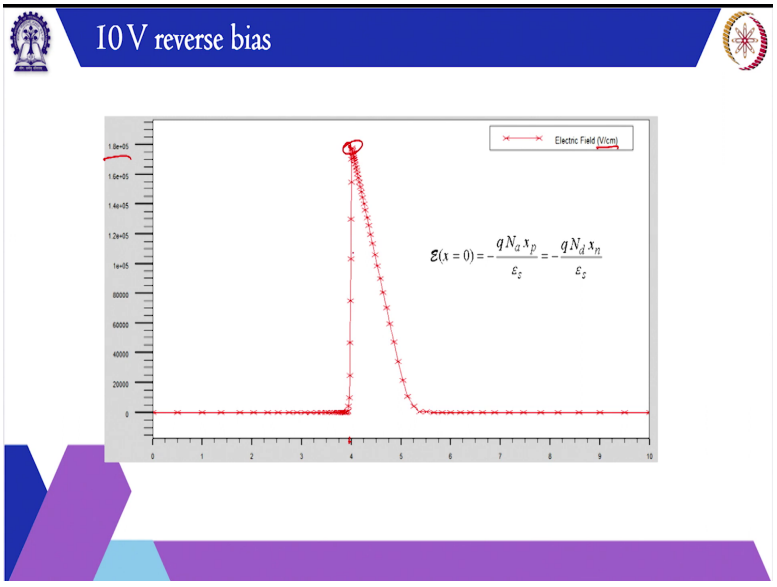

Then this is the electric field. So, you see at 4 this as a meta metallurgical junction the field is quite high is for 10 voltage wise you already have 1.8 10 raised to power 5 volt per centimetre. The unit is also given volt per centimetre and these things basically can be analytically calculated and matched with the simulation.

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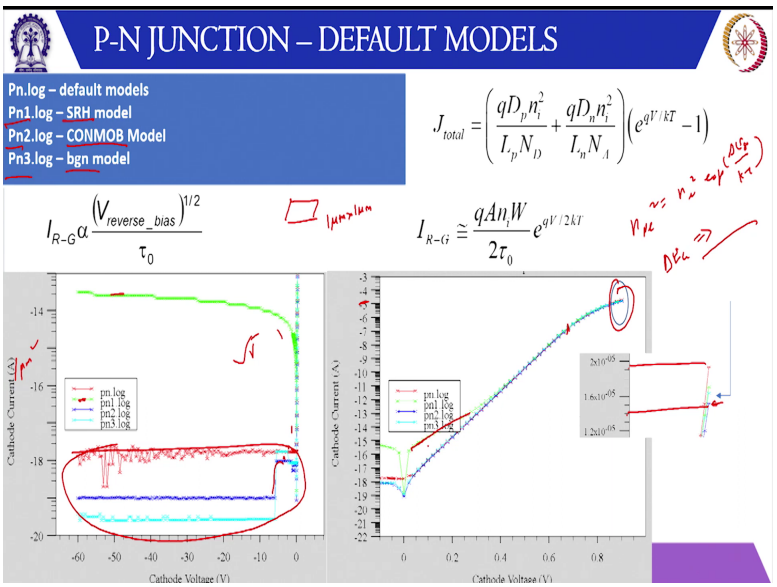

Now if you want to have a realistic diode characteristic then what you have to do, you have to include the certain models. So, for example here I have shown three examples with three modifications. So, in one modification P n 1 dot log is we have included SRH model for P n 2 dot log we have included the concentration dependent mobility model and P n 3. We have included a band gap narrowing model.

So, this SRH model basically will help us to include all the effect due to the generation recombination effect. So, you see here this P n 2 dot log which is green P n 1 dot log which is green in colour, so this is the green one. So, you see here for the reverse bias you have this square root of V dependent increase in current. So, it is increasing from 10 to - 18 to 10 **(()) (21:23)** - 14 here and this is the current density.

Anything you can notice about this device it is 1 micron thick and it is a 2d. So, in third dimension also it assumes 1 micron, so the area is basically 1 micron y 1 micron. So, this is our density, so the current density is basically this many ampere per micrometre square. So, if this device is the order of millimetre centimetre, then this value will basically increase. So, from micrometre if you make it centimetre then it will increase 10 is to power 4 and **(()) (21:55)**.

So, 10, so 8 if it will increase so it will become 10 is to power 6 so the current will be order of micro ampere and in the forward wise it is already 10 to the power - 4. So, again, it will be you know quite high actually. So, we you typically operate around 0.6 or 0.7 you know we do not go to higher voltage because the current actually it becomes quite high. And then this is

the forward wise region you can see the green curve it include that you know q b by 2 kT that non-identity.

Then you can see this is basically everything below 10 is to power 18. So, you can see this is basically just the tolerance related error basically, so you can ignore this thing. Then CONMOB is the consultation dependent mobility. So, it basically include the effect of the carrier consultation on the mobility. So, as the consultation increases or the doping increases the mobility will reduce.

So, that means the mobility which was constant is no more constant. So, it is changing with the doping level. So, now we have doping of **(()) (23:03)** 17 and so the mobility will actually reduce. So, if you see here this region here, we have expanded it so this blue curve is below here. So, that means it is quite a small so you see the corresponding current here is almost you know 1.422 into **(()) (23:25).**

So, this is a significant difference between the current density so because CONMOB reduces the current because it include the concentration dependent mobility. Similarly, you have this band gap narrowing effect band gap narrowing effect is included you have this n i e square = n i square exponential delta E g by kT. So, what happens due to higher doping there is increase in the carrier consultation and that actually affects the band gap.

So, there is a reduction in some kind of band gap. So, this delta easy is calculated in terms of some parameters and these parameters can be set using the command line. So, E g n dot E g dot E g n dot N all these parameters can be set or you can use the default parameters. So, that is about the band gap narrowing model. And so everywhere this current will be slightly less for the consultation dependent mobility model.

And band gambling effect basically if you see it slightly you know the changes very last year but some critical cases it can be experienced that it makes significant effect.

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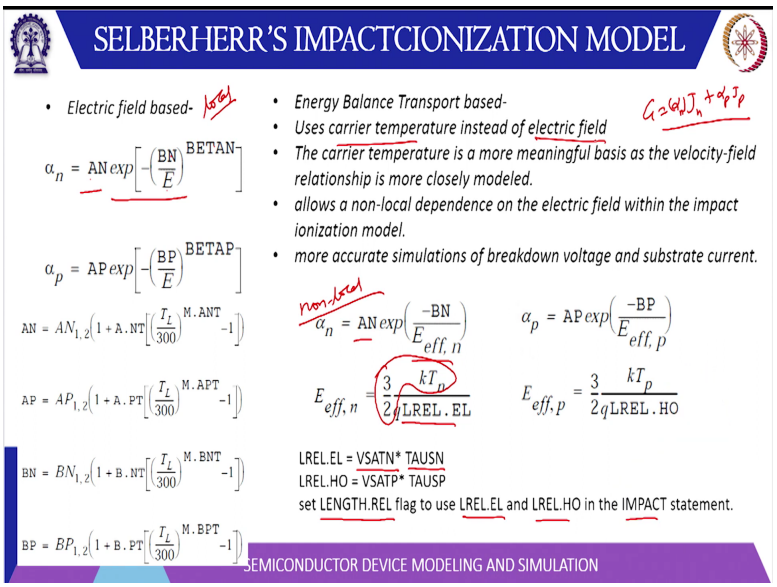

Now let us come to the another part of this PN junction simulation that is the breakdown voltage.

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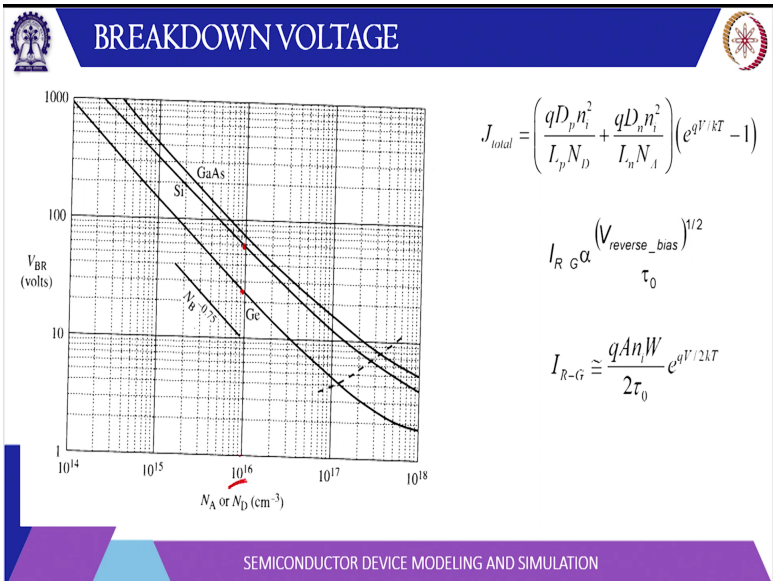

Now if you look at this diagram here this diagram here, we have doping of 10 power 17 and 10 power 16. So, your breakdown voltage should be somewhere here this is basically proportional to the 1 by the lowest doping, so lowest doping is 16. So, corresponding breakdown voltage this is for silicon this was this is for silicon, germanium this was silicon. So, it should come around 60, so around 60 or 50 60 it should come basically corresponding to this dropping.

Now you can simulate this one by including the impact ionizing models. All other models are included using the model statement but impact ionization models are included during the

impact statement. So, if you see here the current density is let us say is some J n is the current density, so the generation it will generate some carriers and that generation will be proportional to J n times alpha n.

Alpha n is basically some kind of ionization coefficient and then similarly you can have similar effect from the holes. So, you can write alpha p times J p, so now this alpha and alpha p have to be modelled. So, alpha and ionization coefficient can be modelled like this some coefficient AN exponential BN by E to the power some BETAN. So, these are parameters AN BN and BETAN where E is the electric field.

Now this is basically a local type of model so that means this ionization coefficient is dependent on the local electric field. This is one such model and these parameters have to be set. And you can simulate it accordingly or you can use non local models where this is not the function of local electric field but some effective electric field you can say. So, you can say alpha N s AN times E to the power - BN by E effective N.

And this E effective is basically you should recall 3 by 2 kT is the energy of the electron divided by relaxation length of the electron and this you can set relaxation length of electron and hole in the impact statement you can set this length dot REL. So, that means you are setting the relaxation length not the relaxation time. Otherwise, it is calculated using saturation velocity times the relaxation time TAUSN and TAUSP.

So, this is basically non local or you can say this is basically energy balance related simulation, so this is based on energy balance transport and we use carrier temperature instead of the electric field. So, in the energy balance transport the mobility or the drip velocity is not the function is not just a function of the local electric field but it is dependent on the carrier temperature.

So, that carry temperature is different from the normal lattice temperature and that is included using a command called SCTE. Then and in case of impact ionization this carry temperature is more meaningful than the local field bias model.

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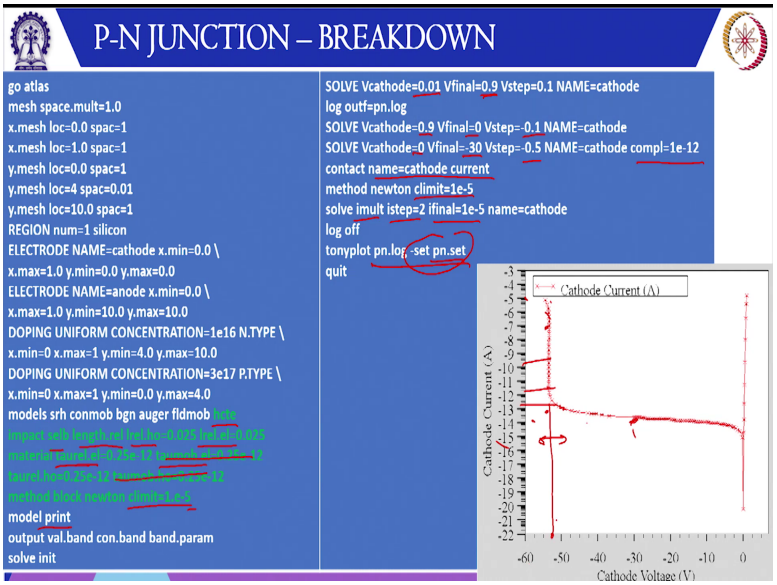

And then this model is included in the code here, you can see so model SRH **(()) (28:36)** field mobility and there is a HCTE so that means carrier temperature is included. So, it is basically corresponding to the energy balance simulation. So, it will have electron temperature hole temperature. Then the impact ionization model we have this **(()) (28:52)** model and then length REL means the length are set.

So, l REL whole relaxation length for electron aerial parameter relaxation time for electron relaxation time for electron hole and so on. Then Tau mobility for hole, so just written twice but this part of the code then method block Newton and this is a c limit. So, that means below certain default values I think some other value. So, below that consultation it kind of ignores does not consider but in case of breakdown even one electron is significant.

So, that this limit of the consultation that have to be taken into account is reduced in case of breakdown simulation because these electrons get multiplied. So, this limit has to be reduced in case of breakdown simulation. Then of course model print will again print all these parameters, then solving it and V cathode and so on. You can also notice one more thing here we solve for V cathode then if you note here this is V cathode is 0.01 final is 0.9.

So, this is **(()) (30:03)**. Then what I am doing here? I got to this 0.9 then I am backtracking basically from 0.9 I am going to 0 in the step of - 0.1, then from 0 to I am going to - 30 in the step of 0.5 and there is a compliance parameter that means if my current is more than this one then it will stop. So, if it my current is more than 10 is 1 - 12 it will stop then I change the

contact to the current contact because see I do not know what is the breakdown voltage exactly.

So, at that point if I change slightly the voltage there is a significant change. So, there will be convergence SEO. So, now my contact is a current contact. So, what I will do? I will simulate in terms of the current. So, now current I can easily set here this current, this current, this current. So, the voltage change will be small, so now it is solve imult, istep double the current ifinal is 1 e – 5.

So, this is the value and it is start with the current that was previously existing. So, maybe a 30 this is the current something **(()) (31:09)** is 13 or 14 and then c limit is 1 e - 5 and then you know in log file all this value is recorded. Then I do the tony plot p n dot log set is basically, if you want to get this plot in certain format. So, that is basically the job of the set file. Then you can see in the reverse bias you can easily see the breakdown is somewhere around 50 of something 52 or 53 does the breakdown voltage or you can do non isothermal.

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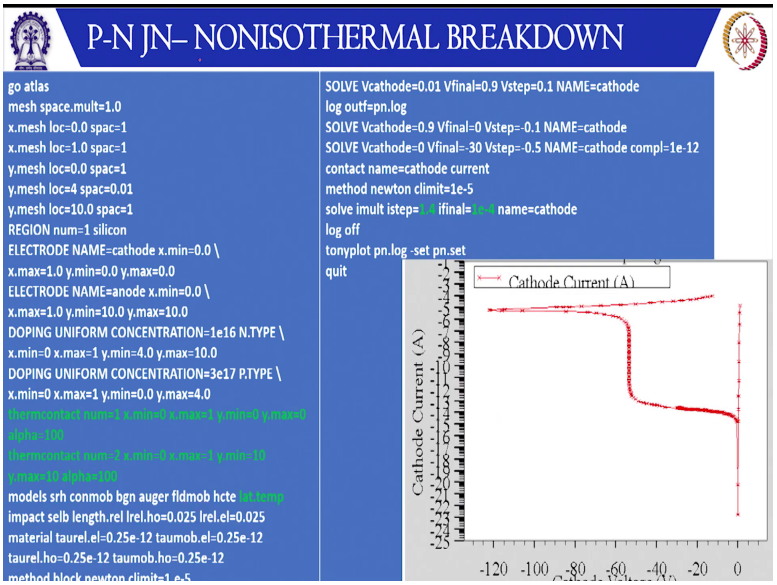

So, in previous case it was isothermal that means the lattice temperature was constant. But in non-isothermal you have to increase lattice temperature parameter. So, here one extra parameter is the area is the lattice temperature. So, we are we are also simulating the change in latest temperature. So, in that case what will happen? So, this is the let us say breakdown voltage somewhere here.

Then it increases then after certain point what happens if you increase the voltage further this current will kind of you know remain at the sufficiently high value but now the it is affecting the temperature of the lattice. So, now lattice temperature will increase and once the lattice temperature increases this voltage will actually reduce and here there is a more issues with respect to the convergence.

So, stay the imulti step is the next current to be simulated is not the double is not two times the I 1 but is 1.4 times. So, we have reduced the step so that we can easily get a convergence, so these are the obviously simulations for the breakdown case. And this we already discussed that you know these are experimental values for the breakdown voltage for different materials germanium silicon and **(()) (33:02)** with respect to the doping.

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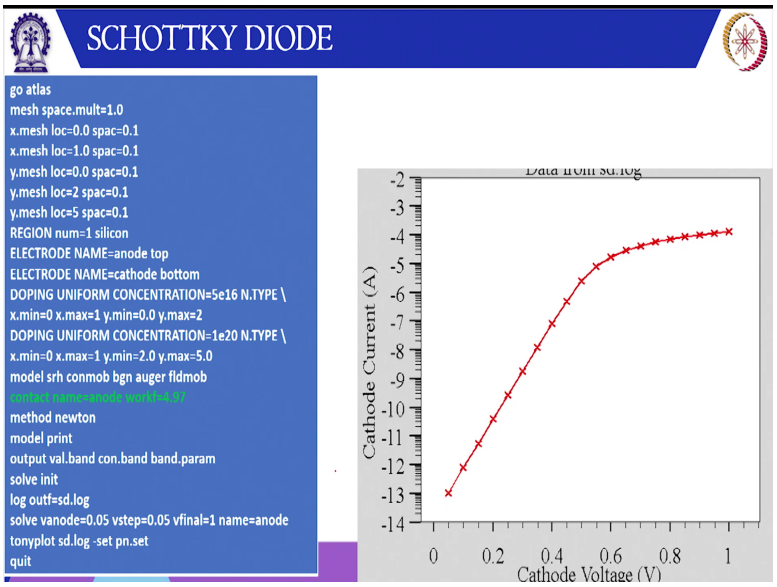

Then Schottky diode is a metal semiconductor diode this is basically the main difference is that now you have to define a Schottky contact. So, here if you see the structure is 0 to 5 is there, so it is a silicon only then anode is defined on the top cathode is defined as the bottom. So, we have not included any metal layer but for the contact anode we have to find the work function.

So, once you include the work function the contact becomes Schottky contact, it is no more ohmic contact. So, then of course when you do simulation you will get the IV characteristics of Schottky. Now you can see here that you know it start to increase for even smaller voltage, so you know for Schottky you have 0.3 or 0.4, you already have significant current basically.

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So, in this lecture we have discussed the metal semiconductor junctions partly and mostly how to get the different regions of IV characteristic for PN junction, so thank you very much.