Semiconductor Device Modelling and Simulations

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Lecture - 59
TCAD Tools

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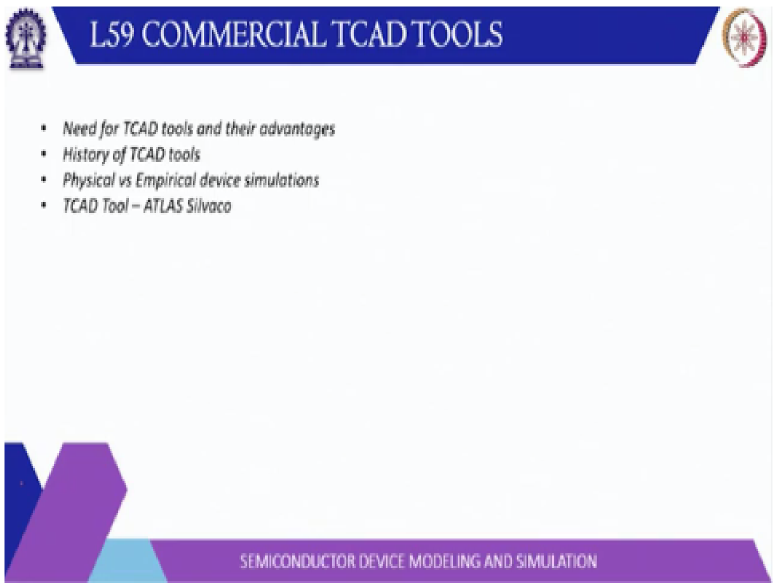

Welcome to lecture number 59. So, far we have discussed about semiconductor devices, their different models starting with the drift diffusion model hydrodynamic model then quantum transport and some solving procedures how to solve the numerical equations. And before that we discuss different types of devices such as PN junction, BJT, MOSFET. Now what we will do? There are so many governing equations there are so many models.

If you want to work on certain topic, you can develop your code. But if you want to have a comprehensive overview or comprehensive view for you know all the devices. Then there are commercial tools that are available. In this lecture we will discuss what is the need for this TCAD.TCAD refers for technology computer added design tools and their advantages, history of TCAD tools how they have developed over the years.

And then physical versus empirical device simulations and at last we will introduce Atlas Silvaco TCAD tool using which we will take some example in incoming classes.

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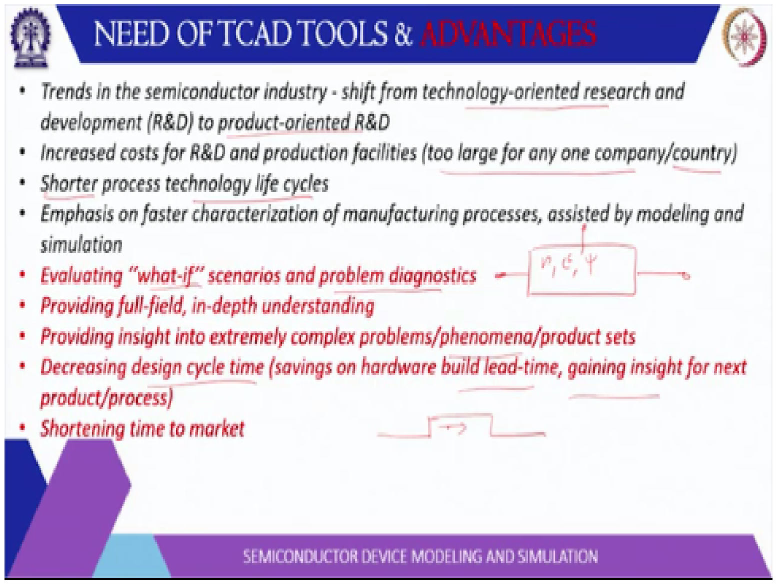

So, need for TCAD tools and the advantages. Now if you look at the focus in the semiconductor industry, they shift from technology-oriented research to product-oriented research and development. So, our product it means that the technology that is developed for the device simulation that is getting refined. But a greater emphasis is on how to use those devices to design a hardware the concerning software code to operate that hardware.

So, that it becomes a whole package starting with material, device, circuit and then you have a system. So, now the focus is basically on the system level design. Now in this process there is a cost for this research cycle than the development cycle and their requirement of production facilities. So, the requirement of this facility is actually too large for any one company or even one country because it involves the investment of several billion dollars.

So, it is not just one company which does all the job; it is basically distributed. So, there are device level company, there are the fabs, there are the circuit design company, they are the product design company so, that way is a supply chain. The purpose of this TCAD tool they sorter the process of technology life cycle. So, if you see you know every two three years a new model basically or new processor is coming in the market.

So, this is due is a result of shortened technology life cycle. Now emphasis is on faster characterization of manufacturing process assisted by modelling and simulation. So, this is basically the need of the TCAD tool and TCAD tool also offers the advantages in terms for example evaluating what if scenario and the problem diagnostic. Let us consider one device so when you have fabricate the device you can get the terminal characteristic of the device.

But you do not know what is happening inside. But the TCAD tool solves the governing semiconductor device equations and it tells you what is the carrier consultation, what is the electric field what are the potentials. So, inside you can probe that where the field is too much, where is the possibility of breakdown, where is the leakage happening all those things inside the device you can see.

So, that is basically and you can also have you know devices which are impossible to fabricate or some scenario that you want to study. So, this is all enabled by the a TCAD tool. It provides the full field in depth understanding, it also improves inside into a extremely complex problem or phenomena or some product is giving some erroneous result you can debug it also. It shortens or decreases the design cycle time.

So, it saves on hardware building time and it also provides the insight for the new product. For example, if you have this MOSFET then property of this current flow when you shorten it how it changes from diffuser transport to ballistic transport and so on. It actually gives you some idea that how the next device will be designed. So, these are the basically advantages and the need of the TCAD tool.

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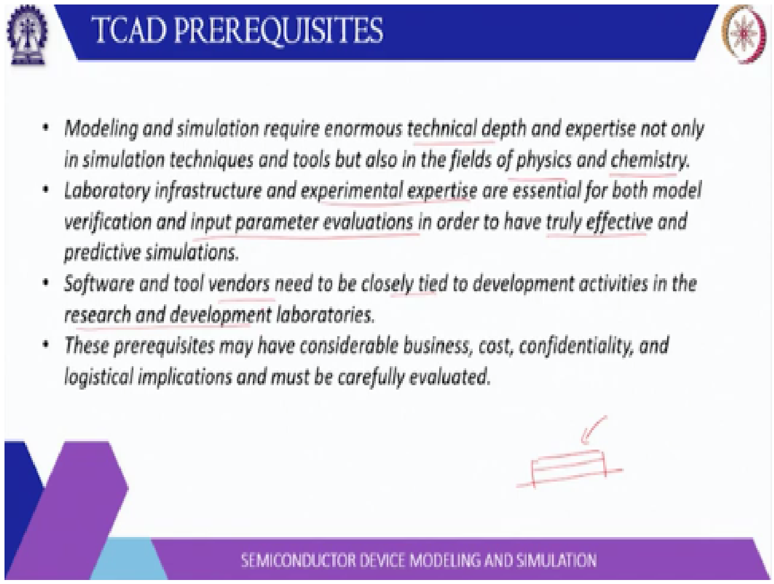

Then prerequisite, so, prerequisite for any TCAD tool basically modelling and simulation that requires enormous technical depth as we have discussed in the previous lecture and expertise not only in simulation but although in the fields of physics and chemistry. Because when you design a device, you have to start with the material then different chemical processes or physical processes to make the whole structure.

Then inside the device what equation to solve which model to consider so all these things are required basically. And to assessed the software development or the tool development laboratory infrastructure is required at least for some part and this experimental expertise are essential. So, that you can verify your model and you can fine tune the input parameters. Because these sometimes these different types of parameters are required the fitting parameters and all to have a truly effective and predictive simulation.

Of course, software tool and vendors they need to closely tie to the development activities in the research and development laboratories. So, this predicate may have considerable business, cost, confidentiality and logic logistical implications they have to be evaluated.

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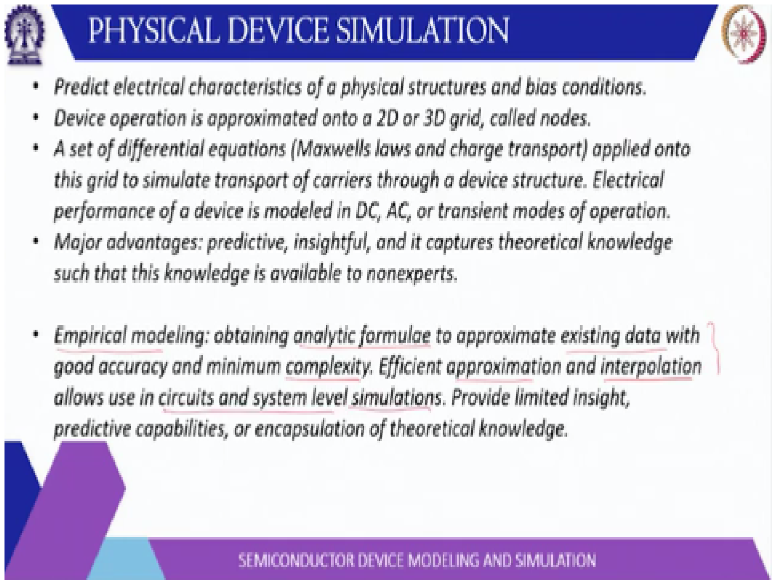

Now physical based device simulation. There are two types of the techniques that are prevalent one is physical modelling another is empirical modelling. So, in empirical modelling what we do? We obtain the analytical expression. So, that this analytical expression it approximate the existing data with good accuracy and minimum complexity and efficient approximation and the interpolation.

So, this allows these empirical models to be used in circuit and system level simulations. Because if you consider any processor in current generation, they have brilliant transistors and of course if you sit down and do the physical device simulation for the brilliant transistor it will take you know lifetime. Even more than that so physical models are not good for circuit level simulation. So, they have to use some models which are good for the empirical modelling.

So, these are the basically properties of those empirical models. But they provide a limited insight or the predictive capabilities or the theory is not there in those models basically. It is more or less like a mathematical exercise and compared to empirical model the physical device model or the physical device simulations they predict the electrical characteristic of physical structure under bias conditions and there we actually solve the governing semiconductor equations.

So, what we do? We approximate these equations; these equations are approximated on 2D or 3D grid and these are called nodes basically. And these equations so the Maxwell laws especially the

Poisson equation and the charge transport equation for example bolts when transport or continuity equation they are applied onto this grid to simulate the transport of carriers through the device structure.

Then it enables the simulation of the performance of a device for DC bias, AC bias or transient mode these are different modes in which you can do the physical device simulation. The major advantage of the physical device simulation is basically they are predictive. So, even if you are not fabricated it, they can give you the insight, they can predict the performance of the device and it of course captures the theoretical knowledge.

And using the TCAD is available to non-experts also. So, somebody who does not have the knowledge of the physical models they can also use the TCAD models.

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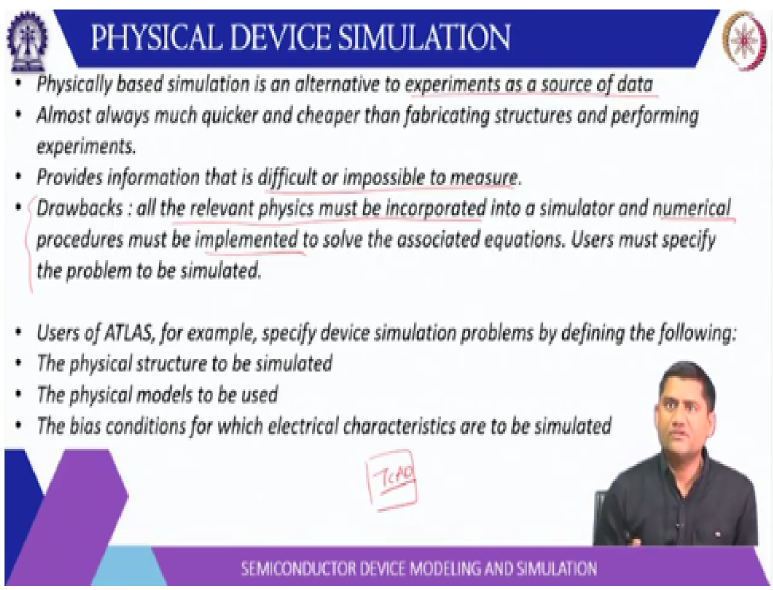

Now physically based simulation is an alternative to experiment as a source of data. So, and of course they are much quicker and cheaper than fabricating restructure and performance experiment. And provides information that is difficult or impossible to measure. And the drawback is that all the relevant physics must be incorporated. So, by mistake if you leave out any model or you do not consider any phenomena then result will be entirely different.

So, all the features must be incorporated and the numerical stimulation must be implemented to solve the associated equations and that again requires the expertise of mathematics because this equation should be solvable and there are different techniques to solve these equations. So, this two expertise are required and this two expertise are actually basically taken care of the by the TCAD tools. So, that you know different people can use this TCAD tools.

So, the purpose of this last week is basically the students should not use a TCAD tool as a black box. They should actually know what is happening inside and if they want to actually particular device, they should be aware of the relevant physics or which model to include. Although they are not required to write down the equation and solve it but they should be available that there is a model for this effect and this has to be included in certain scenario.

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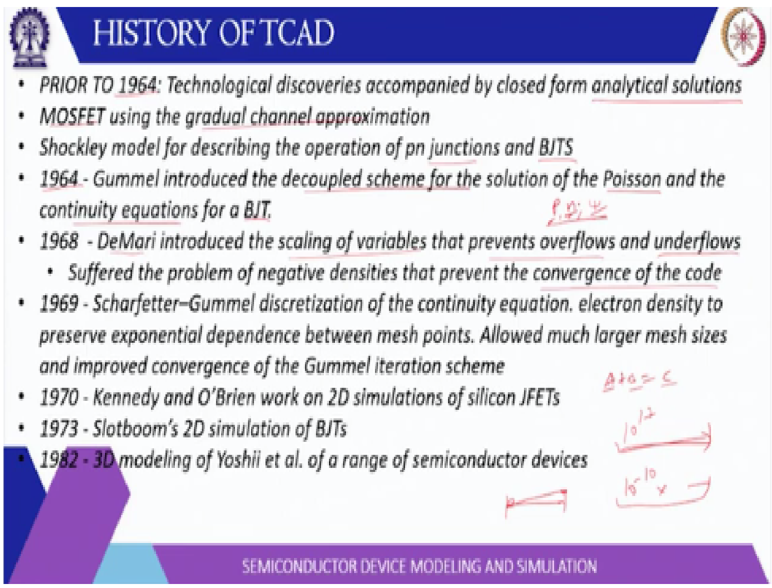

Now the history of TCAD. Prior to 1964 when the devices were discovered they were accompanied by analytical formula such as for MOSFET there was gradual channel approximation. So, ID was given by mu and c u x w by L and so on and Shockley gave a equation describing the operation of PN junction and bipolar junction transistors. Then in 1964 Gummel introduced the decoupled scheme for the solution of Poisson and the current equation for a BJT.

So, that time you know people has already started working on these numerical procedures and they were hopeful that you know the processes that are coming or going to come they will look capable enough to solve these numerical equations. Then there are some shortcomings with the very preliminary model. So, in 1968 DeMari introduced the scaling of variables that prevents overflow and underflow.

Now what is overflow and underflow? Let us say you have a number let us at 10 raise to power 17 is the carrier consultation. And if you have some multiplication of such numbers this can easily go very large and it may go beyond the storage capacity. So, that is called overflow or if the number is let us say 10 raise to power - 10 and then again you due to some reason you have some multiplication of these such terms it will go very small.

And then there may be a you know again it may not be able to fit in the finite bite size. So, this overflow and underflow this was there because if you see p the carrier consultation p and n then your potential psi so if you solve for this now p n is out of 10 raise to power 15 to 20 and psi is order of few millivolts few volts so this order of difference. So, if you write the equation then in equation let us say a + b = c.

So, these numbers are actually you know ranging from you know they have a broad range. So, this actually cause that this issues in the numerical issues. So, DeMari it is scaled it basically so it is scaled p, it is scaled n, it is scaled say that we have I think we have discussed that one in when we discuss the numerical modelling for the solving the diffusion model. So, now what happens? They support the problems on negative densities that prevented the convergence of the code.

Now negative densities appear because let us say you are this is your grid and you are approximating from one grid point to second grid point. And if you assume the linear then this p and n will change by magnitude of transverse 16 or 17. So, when you estimate it may easily go negative. So, these kinds of problems were coming. So, then you have to actually reduce the grid size to a very small value and that is not feasible because now you will have too many grid points.

So, to address this issue in 1969 Scharfetter Gummel gave a discretization of the continuity equation. There he said that between the two-grid points potential is varying linearly and because the electron and hole consultation depends on the exponential of this potential. So, this carrier concentration has to vary exponentially between two grid points. So, based on that theory he gave the discretization and that allowed a larger mesh size and improves the convergence of Gummel iteration scheme.

Then of course by 1970 Kennedy O'Brien they worked on 2D simulation of silicon junction field effect transistor. In 1973 Slotboom again they work on 2D simulation of BJT, 1980 to 3D modelling of range of semiconductor devices by Yoshii et al. So, that this were basically development continued.

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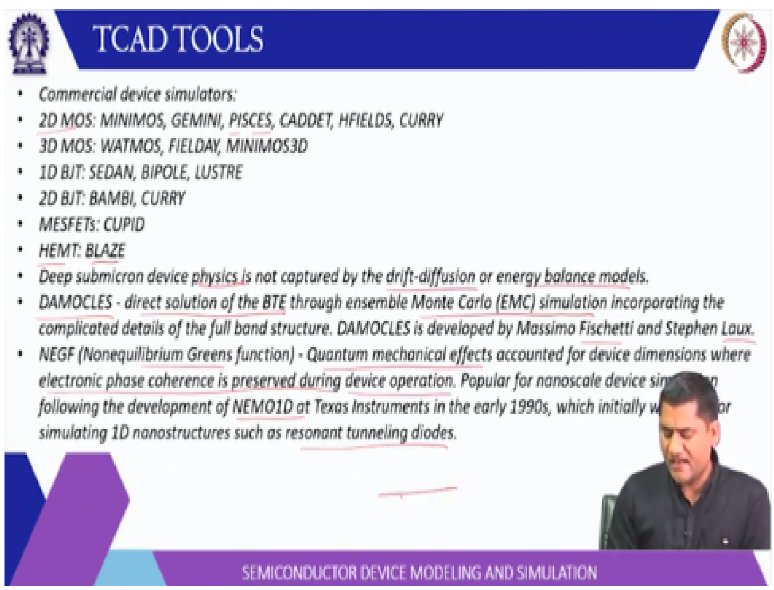

Then there are several commercial device simulators they cater to different devices. So, for 2D most structure there is MINIMOSE, GEMINI, PISCES. So, this Atlas Silvaco user process simulator then CADDET, HFIELDS, CURRY. Then 3D MOS there is a WATMOS, FIELDAY then MINIMOS 3D. For one dimensional BJT there is a SEDAN, BIPOLE, LUSTRE then 2D BJT BAMBI and CURRY.

For MESFET there is a CUPID, for HEMT there is a BLAZE simulator. So, this BLAZE is also used in Atlas Silvaco. So, Atlas Silvaco is basically kind of umbrella which houses these softwires for different devices. Then deep sub-micron devices their physics is not captured by the drip diffusion or the energy balance model. So, you have to go for higher order models and one is this ensemble Monte Carlo simulations that we have discussed.

So, it solves directly the Boltzmann transport equation. So, you choose some number of carriers and you track them basically and then based on that construct the probability distribution curve. So, this software is DEMOCLES which basically solves the Boltzmann transport equation for through Monte Carlo simulation and it was developed by Fischetti and Laux. Then for quantum simulations there is a non-equilibrium greens function.

So, this basically takes into account the quantum mechanical effect accounted for device dimension. And there is another one the popular for non-scale device simulation is following the development of NAMO1D at Texas instrument in early 90s which was initially used for simulating 1D nanostructure such as resonant tunnelling diode. Then this quantum mechanical devices device simulation is used when electronic phase coverage length is preserved during device operation.

That means the length scales are you know order of the space coherence length. So, this presence length can all this we have discussed in one of the lecture.

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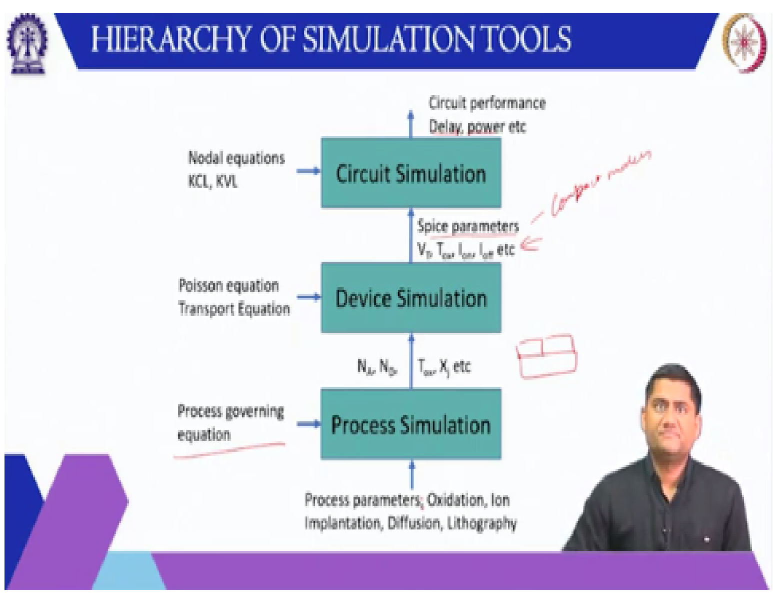

Now this is the hierarchy of different simulation tools. So, there is a process simulation, it solves the process governing equations and the input can be the process parameters such as oxidation, iron implantation, diffusion, lithography. So, all those physical processes then at the end you have a structure with the dimensions with the doping and different junction thickness, oxide thickness all those and that is the input to the device simulation.

So, in device simulation we solve the Maxwell Poisson equations and the transport equations and then this gives you the parameters of the device, device parameters. So, for example for MOSFET your threshold voltage, oxide thickness, on current, off current and they are used by spice simulators. So, this is like basically you have some you have analytical models here or you have compact models here they are given to the circuit.

So, in circuit these nodal equations Kirchhoff current, Kirchhoff voltage the salt to obtain the circuit performance. So, circuit performance is characterized by the what is the power consumption what is the delay you know propagation delay all those characters are calculated.

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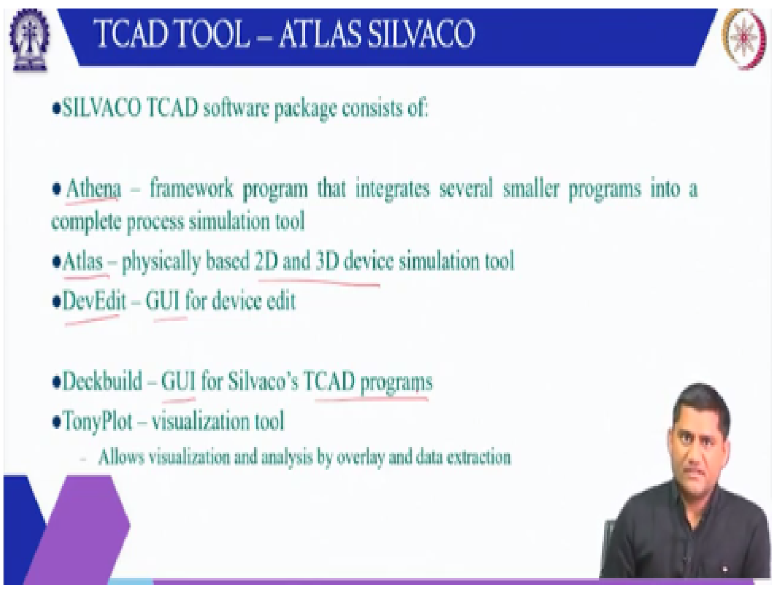

Now let me introduce the SILVACO ATLAS TCAD tool. So, this SILVACO TCAD software is consists of a process simulator which is Athena. So, it is a framework program so which integrates several small programs. So, there is a program for oxidation simulation, there is a program for diffusion, there is program for iron implantation. So, they are you know inside this framework program Athena.

Then there is a similar program for device simulation that is Atlas and it is used for physically based simulation of 2D and 3D devices. Then there is a Dev Edit which is graphical user interface for editing the device structure. Device structure consists of the dimensions, dopings and contacts. Then there is a Deck build which is the graphical user interface for SILVACO to use the TCAD programs.

Then once you have run the TCAD program you have obtained the output. So, to visualize the output there is a Tony plot so this is a visualization tool. So, it also allows the visualization analysis of overlay and data extraction.

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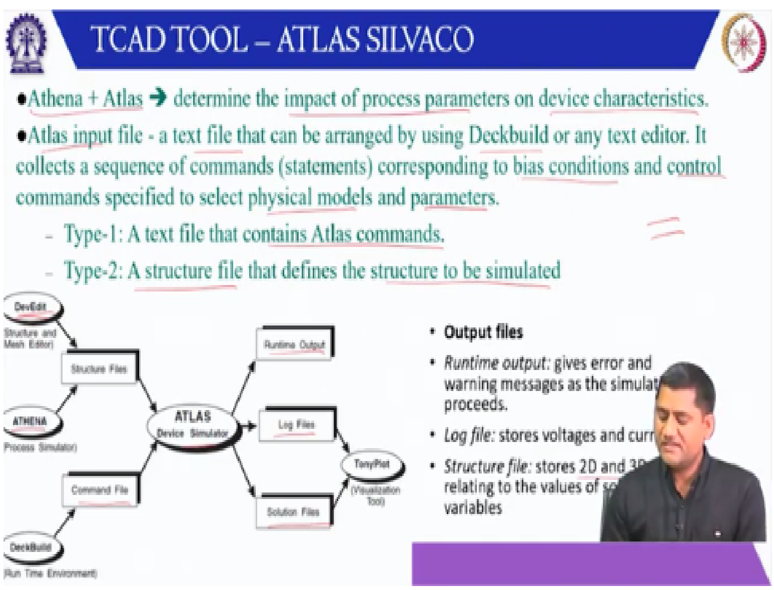

Now if you use Athena + Atlas then you can determine the impact of process parameters on the device characteristic. So, it is basically like a holistic approach and the input file for the Atlas it consists of this is a text file which is you know you can type in the Deck build or you can type in any text editor. It is a sequence of commands like MATLAB, it is a sequence of commands basically.

So, these commands they correspond to certain bias condition, the control commands specify just select the physical models and the parameters. So, either you can have a text file that contains all the Atlas commands or you can create a structure file using the Dev edit and then you can simulate it for a different bias condition all. So, this structure file you can obtain from the Dev Edit or from the Athena the process simulator or you can write the commands to get this structure file and this is input to the device simulator.

Then when you run this device simulator you get basically three types of output. So, one is the runtime output which basically you know goes through every command and tells you the status of the command. If there is a warning, error message all those things are listed here and if the simulation does not converge it is also a state if it does not converge then whether the potential step is reduced or what is done that is also mentioned.

So, runtime log basically contains all the information related to the running of the code. Then there are log files that are specified in the code they store the IV relationship. So, for a given device if you change the bias voltage what is the current or if you have current boundary condition you change the current different values of current what is the values of voltage you get. So, these are stored in the log file.

Then for each simulation there is a structure file that of course if you want to say if you then the latest run is actually saved. So, it stores a 2D and 3D data related to the values of solution variable.

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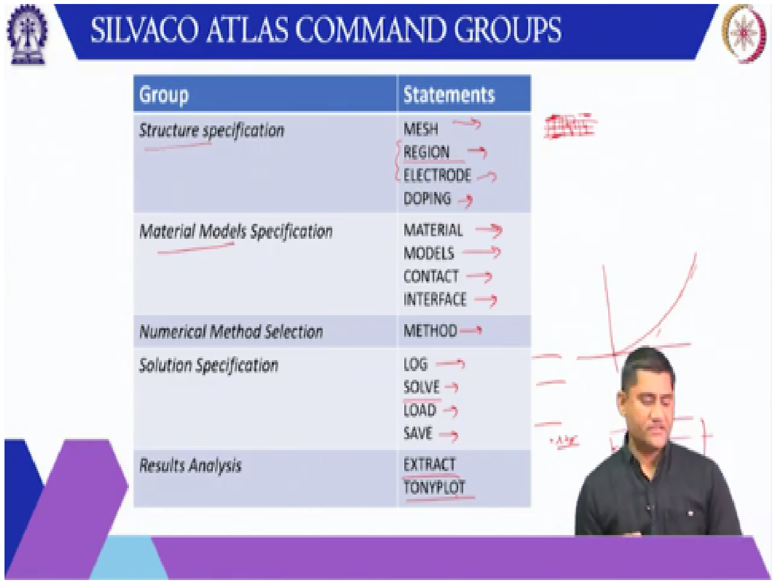

There are five command groups. So, first group is the structure specification so to specify the structure and it begins with the MESH. So, you have to first define the MESH then in the MESH every point has to be as uncertain region. So, this is less silicon this is silicon dioxide and so on so this region has to be assigned then the contacts or the electrodes have to assign. Let us say anode, cathode or source drain gate and then you have to also expect.

So, this region and this electrode is also one kind of region basically then you have to define the doping. So, what are the doping level in each region then once you define the doping so for region let us say you expect the material. So, you can change the material properties so that is done through the material model specification. So, material properties can be specified here. Let us say you have this describe a material what is a band gap, what is effective mass, what is the you know second band gap and so on or whether it is a direct, indirect band gap.

So, other parameters also can be specified. What is a lifetime then the models that are used in solving the concerning the governing equation whether you are using division model or the hydrodynamic model so or you are using the impact organization model. So, these models can be specified under model statement. Then you have to specify the nature of the contacts, it is a ohmic contact or it is an interface with some charge, what is the charge density or is a Schottky contact, what is the work function of the metal and the interface properties.

So, these are specified through the material model specification. Then of course you can choose the method, default is Newton method which has quadratic convergence and but you can choose the Gummel method, block metal method or Newton method. Then once you choose the metal then you basically define list the LOG file that you name the LOG file where you want to store the current voltage values.

Then after the special LOG file you can write a solve statement and that gives you the data from the simulation. Let us say you want to have multiple runs of the simulation then you can load one structure file again do commands and then again create a log file. So, you can basically create multiple log files. So, between one LOG file and two LOG file you have to write LOG of so LOG of the list of that previous log file and then you can use a second LOG file.

And then of course for a particular solution you can also solve the SAVE the structure file. So, it will save that dot str file. You can also extract the data related to the structure or related to the performance let us say you have this IV curve; you can extract out the threshold voltage. If you have this structure this unless p doping is there then n doping is there so it can basically extract out the junction depth and so on and you can also plot them in TONYPLOT. So, these are the main groups.

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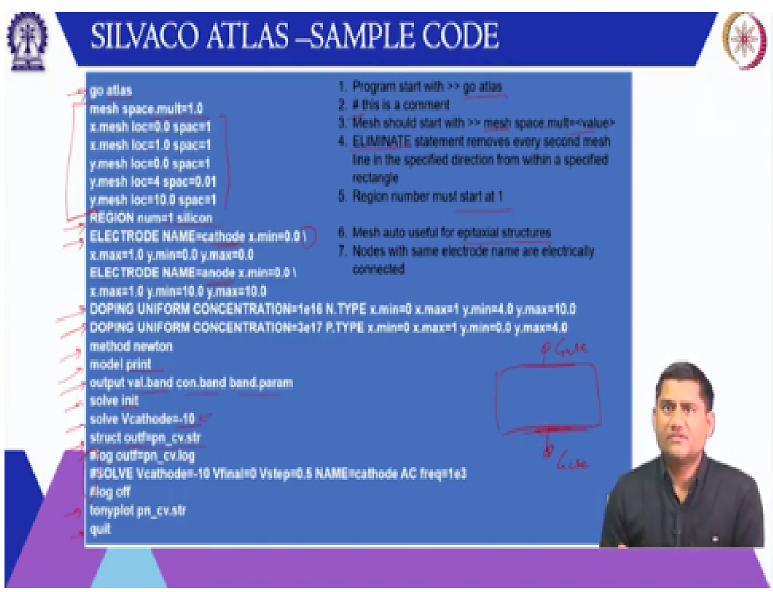

So, this is one sample program. Here I can show you all the regions. So, it is start with the go Atlas so there is a first command that means you are invoking the Atlas simulator or the device simulator. Then this first region is the mesh specification then this is the REGION here then there is ELECTRODE here. Now this is basically continuity of the command. So, this electrode command is continued to the two lines and then this is the cathode, this is anode then there is a doping.

So, this material qualities the doping is specified then there is a method then there are models. Here I am not include any model it just print. Print basically in the runtime LOG it will print all the data that is used in the simulation. So, this is the purpose of this print model. So, no other models are used that means all the default models are used in the simulation. Then output basically tells you what are the parameter you want to see.

So, here I have written the valence band, conduction band and the other band parameters then solving it solves for all the terminals set to zero volt. So, there are two terminals here anode and cathode and both are zero so that is solving it. Then of course you can solve weak cathode for minus ten volt then you can for this solution you have this structure file p n underscore cv dot str. This is a name you can use any arbitrary name so this save the structure file.

So, this is structure file has all the information about this solution at - 10 volt then hash means these are commented. So, this code is not executed. Then TONYPLOT again plots this structure file and this quit means it ends the simulation. So, there are few salient point program must start with go Atlas and ash it is a command and start with a mesh command, mesh space mult basically tells you whether you want to have a **(()) (28:19)** mesh or the fine mesh.

So, bigger the number coerce are the mesh and smaller the number less than one then this great that you specify here is basically doubled basically. There is another command eliminate so if you get the mesh from the simulation then you can basically re mesh it. And if there is some extra mesh then you can eliminate those some of the mesh points there is also possible. And the region number here is there is only one reason but it can go up to you know a large number.

So, it must start with one so region number has to start with one and then mesh is auto for useful for epitaxial structure and nodes that with the same electron name are electrically connected. So, let us say your this is a restructure and let us say dual gate some time thing. So, this is again this is one gate to write. So, if you name it let us say this is also named as gate, this is also named at gate. So, that means these both are electrically connected.

So, we specify any voltage this both terminal will get the same volt. So, that is a meaning of it is electrically connected. So, if you specify the same name then they will be electrically connected.

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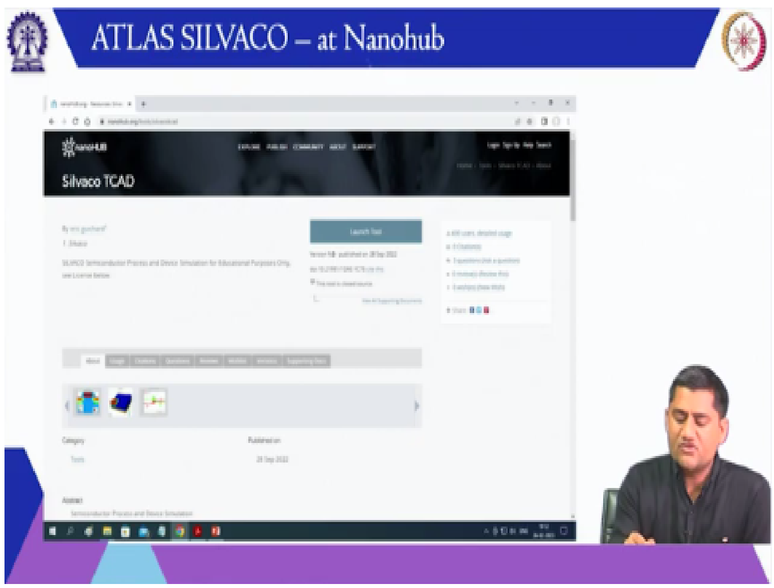

Now for your information this ATLAS SILVACO is also available at Nanohub. So, you go to this URL nanowup.org silvaco TCAD then you click the launch tool.

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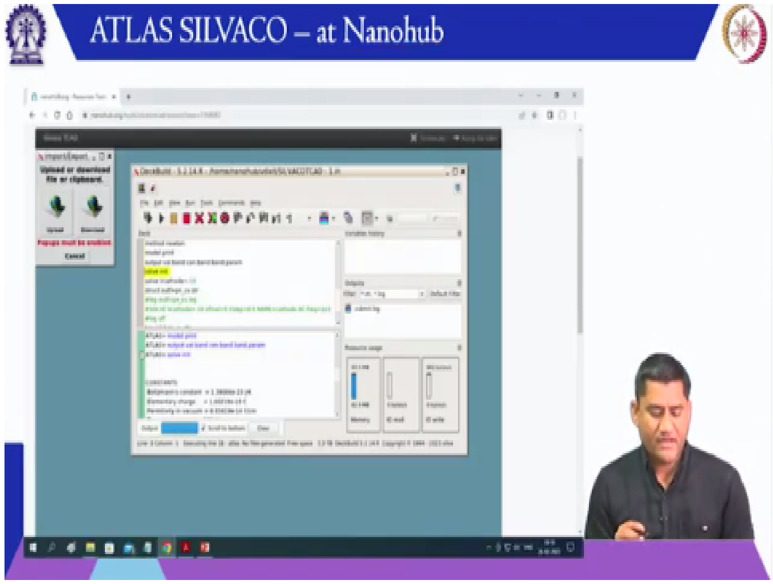

So, when you clock it, you can type your program here and then you can run it. But there is some issue of this license is there. Not all the time you will get the license but sometimes you are lucky you can get the license and you can also upload the file download the file that facility is there.

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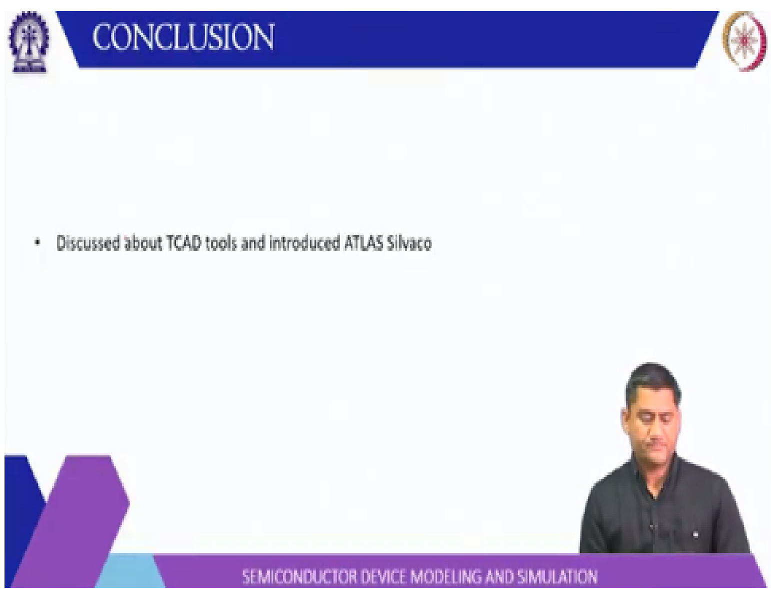

So, in this lecture we have discussed some of the TCAD tools and introduce the ATLAS SILVACO. In next lecture we will give the overview of how to use SILVACO and then we will take up the examples from the theory that we have discussed. Thank you very much.