Semiconductor Device Modeling
Prof. Shreepad Karmalkar
Department of Electrical Engineering
Indian Institute of Technology – Madras

Lecture - 16
Drift-Diffusion Transport Model: Equations, Boundary Conditions, Mobility and Generation / Recombination

In today's lecture, we are beginning a new model.

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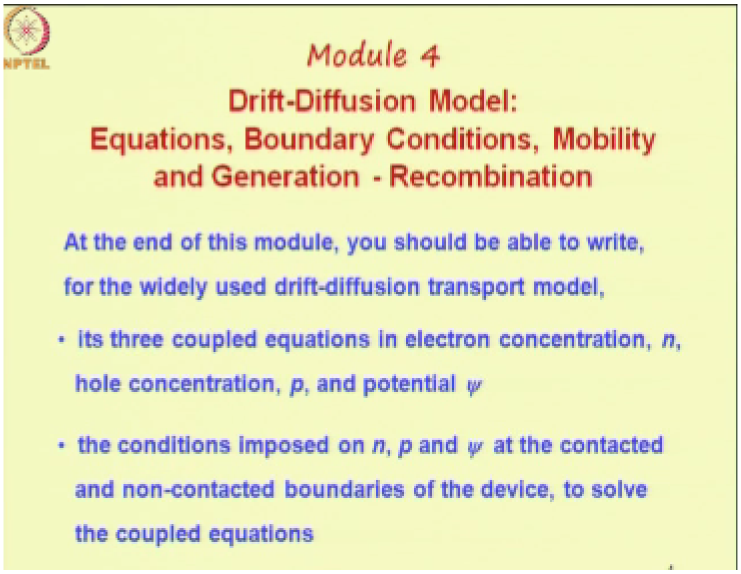

Module 4

Drift-Diffusion Model:
Equations, Boundary Conditions, Mobility and Generation - Recombination

At the end of this module, you should be able to write, for the widely used drift-diffusion transport model,

- its three coupled equations in electron concentration, *n*, hole concentration, *p*, and potential ψ
- the conditions imposed on *n*, *p* and ψ at the contacted and non-contacted boundaries of the device, to solve the coupled equations

This model is on the widely used Drift-Diffusion model diffusion model. For this model we will be discussing the Equations, Boundary Conditions, Mobility and Generation-Recombination mechanism. So we will discuss a formula for these quantities. At the end of this module you should be able to write for the widely used Drift-Diffusion transport model. It is ix coupled equations in electron concentration, n, hole concentration p, and potential Psi.

You should be able to write the conditions imposed on n, p and Psi at the contacted and non-contacted boundaries of the device to solve the coupled equations.

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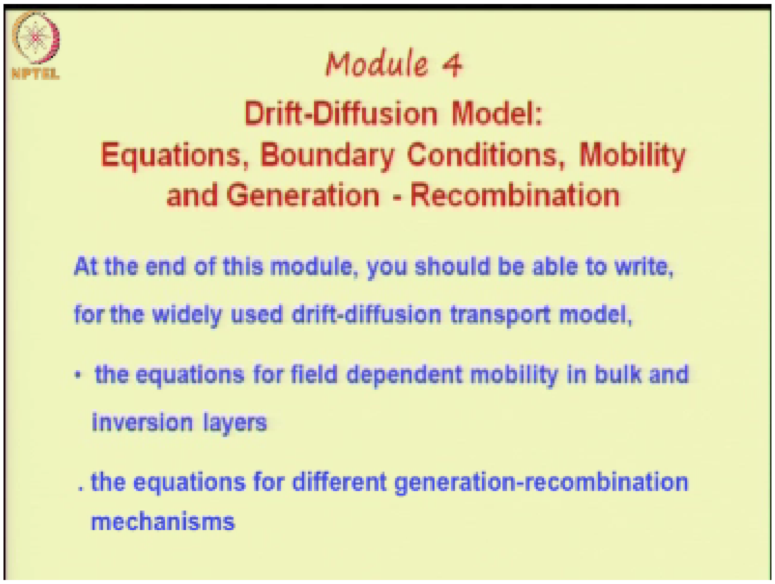

Module 4

**Drift-Diffusion Model:
Equations, Boundary Conditions, Mobility
and Generation - Recombination**

At the end of this module, you should be able to write, for the widely used drift-diffusion transport model,

- the equations for field dependent mobility in bulk and inversion layers
- the equations for different generation-recombination mechanisms

Then you should be able to write the equations for field dependent mobility in bulk and inversion layers. And finally, you must also be able to write the equations for the different generation-recombination mechanism.

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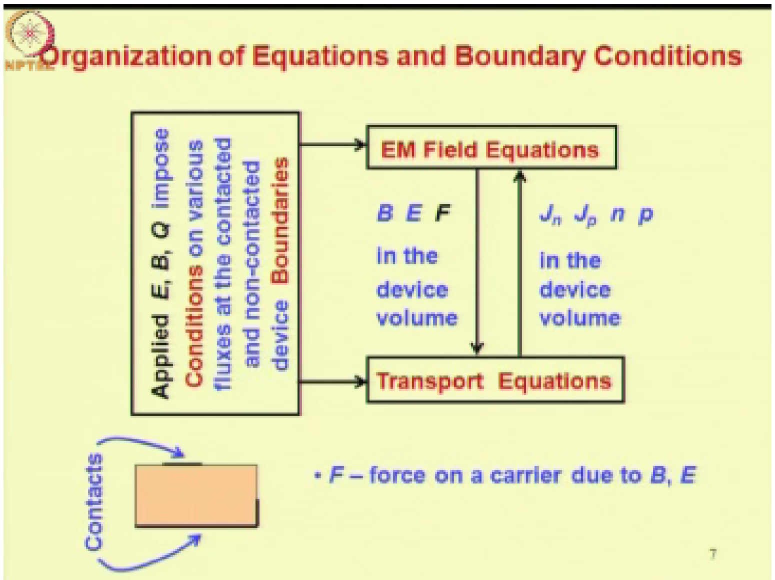

Organization of Equations and Boundary Conditions

Applied E, B, Q impose Conditions on various fluxes at the contacted and non-contacted device Boundaries

EM Field Equations

B E F in the device volume

J_n J_p n p in the device volume

Transport Equations

Contacts

- F – force on a carrier due to B, E

So let us look at the organization of the equations from the previous module. So you have the Electromagnetic field equations fielding into the transport equations. The information about B, E and the Force F on the electron due B and E and the transport equation yielding the current density of electrons and holes and the carrier concentration of electrons and holes. Now this information is fit into the Electromagnetic equations to get the solutions of B E and F.

And then the equations are solved subjected to some boundary conditions on E, B and heat flux Q at the boundaries of the device.

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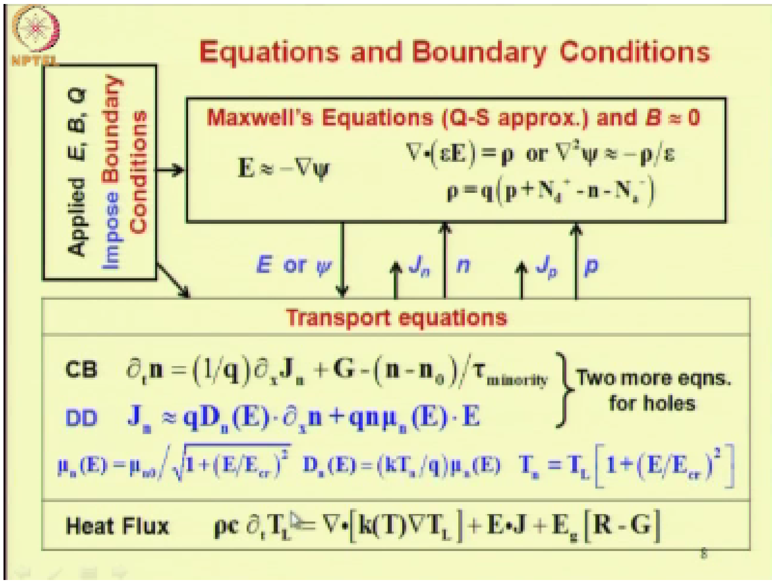

Equations and Boundary Conditions

Applied E, B, Q

Impose Boundary Conditions

Maxwell's Equations (Q-S approx.) and $B \approx 0$

$$\mathbf{E} \approx -\nabla\psi \qquad \nabla\cdot(\varepsilon\mathbf{E}) = \rho \text{ or } \nabla^2\psi \approx -\rho/\varepsilon$$

$$\rho = q\left(p + N_d^+ - n - N_a^-\right)$$

Transport equations

CB $\partial_t n = (1/q)\partial_x J_n + G - (n - n_0)/\tau_{minority}$

DD $J_n \approx qD_n(E)\cdot\partial_x n + qn\mu_n(E)\cdot E$

Two more eqns. for holes

$\mu_n(E) = \mu_{n0}/\sqrt{1+(E/E_{cr})^2}$ $D_n(E) = (kT_n/q)\mu_n(E)$ $T_n = T_L\left[1+(E/E_{cr})^2\right]$

Heat Flux $\rho c\, \partial_t T_L = \nabla\cdot[k(T)\nabla T_L] + E\cdot J + E_g[R - G]$

Now the Drift-Diffusion equations which we arrived at in the previous module are repeated here. When we use the term Drift-Diffusion model it incorporates not only the equations on Drift and Diffusion current but also all the other equations which are used together with this equation to derive the current and as a function of voltage for a device. Therefore, while the Drift-Diffusion equations are only those which are shown here in blue color.

The equations of the Drift-Diffusion model would incorporate all the equations that are shown here such as the Maxwell's equations under the Quasi-Static approximation and Negligible Magnetic Field and the Carrier Balance equation and also the equation of Heat flux. Similarly, we will also include equations for holes apart from the equations for electrons. Thus, you find that the Drift-Diffusion model will consist of 2 of these equations = - gradient of Psi and diversions of Epsilon E = Rho or delta square Psi = -Rho/epsilon.

So 2 of these equations. Then, Carrier Balance equation and Drift-Diffusion equation. For electrons as well as holes so that makes it 4 more and then the equation for heat flux. So you have 2+4+1, so the 7 equations in total. Now very often, we do not use the heat flux equation. Now that leaves us with 6 equations.

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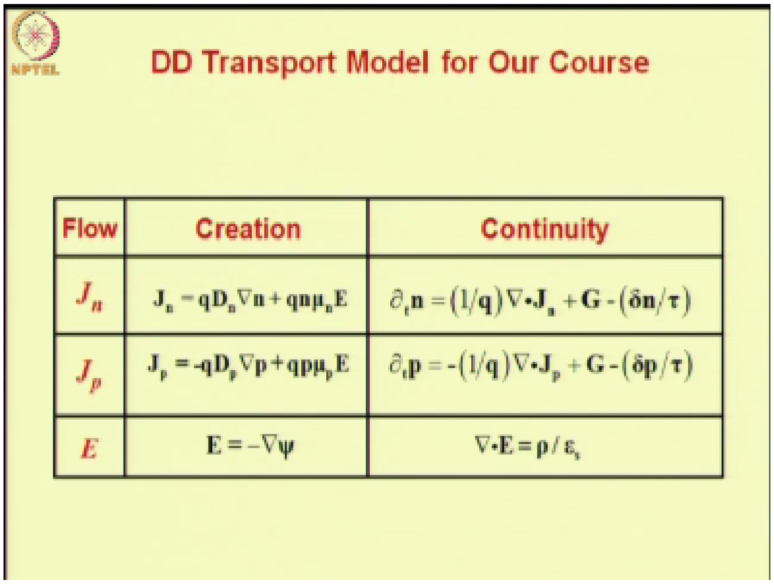

DD Transport Model for Our Course

Flow	Creation	Continuity
J_n	$\mathbf{J}_n = q\mathbf{D}_n\nabla n + qn\mu_n\mathbf{E}$	$\partial_t n = (1/q)\nabla \cdot \mathbf{J}_n + G - (\delta n/\tau)$
J_p	$\mathbf{J}_p = -q\mathbf{D}_p\nabla p + qp\mu_p\mathbf{E}$	$\partial_t p = -(1/q)\nabla \cdot \mathbf{J}_p + G - (\delta p/\tau)$
E	$\mathbf{E} = -\nabla\psi$	$\nabla \cdot \mathbf{E} = \rho / \varepsilon_s$

These 6 equations are shown here and they have been organized into 2 sets, one set that we can call as flow creation equation and another set that we can call as flow continuity equations. So for instance, the equations of Jn, Jp and electric field shown in this column are referred to as creation because they talk about how the flow is created.

For instance, equation for Jn here says that the electron current density is created by the diffusion and drift, same is true for the hole current density here. And similarly, this equation tells you that the electric field E is created by a potential gradient. The Continuity equations, on the other hand, talk about conservation of quantities during flow. The continuity equation for electrons is the things that the Carrier Balance equation for electrons.

And similarly, the continuity equation for holes is a carrier balance equation for holes. And as we have already argued in the previous module the equation of Gauss's Law is also an equation of conservation of electric flux. Commonly the equations of Jn and Jp involving the creation of these current densities and continuity of electron and hole concentrations are refer to as transport equations.

Now, I would like to point out that the excess concentrations of electrons and holes are shown here using separate symbols because in general a semiconductor may not be neutral, so excess electron concentration at a point can be different from the excess hole concentration. Though if you take the device as a hole it will be neutral but at local points there can be space charge. So the positive space charge at one point of the device maybe compensated by negative space charge at other points to provide an overall neutrality.

However, the generation rate of electron hole pairs G is the same in both these equations, okay the Hole Continuity equation and the Electron Continuity equation. The set of equations related to the electric field are called Electrostatic equations. Because these equations are derived assuming that there is no time varying electric field and there is no time varying magnetic field that is why these are referred to as static equation, so Electrostatic.

You obtain the current voltage characteristic by integrating the current density J which is nothing but the some of the electron current density and hole current density, so integrating the current density J over any contact area dS is the contact area then you get the current. And similarly, you get the voltage across a device or potential between the 2 points, 2 terminals by integrating the electric field from one end one contact to the other contract.

So dL is a line moving from one contact to the other contact. Often, the equations of Jn and Jp are referred to as current density equations and those equations of carrier balance the electron balance and the whole carrier balance that is dou n/dou t and dou p/dou t equations involving these are refer to as continuity equation. And this equation is the Gauss' law diversions of E = Rho/epsilon.

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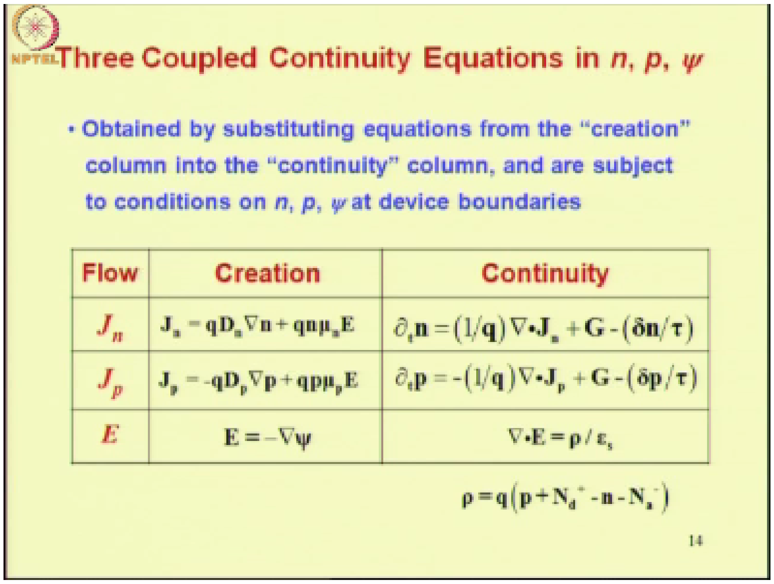

Three Coupled Continuity Equations in *n*, *p*, ψ

- Obtained by substituting equations from the "creation" column into the "continuity" column, and are subject to conditions on *n*, *p*, ψ at device boundaries

Flow	Creation	Continuity
J_n	$\mathbf{J_n = qD_n \nabla n + qn\mu_n E}$	$\partial_t \mathbf{n} = (1/q)\nabla \cdot \mathbf{J_n} + G - (\delta n/\tau)$
J_p	$\mathbf{J_p = -qD_p \nabla p + qp\mu_p E}$	$\partial_t \mathbf{p} = -(1/q)\nabla \cdot \mathbf{J_p} + G - (\delta p/\tau)$
E	$\mathbf{E} = -\nabla\psi$	$\nabla \cdot \mathbf{E} = \rho / \varepsilon_s$

$$\rho = q\left(p + N_d^{\,+} - n - N_a^{\,-}\right)$$

Now, though we have 6 equations ultimately they can be reduced to just 3. So in a sense actually in the Drift-Diffusion model there are just 3 coupled equations and this are continuity equations in n, p and Psi. So how do you get this? So these equations are obtained by substituting the equations from the Creation column into the Continuity column and are subjected to conditions on n, p and Psi at device boundaries.

So you take the equation for Jn from this column and put this equation for Jn here in the continuity equation in the diversion of J in term. Now Jn is given in terms of the carrier concentration and the electric field, the electric field is in turn is dependent on the potential Psi. So if I combine this equation the equation for Jn and substitute it here ultimately I will get an equation for n in terms of Psi and other quantities.

Same thing I can do for Jp, I take Jp and substitute it here in the whole continuity equation and finally I take this equation e grad Psi and put it here in the Gauss' Law I get the Poisson's equations in Psi; that is how I will reduce the 6 equations into just 3 coupled equations. So ultimately I need to solve only these 3 coupled equations for getting the device current as a function of voltage that is what most of the simulators which are based on the Drift-Diffusion model, they do.

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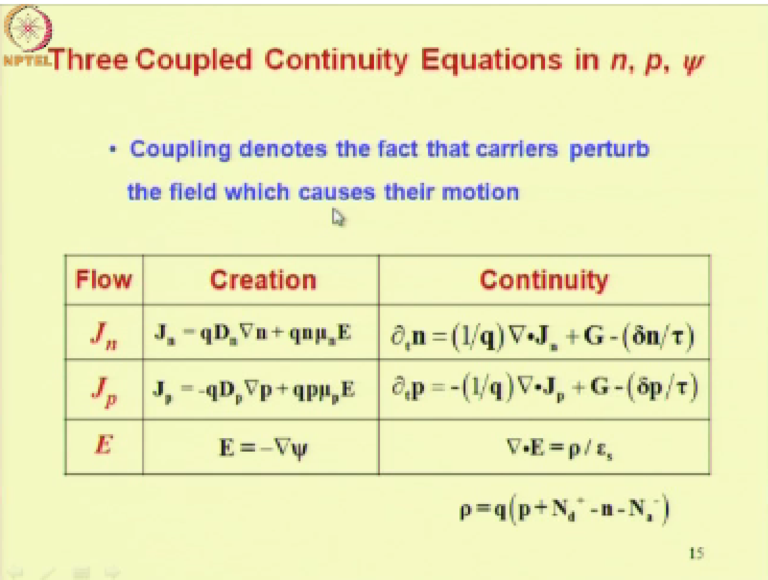

Three Coupled Continuity Equations in *n*, *p*, *ψ*

- Coupling denotes the fact that carriers perturb the field which causes their motion

Flow	Creation	Continuity
J_n	$\mathbf{J_n = qD_n \nabla n + qn\mu_n E}$	$\partial_t \mathbf{n} = (1/\mathbf{q})\nabla\cdot\mathbf{J_n} + \mathbf{G} - (\delta\mathbf{n}/\tau)$
J_p	$\mathbf{J_p = -qD_p \nabla p + qp\mu_p E}$	$\partial_t \mathbf{p} = -(1/\mathbf{q})\nabla\cdot\mathbf{J_p} + \mathbf{G} - (\delta\mathbf{p}/\tau)$
E	$\mathbf{E} = -\nabla\psi$	$\nabla\cdot\mathbf{E} = \rho/\varepsilon_s$

$$\rho = q\left(p + N_d^+ - n - N_a^-\right)$$

Now, what is the physical meaning of mathematical coupling, so when we say these equations are coupled the coupling denotes the fact that carriers perturb the field causes their motion. So the motion of carriers is because of the field but as the carriers move they redistribute the concentration and the redistribution of the concentration sets up a space charge and this space charge creates an electric field according to the Gauss' Law, so that is how it is a coupled situation.

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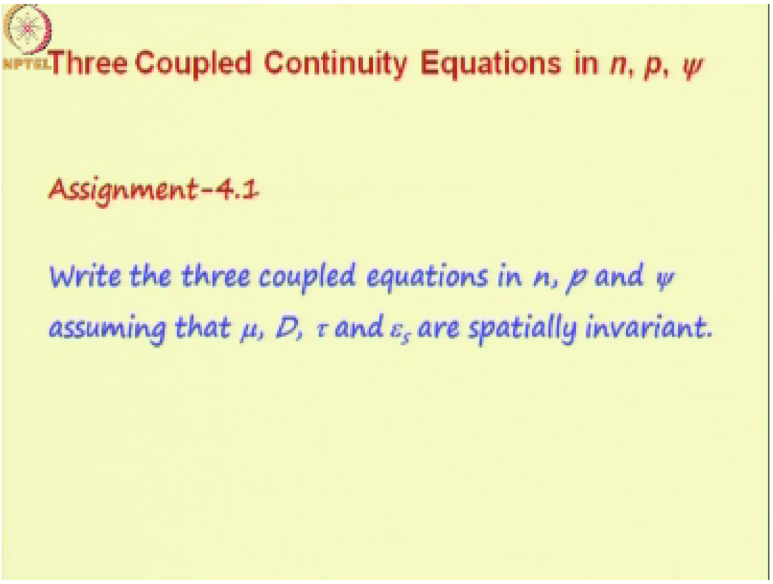

Three Coupled Continuity Equations in *n*, *p*, *ψ*

Assignment-4.1

Write the three coupled equations in *n*, *p* and *ψ* assuming that *μ*, *D*, *τ* and ε_s are spatially invariant.

Now, we have written down the 3 coupled equation I am leaving it to you as an assignment. Write the 3 coupled equations n, p and Psi assuming that the mobility's of electrons and holes mu, the Diffusion coefficient of electrons and holes D, the lifetime of minority carriers and the dielectric constant of the semiconductor epsilon s are spatially invariant.

Now in the previous module we had used the symbol epsilon for the dielectric constant of the epsilon semiconductor, in this module we are putting a suffix s because we will encounter a dielectric constant of the ambient that is the surrounding of the device and that we will denote as a epsilon suffix a to distinguish and to have clarity on which dielectric constant we are referring to; we are using a suffix s for the semiconductor dielectric constant.

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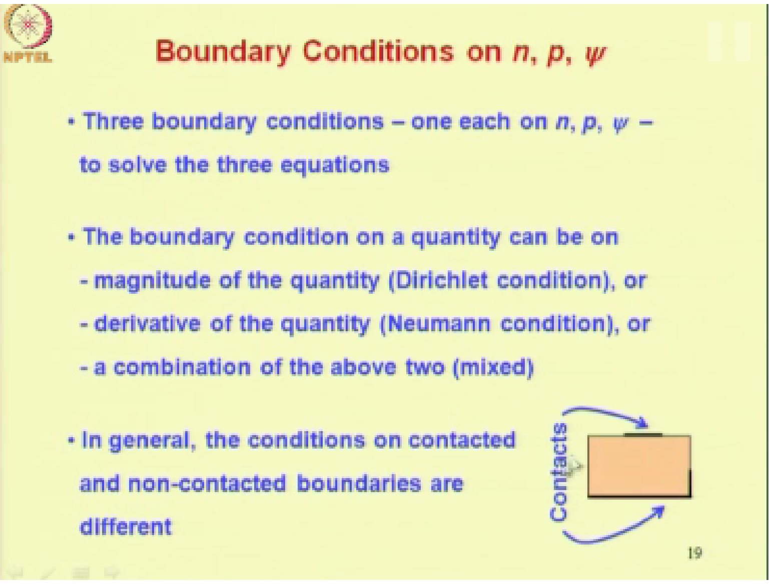

Boundary Conditions on *n*, *p*, ψ

- Three boundary conditions – one each on *n*, *p*, ψ – to solve the three equations
- The boundary condition on a quantity can be on
  - magnitude of the quantity (Dirichlet condition), or
  - derivative of the quantity (Neumann condition), or
  - a combination of the above two (mixed)
- In general, the conditions on contacted and non-contacted boundaries are different

Let us look at the boundary conditions on n, p and Psi. So, the 3 boundary conditions one each on n, p and Psi are required to solve the 3 equations. Now, the boundary condition on a quantity suggest n or p or Psi can be on either the magnitude of the quantity, now such a condition is called Dirichlet condition or the derivative of the quantity such a condition is called the Neumann condition or a combination of the above 2.

So the combination of the above 2 would be referred to as a mixed condition. In other words, we are saying the boundary condition can be on n, p and Psi or gradient of n, gradient of p and gradient of Psi or on a combination, so you can have a boundary condition on n on the electron concentration which is given in terms of an equation which consists of both n as well as gradient, right. So that is the mixed condition.

In general, the conditions on contacted and non-contacted boundaries are different. So here is conceptual device showing the contacts and the non-contacted boundaries.

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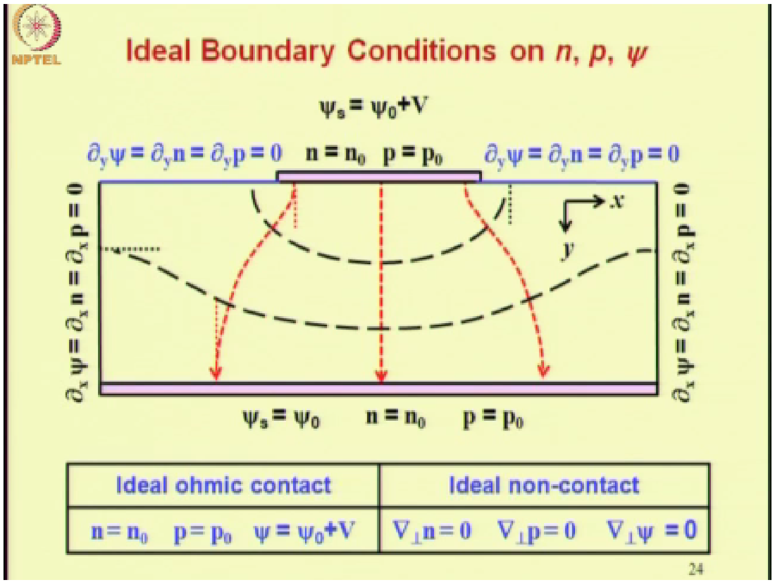

Ideal Boundary Conditions on *n*, *p*, *ψ*

$\psi_s = \psi_0 + V$

$\partial_y \psi = \partial_y n = \partial_y p = 0$ $\quad n = n_0 \quad p = p_0$ $\quad \partial_y \psi = \partial_y n = \partial_y p = 0$

$\partial_x \psi = \partial_x n = \partial_x p = 0$ $\quad \partial_x \psi = \partial_x n = \partial_x p = 0$

x

y

$\psi_s = \psi_0 \quad n = n_0 \quad p = p_0$

Ideal ohmic contact	Ideal non-contact
$n = n_0 \quad p = p_0 \quad \psi = \psi_0 + V$	$\nabla_\perp n = 0 \quad \nabla_\perp p = 0 \quad \nabla_\perp \psi = 0$

Let us look at Ideal Boundary Conditions on n, p and Psi. This we shall illustrate with the help of an example. So let us say you have a uniform semiconductor block with a short contact on the top surface and a contact covering the entire bottom surface. Okay. And you are applying a voltage between these 2. This situation is referred to as a spreading resistance, right because the current spreads from a smaller contact to a larger contact.

Now at the contacts the ideal conditions on n, p and Psi are the carrier concentrations are uniform at their equilibrium values. So you see here n = n0, p = p0 so uniform concentration at this end wherever you have the contact. Similarly, you have uniform concentration equal to the equilibrium concentration at the bottom contact as well n = n0, p = p0. The potential is assumed to be uniform, so uniform potential. Like the uniform concentration.

At the top contact the potential is assumed to be Psi s = Psi not+V so s here refers to the surface. Okay. So Psi s is nothing but the potential at the semiconductor surface. This is equal to a built-in potential + applied voltage. Since in general the semiconductor maybe non-uniform, there can be a built-in potential. So that is also incorporated here, so V is Applied voltage.

Now as again this, the bottom surface the potential is equal to the just the built-in potential because we are assuming the applied voltage is 0 so bottom is the reference. Now what implications do these boundary conditions have? Let us for example draw the flow lines in the device which show the current flow. So you find that the flow lines eminent perpendicular to the contact surface.

So here the flow line is perpendicular and here also the flow line is perpendicular. Current is flowing from top contact to bottom contact. Now fact that the flow line emanates emerges perpendicular to the contact surface is because of the conditions that we have imposed. Since potential is uniform the electric field at the surface can only be in the vertical direction or in the y direction. There can be no electric field in the x direction because if any electric field in the x direction would mean potential along the contact is not uniform.

Similarly, since we have assumed that the carrier concentration is uniform there can be no carrier concentration gradient in the x direction. Okay. So any gradient has to be in the y direction therefore even if there are diffusion currents in addition to drift currents the sum total of this currents will be in the direction perpendicular to the surface, so in the y direction only. So that is how the boundary conditions have a bearing on the way the flow emerges from the contact or terminates into the contact.

Let us look at the non-contact boundaries. Now here, you have Neumann condition or the condition on the derivatives of the quantities. So at the contact, the conditions Dirichlet because they were on the values of the magnitudes of the quantities. For example, let us take this non-contact surface what you are saying is that the potential gradient along the y direction that is along vertical direction is 0 at this boundary this means no electric field either enters or leave the surface normal to the surface.

Similarly, no concentration gradient of electrons or holes can exist in the y direction because that would mean electrons or holes are leaving the surface or entering the surface from outside. Similar conditions are imposed on the vertical walls as well. So you can see that along this wall or this edge of the device you have no gradient in the x direction for either potential or carrier concentration.

So in this direction you have no gradient so no field can escape out of the device or come into the device. No current can go out of the device or in into the device. Now this boundary condition in the non-contact will have a bearing on for example the potential lines so here we have drawn the Equipotential lines. When you find that the potential line emerges perpendicular to the surface at the non-contact surface.

Now this is a direct result of imposition of the condition that dou shi/dou y is 0 so there can only be dou Psi/dou x. Same thing applies to the potential line emerging from the sides. So even here the potential line is perpendicular. So this means in this direction there is no field. Summarizing the boundary conditions the ideal boundary conditions you have at an ideal ohmic contact, carrier concentration is equal to the equilibrium value and uniform and the potential is also uniform at the applied voltage + the built-in voltage.

At an Ideal non-contact, the gradients of the concentrations n and p which are perpendicular to the surface, so the perpendicular sign here means perpendicular to the surface. And similarly, the perpendicular gradient of the potential all these are 0 because no current can escape or no field can escape out of the device or enter the device.

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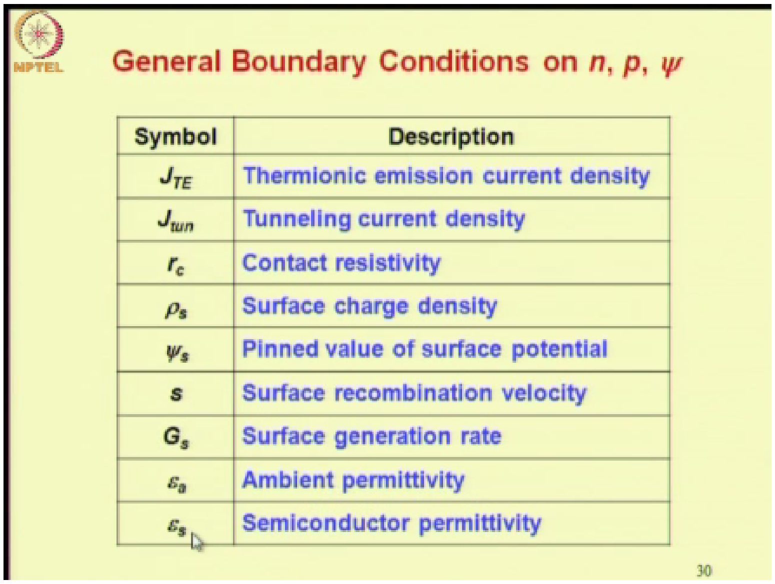

General Boundary Conditions on n, p, ψ

Symbol	Description
J_{TE}	Thermionic emission current density
J_{tun}	Tunneling current density
r_c	Contact resistivity
ρ_s	Surface charge density
ψ_s	Pinned value of surface potential
s	Surface recombination velocity
G_s	Surface generation rate
ε_a	Ambient permittivity
ε_s	Semiconductor permittivity

Now let us look at General Boundary Conditions. Now what we have discussed so far are Ideal conditions, okay which may apply in many of the devices particularly large size devices. Okay. However, as we shall find there can be instances when you do not have Ideal conditions existing. Now let us look at in general, what are the factors that can influence the conditions on n, p and Psi at the boundaries. We would like to define a few quantities here.

JTE is Thermionic emission current density, Jtun is Tunneling current density. R suffix c is contact resistivity. Rho suffix s is Surface charge density, so Rho without suffix s is space charge that is charge for unit volume but Rho suffix s is the charge for unit area. Psi s is the pinned value of surface potential. They are already used in terms in the ideal boundary condition. S is Surface recombination velocity.

Now G suffix s is surface generation rate. Epsilon suffix a is Ambient permittivity and Epsilon suffix s is Semiconductor permittivity. So these epsilon include the permittivity if vacuum. So the Epsilon s for example would be equal to the dielectric constant of the semiconductor multiplied by the permittivity of free space.

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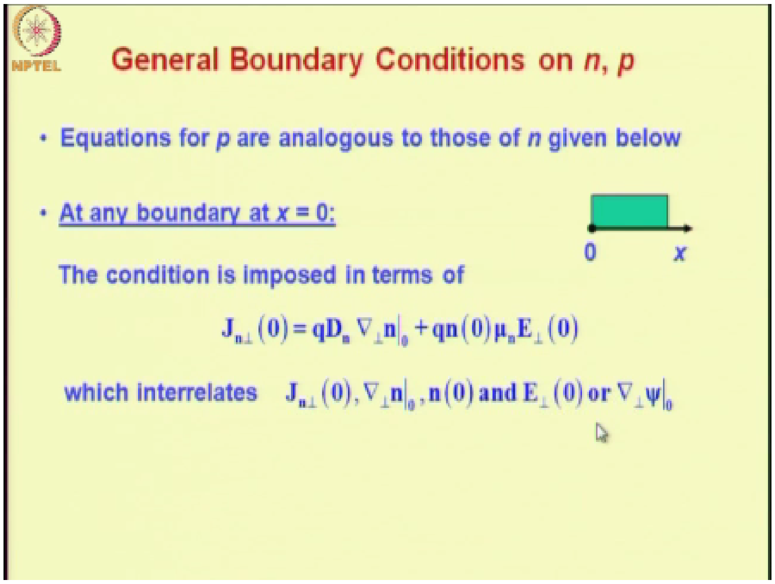

General Boundary Conditions on *n*, *p*

- Equations for *p* are analogous to those of *n* given below
- <u>At any boundary at $x = 0$:</u>

The condition is imposed in terms of

$$J_{n\perp}(0) = qD_n \nabla_\perp n\big|_0 + qn(0)\mu_n E_\perp(0)$$

which interrelates $J_{n\perp}(0), \nabla_\perp n\big|_0, n(0)$ and $E_\perp(0)$ or $\nabla_\perp \psi\big|_0$

Now we shall write the equations for n and similar equation would be used for p. So whenever we are writing equations involving both p and n that would be evident. At any boundary at x=0 let us assume that you have a semiconductor block as shown here and we are assuming a one dimensional situation in the x dimension and the boundary that we are talking about is at x=0 so this vertical boundary.

Now at any boundary the condition is imposed in terms of the perpendicular current density. This is the important point. Why? Because we can talk in terms of how much current is leaving the boundary or entering the boundary perpendicular to the boundary; at contacts you will have a non-zero current leaving the boundary perpendicular the boundary or entering the boundary.

On the other hand, at non-contacts you will have no current entering the boundary or leaving the boundary, right. Therefore, though ultimately we want conditions on n, p and Psi basically the conditions are on the current density and from there we can derive the conditions n, p and Psi. Now any current density you know is composed of the diffusion current and drift current in our diffusion model.

Let us explain the symbol the symbolism here, so what does Jn perpendicular 0 mean, what does Q sorry what does perpendicular gradient of n at x=0 mean, right and so on. So this equation inter relates the perpendicular current density at x=0; the perpendicular gradient of carrier concentration, electron concentration at x=0; the value of electron concentration at x=0 and the perpendicular component of the electric field at 0 or the perpendicular gradient of the potential at x=0. Let us explain this the terms with the help of a figure.

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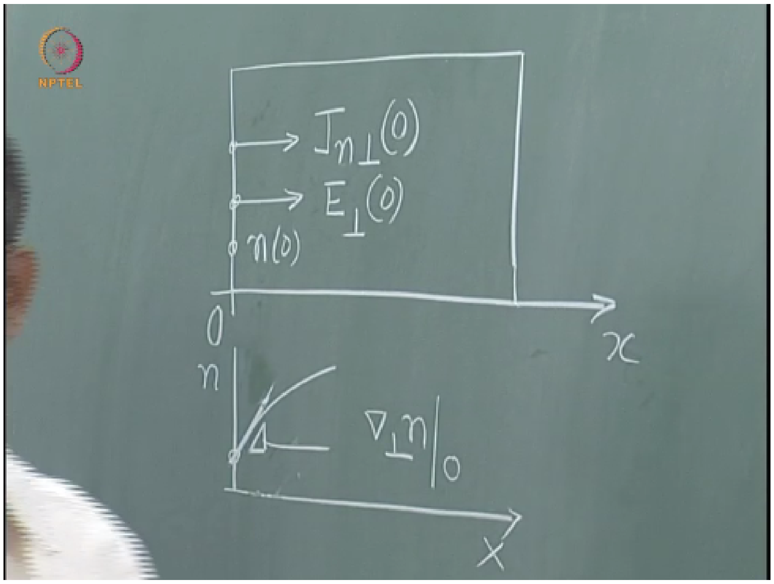

So this is your semiconductor. And let us say this is the x direction, and this is the origin. The current at this point in this direction is referred to as Jn perpendicular with 0 there. So this means the value of this current at this point. Similarly, the electric field perpendicular means the electric field in this direction at 0 that means a field here. n of 0 means in electron concentration at this point so that would be n of 0.

Now what about the perpendicular gradient of n? So for example, if within the device your carrier concentration of electrons is changing like this then this is the gradient of the electron concentration right at the origin; so this gradient is referred to as the perpendicular gradient of electrons and since it is at this point they are calling it as a suffix at x=0. So this is the meaning of the various terms which are used in the equation.

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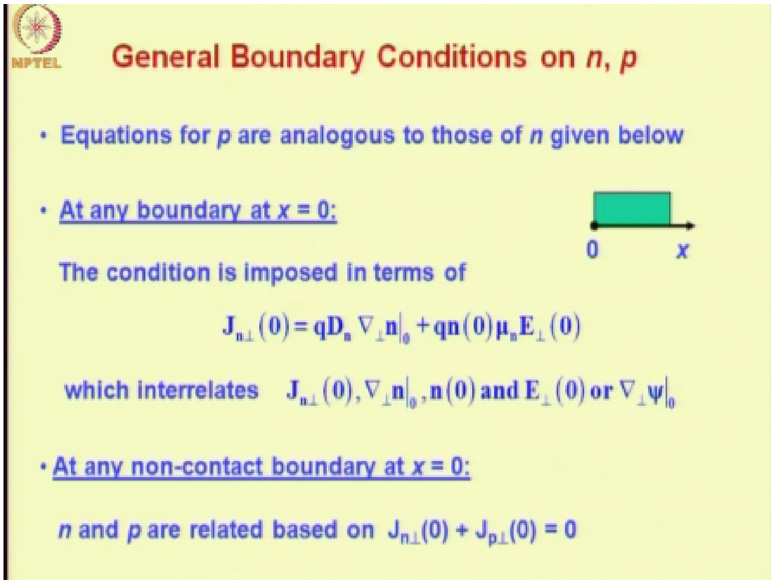

General Boundary Conditions on *n*, *p*

- Equations for *p* are analogous to those of *n* given below
- At any boundary at *x* = 0:

  The condition is imposed in terms of

$$J_{n\perp}(0) = qD_n \nabla_\perp n|_0 + qn(0)\mu_n E_\perp(0)$$

  which interrelates $J_{n\perp}(0), \nabla_\perp n|_0, n(0)$ and $E_\perp(0)$ or $\nabla_\perp \psi|_0$

- At any non-contact boundary at *x* = 0:

  n and *p* are related based on $J_{n\perp}(0) + J_{p\perp}(0) = 0$

At any non-contact boundary again assuming that the boundary at x=0; the n and p are related based on the condition the total current J = 0 that Jn perpendicular 0+Jp perpendicular at x=0 is equal to 0. Now this is important. Actually at a non-contact boundary no current can enter and when we talk about no current you must consider the combination of electron and hole currents, right? Not just individual currents.

Let me give you an example where the individual currents of electrons and holes are non-zero but there sum contributing to the total current is 0.

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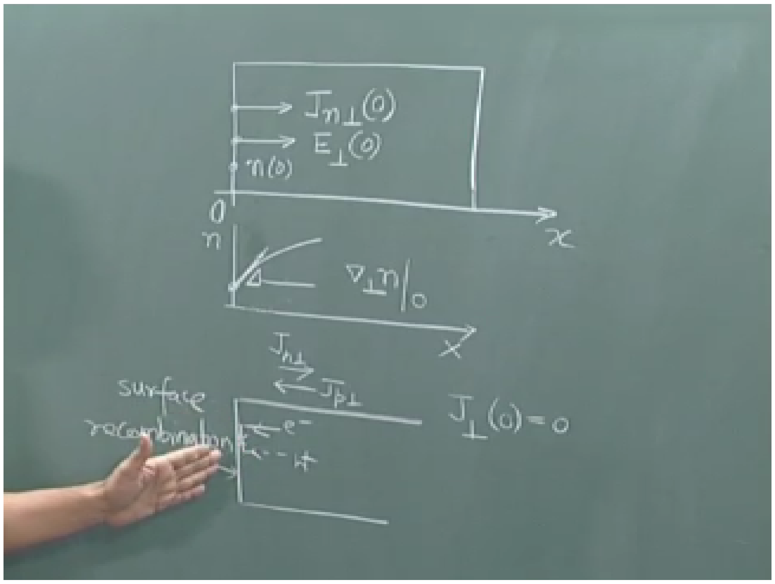

Suppose I have surface recombination at this surface and this is your semiconductor, then what will happen is the electrons will tend to move in this direction and holes will also tend to move in this direction. And here at the surface they will recombine. So you see because of the electron moment into the surface you have an electron current so Jn and that Jn is in this direction—the electrons are moving in this direction your Jn perpendicular is like this.

And if the holes are moving in this direction it contributes to Jp perpendicular like this. And these 2 currents are canceling each other. Okay. That is how it is resulting in the condition J perpendicular at 0 = 0. Okay. So this an example where this is a non-contact surface with a surface recombination you have both electron currents and hole current at the surface. But sum total of them is 0.

Therefore, at a non-contact surface we must think in terms of the total current to begin with and later on we may find that if those surface recombination then individually also the currents can be 0.

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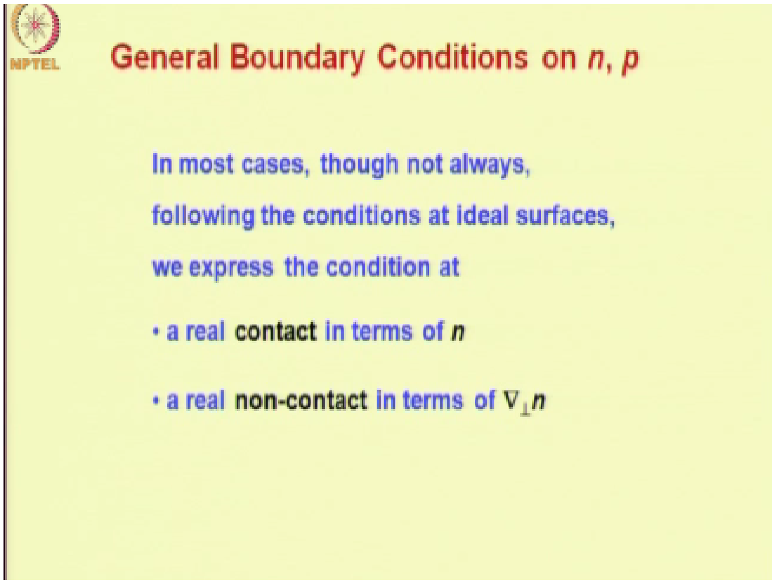

General Boundary Conditions on n, p

In most cases, though not always,
following the conditions at ideal surfaces,
we express the condition at

- a real **contact** in terms of n
- a real **non-contact** in terms of $\nabla_{\perp} n$

In most cases, though not always, following the conditions at Ideal surfaces, we express the condition at a real contact in terms of n and a real non-contact in terms of the perpendicular gradient of n at the surface. So we have said that under Ideal conditions and an Ideal contact; the electron concentration n = equilibrium value. Therefore, it makes sense to see under non-ideal conditions how much does n differ from n0.

Similarly, ideal condition at non contact is in terms of gradient of n the perpendicular gradient of n = 0. It therefore makes sense to see how the perpendicular gradient in term of n differs from 0.

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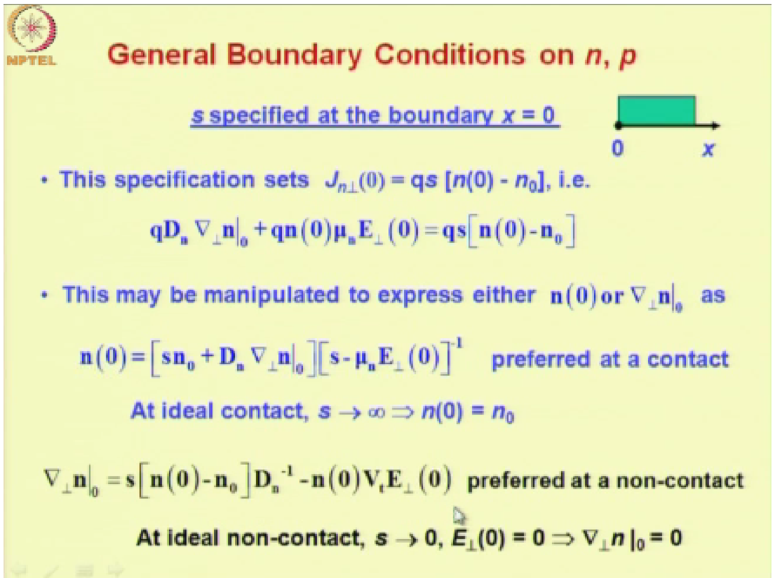

General Boundary Conditions on n, p

s specified at the boundary $x = 0$

- This specification sets $J_{n\perp}(0) = qs\,[n(0) - n_0]$, i.e.

$$qD_n \nabla_\perp n|_0 + qn(0)\mu_n E_\perp(0) = qs[n(0) - n_0]$$

- This may be manipulated to express either $n(0)$ or $\nabla_\perp n|_0$ as

$$n(0) = [sn_0 + D_n \nabla_\perp n|_0][s - \mu_n E_\perp(0)]^{-1}$$ preferred at a contact

At ideal contact, $s \to \infty \Rightarrow n(0) = n_0$

$$\nabla_\perp n|_0 = s[n(0) - n_0]D_n^{-1} - n(0)V_t E_\perp(0)$$ preferred at a non-contact

At ideal non-contact, $s \to 0$, $E_\perp(0) = 0 \Rightarrow \nabla_\perp n|_0 = 0$

Let us take some specific cases. Suppose we have a surface recombination velocity specified at the boundary x=0 then how would be a condition look like. Specification of s sets this equation up. The perpendicular component of Jn at x=0 is equal to 2 times the surface recombination velocity into the electron concentration at 0 - the equilibrium value of electron concentration at 0.

So L0 - n suffix 0 this term is the excess electron concentration at the boundary. So the current is prepositional to the excess electron concentration. Therefore, you write the equation for Jn perpendicular including diffusion and drift and this is the equation that is setup by the surface recombination velocity. Now this equation can be manipulated to express either n of 0 which is what will be the preferred equation at contact or perpendicular gradient of the n at origin.

So the manipulation will give if you write n of 0 then it will turn out to be given by this formula. This is a very straightforward algebraic manipulation so I am not working it out here. It is obtained from this formula. Now this is the formula preferred at a contact. Now note that you can recover the condition for the ideal contact by setting s tending to infinite so in this formula if you set s tending to infinite you will get the electron concentration at boundary is equal to equilibrium concentration.

Thus, an ideal contact ohmic contact corresponds to infinite surface recombination velocity. If you want to specify in terms of the surface recombination velocity. Now you can manipulate the same equation but now you try to express the perpendicular gradient of electrons. Now that is given by this formula. And this would be the preferred formula to us at non-contact to find out how much thus this quantity differ from 0 for the ideal contact.

Now you can recover the condition for the ideal contact. Sorry the ideal non-contact. So at the ideal non-contact this quantity is 0. So we would like to see a real non-contact how much does it differ from 0. So if you-- you can recover the ideal conditions if you set s = 0 and the perpendicular electric field also = 0. So look at it here if I set s = 0 this term drops off and I will have to set perpendicular also = 0 to get perpendicular gradient of n = 0.

So you see you need a combination of 2 conditions to define an ideal non-contact. Surface recombination velocity is 0 and the perpendicular electric field also is 0, only then you will get the condition the gradient of the concentration perpendicular to the surface is 0.

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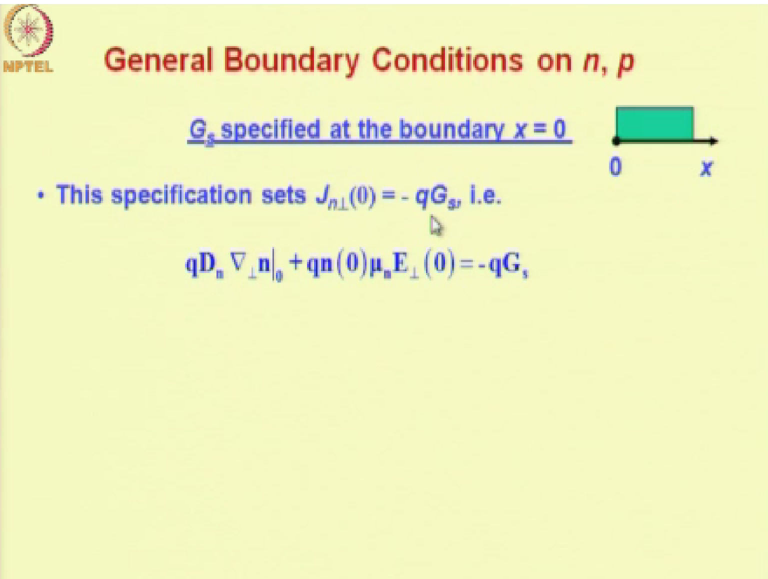

General Boundary Conditions on n, p

G_s specified at the boundary $x = 0$

- This specification sets $J_{n\perp}(0) = -qG_s$, i.e.

$$qD_n \nabla_\perp n\big|_0 + qn(0)\mu_n E_\perp(0) = -qG_s$$

Suppose you choose to specify surface generation instead of surface recombination at x=0 then what would your formulae be? Now, your setting Jn perpendicular at x=0 = -Q times Gs okay this transforms to this equation; when you split the perpendicular current density into diffusion at drift components. Now let us explain what is the meaning of this Jn perpendicular at x=0 -Q time Gs.

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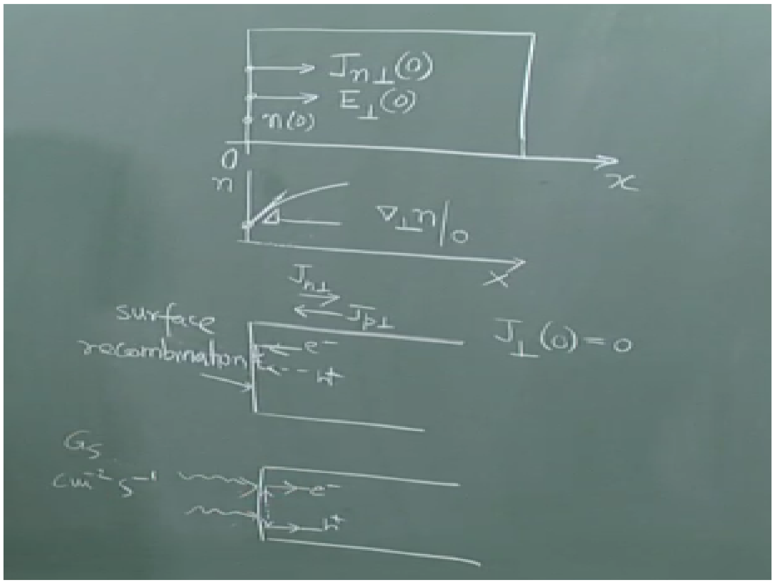

So, here we are assuming a surface generation at this end. Now surface generation the unit is per centimeter square per second. Number of photons impinging per centimeter square per second. And each of them let us assume for simplicity gives as an electron hole pair, so as a result of that you have electrons flowing in so you have generation of electrons and holes and then the holes and electrons they move in. So it is this current that we are relating to this Gs. Okay. That is what we are doing.

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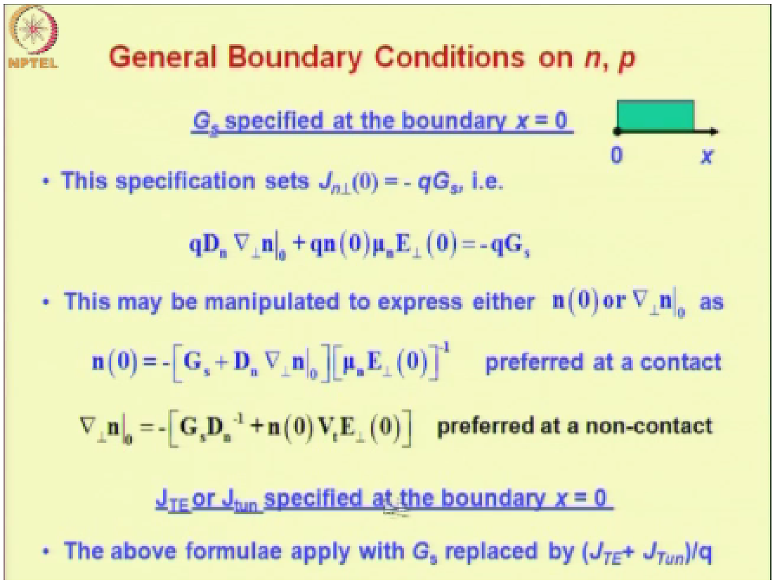

General Boundary Conditions on *n*, *p*

G_s specified at the boundary $x = 0$

- This specification sets $J_{n\perp}(0) = -qG_s$, i.e.

$$qD_n \nabla_\perp n\big|_0 + qn(0)\mu_n E_\perp(0) = -qG_s$$

- This may be manipulated to express either $n(0)$ or $\nabla_\perp n\big|_0$ as

$$n(0) = -\left[G_s + D_n \nabla_\perp n\big|_0\right]\left[\mu_n E_\perp(0)\right]^{-1}$$ preferred at a contact

$$\nabla_\perp n\big|_0 = -\left[G_s D_n^{-1} + n(0) V_t E_\perp(0)\right]$$ preferred at a non-contact

J_{TE} or J_{tun} specified at the boundary $x = 0$

- The above formulae apply with G_s replaced by $(J_{TE} + J_{Tun})/q$

Now you can again manipulate this equation as we did for surface recombination and you will get these 2 equations one in terms of the electron concentration at the boundary or in terms of the perpendicular gradient of electron concentration. So you will choose n of 0 this equation at contact and this equation at non-contact. Now if the Thermionic emission or tunneling currents are specified at the boundary then the equation look in fact very similar to the equation of Gs.

So, all that you need to do is that the above formulae apply with Gs replaced by the Thermionic emission current density + tunneling current density divided by Q. So you set Gs = this value. Then you get the boundary condition in terms of this current density.

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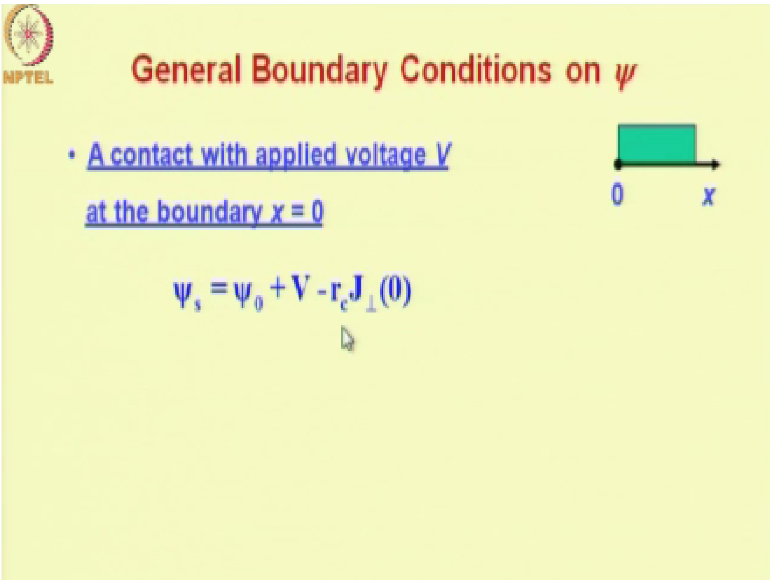

General Boundary Conditions on ψ

- A contact with applied voltage V at the boundary $x = 0$

$$\psi_s = \psi_0 + V - r_c J_\perp(0)$$

Now, so far we have discussed the conditions on n and p. Now let us discuss the conditions on the potential Psi. Now you will recall from the formulae that we derived for the boundary conditions on n and p that there was an electric field term also the perpendicular component of the electric field at the boundary. This was entering into the formulae for the real boundary conditions.

Therefore, we need to understand how we can derive this information that is perpendicular value of electric field. And we also need to know how the applied voltages and so on in imposed conditions. So this is what is done now. So General Boundary Conditions on Psi, considered a contact with applied voltage V at the boundary x=0, so we are applying a voltage at this end. Consequently, the boundary condition on the potential at the surface of the semiconductor.

So, Psi S is happening is inside the semiconductor at the surface. We will shortly explain this so this with a diagram so this equal to built-in voltage or built-in potential solenoid + the applied voltage V- the contact resistance rc into the perpendicular component of the current at the boundary. Now note that this current includes both electrons as well as hole currents. So let us explain this formula with the diagram.

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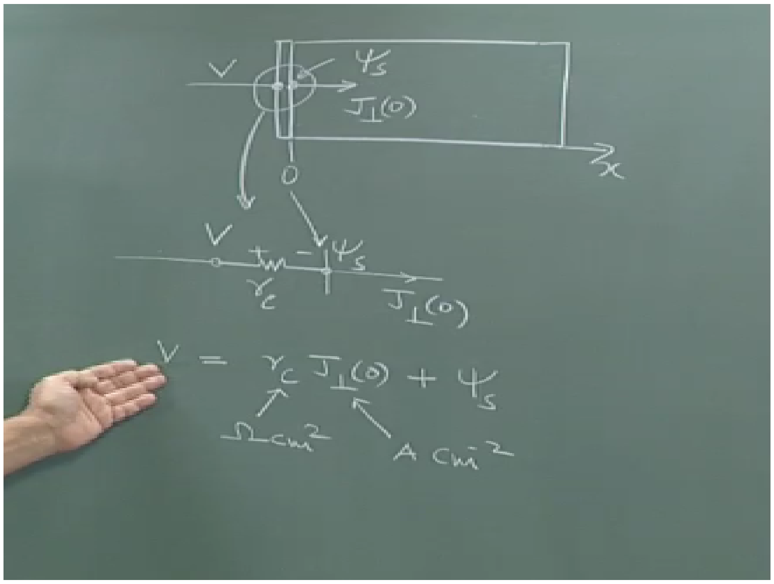

So now this is the contact at this end and the voltage is applied at the outside, right this is the voltage. Now the Psi S is here now from this point to this point when the current is entering the semiconductor and moving across the contact it encounter as a resistance. So if I were to expand this part it is something like this. So this is Psi s, this is V. This is the contact resistance rc and you have a current.

Now the current is in this direction and that is J perpendicular at the boundary. So, this current which is same as this current; this is J perpendicular. So therefore you got the equation that V = rc into J perpendicular at this point 0 so this is the x=0 point. So you have this potential drop +Psi s. Right now I have ignored the built-in potential. Now carefully note the dimensions.

The dimensions of rc is Ohm centimeter square because the dimension of this current density is ampere per centimeter square, so when we multiply this 2 I must get volts. So I can transform this relation to express Psi s. So Psi = V- this quantity and then you can add the built-in potential. Now that is what is done here.

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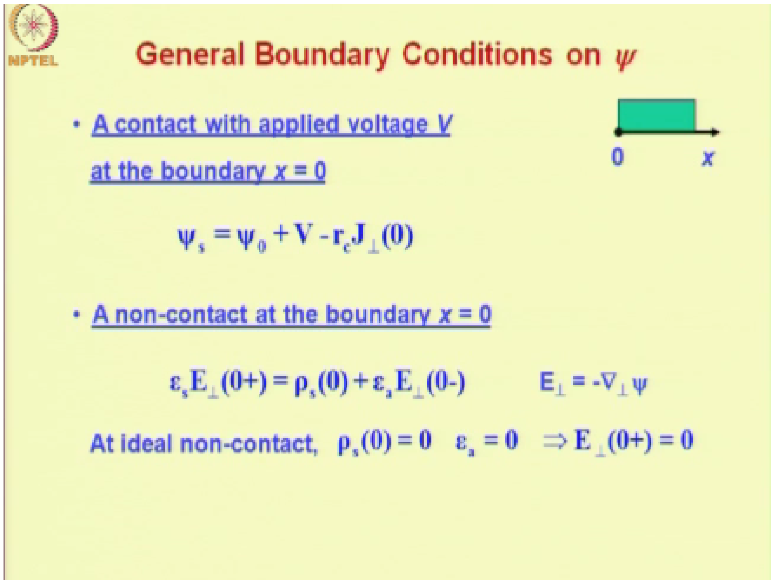

General Boundary Conditions on ψ

- <u>A contact with applied voltage *V* at the boundary *x* = 0</u>

$$\psi_s = \psi_0 + V - r_c J_\perp(0)$$

- <u>A non-contact at the boundary *x* = 0</u>

$$\varepsilon_s E_\perp(0+) = \rho_s(0) + \varepsilon_a E_\perp(0-) \qquad E_\perp = -\nabla_\perp \psi$$

At ideal non-contact, $\rho_s(0) = 0 \quad \varepsilon_a = 0 \quad \Rightarrow E_\perp(0+) = 0$

Let us look at the non-contact. The non-contact again at the boundary x=0. So here in general you may have electric field entering the non-contact region and then leaving the surface so outside you can have electric field as well as inside. So what is why the relation between these 2 fields is expressed here. The field outside the device is in terms of the epsilon A. And the field inside the semiconductor is in term of epsilon s the term here.

And Rho as is a surface charge at the boundary. Let us explain this equation.

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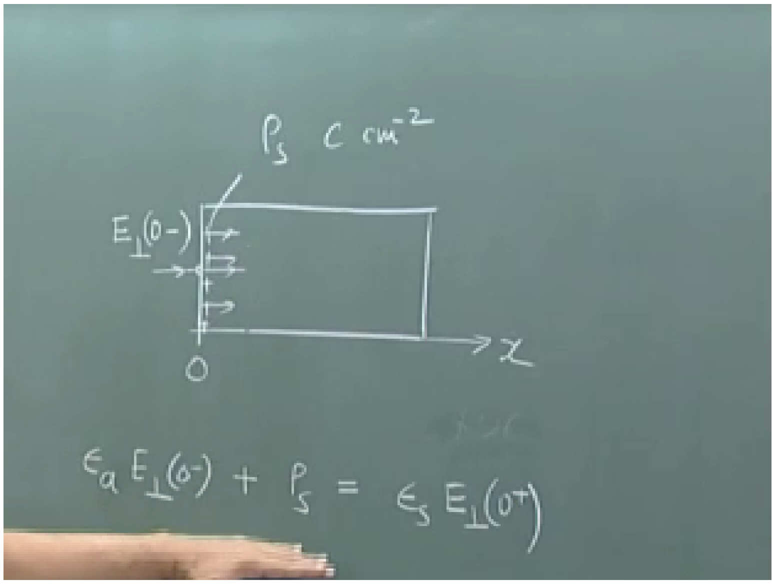

So this is the origin and here you have a surface charge. This is column per centimeter square. The field at this point but from outside this field is referred to as the perpendicular field at 0- - so 0- is this side and 0+ is this side. Now, these lines anyway continue through and each of these positives charges will also contribute field lines right. So the field inside will be more than the field outside assuming that the field is directed in this way because this is our positive x direction that is the convention.

So from here we can write the displacement epsilon A into perpendicular component of electric field 0- that is the displacement here + the contributions of the surface charge Rho s. So this displacement + this will together contribute to the field inside, you can see there are more lines of field inside then outside because each positive charge is contributing therefore this is = epsilon s into E perpendicular 0+, so 0+ means field inside. So that is how you get this relation.

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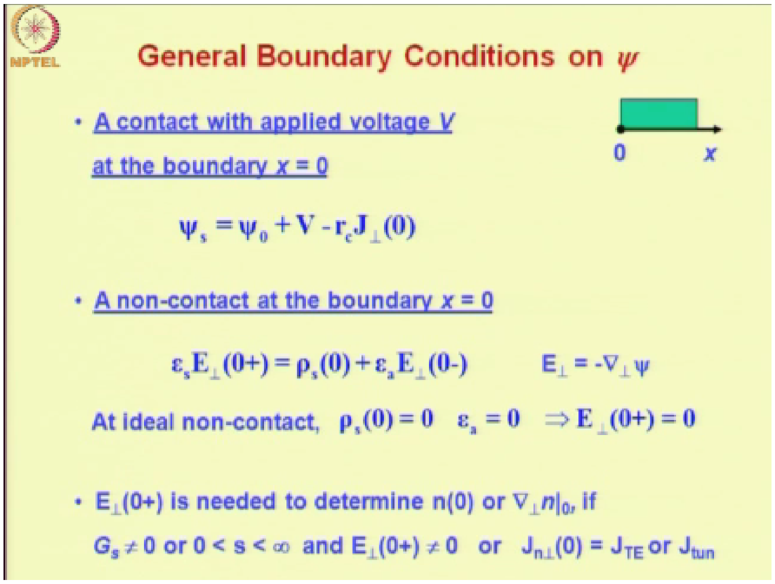

General Boundary Conditions on ψ

- A contact with applied voltage V at the boundary $x = 0$

$$\psi_s = \psi_0 + V - r_c J_\perp(0)$$

- A non-contact at the boundary $x = 0$

$$\varepsilon_s E_\perp(0+) = \rho_s(0) + \varepsilon_a E_\perp(0-) \qquad E_\perp = -\nabla_\perp \psi$$

At ideal non-contact, $\rho_s(0) = 0 \quad \varepsilon_a = 0 \quad \Rightarrow E_\perp(0+) = 0$

- $E_\perp(0+)$ is needed to determine $n(0)$ or $\nabla_\perp n|_0$, if $G_s \neq 0$ or $0 < s < \infty$ and $E_\perp(0+) \neq 0$ or $J_{n\perp}(0) = J_{TE}$ or J_{tun}

Now you can convert this into a relation for perpendicular gradient of the potential by using these formulae. So this formula should be used from each of the electric field so this one as well as this one. You can get then conditions on the potential. Now at an ideal non-contact this condition will correspond to no surface charge. So Rho s at that point, 0 =0 and the ambient electric constant is 0.

So when you say that no field escapes the device or no field enters a device from outside you are indirectly assuming that dielectric constant of the ambient is 0. Now you know that this is evidently not correct. So in general for a device field will always exists even outside the device volume. Okay. Now this point has to be born in mind, we shall shortly so an example, where if you neglect this field in the ambient you can get grossly inaccurate results.

Now before we go onto that example let us make a point that the perpendicular component of the electric field in the semiconductor that is 0+; so 0+ is the semiconductor side of the boundary. Now this electric field is needed to determine the carrier concentration at the boundary or the gradient of the carrier concentration in the real case, right. So this we have seen in the formulae that we derived.

Now this field will be required in the formulae if your surface generation rate is non-zero or your surface recombination velocity lies between 0 and infinite, so you are not having ideal contact nor an ideal non-contact. And in addition the perpendicular component of the electric field is not 0. So in that case you have to use this above results to get this perpendicular electric field and then derive the conditions on carrier concentration or the gradient.

Another situation where you need the electric field information above is when you set the current density condition at boundary in terms of Thermionic emission or Tunneling.

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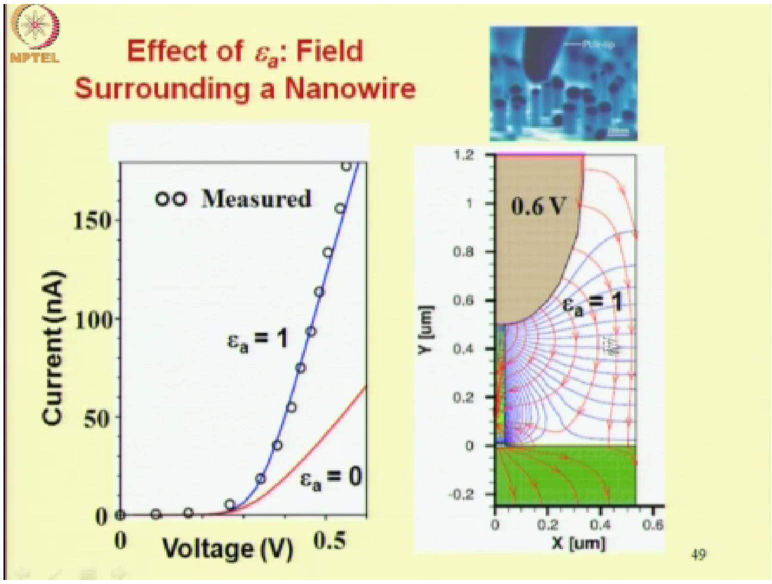

Effect of ε_a: Field Surrounding a Nanowire

Now here is the example which tells you why you must consider the field in the ambient as well. Let me tell you the situation. This is a Nanowire a very, very small scale wire. So Nanowire means the diameter of the wire can be of the order of say (()) (45:42) angstroms. That is the kind of wire that we are considering.

Now this wire, has been deposited on the substrate, and suppose your measuring the current voltage characteristics of this wire by bring in a probe in contact. So the experimental arrangement is shown here and this is the simulation of this situation. Now as you can see when you draw a diagram to scale that a lot of field is going to exist in the ambient for example from the probe you will have field lines entering the semiconductor Nanowire all along the surface.

So because of the potential gradient, so this is 0.6 volts, top is 0.6 volts and bottom is 0 so there is a potential variation along the wire from top to bottom and therefore there are field lines not only inside the semiconductor but outside the semiconductor and they are entering the semiconductor you can see that. Now this field lines will modulate the space charge inside because after all the lines had to be terminate on some charge inside the Nanowire.

So therefore they are going to modulate the conditions of the charge and therefore the conductance of the wire. The blue lines here are Equipotential lines. The field lines and Equipotential lines have been drawn based on the appropriate boundary conditions at the surfaces involved. For example, surface of this contact surface of the Nanowire and also the surface of the substrate.

Now what happens if you do not consider the fielding the ambient? So you will set epsilon a = 0 then this entire field that is shown here will vanished and the field will exist only in the wire, right. Let me illustrate with the diagram.

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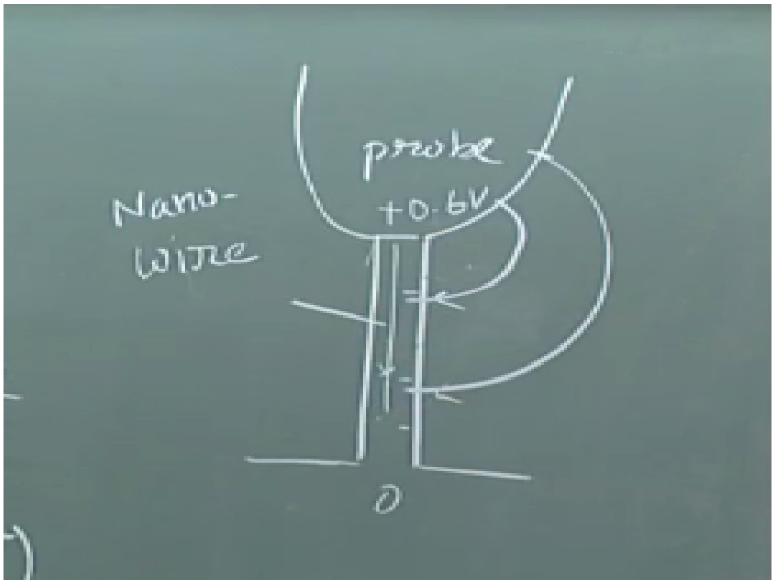

So this is your wire on a substrate and this is your probe. Now if there is no field in the ambient you have just straightforward field picture like this so this is 0.6 volts and this is 0 so your field line like this. But when you consider the field in the ambient the field lines are emanating from here and terminating like this, right. So the emanate perpendicular to the surface here and terminate here.

Now this contribution to charges, so for example lines will terminate on electrons here. In other words, there will be enhancement of the negative charge in the wire. If it is entire pair, you will have more electrons; the conductivity will increase it will be modulated. So that is the effect of the ambient field.

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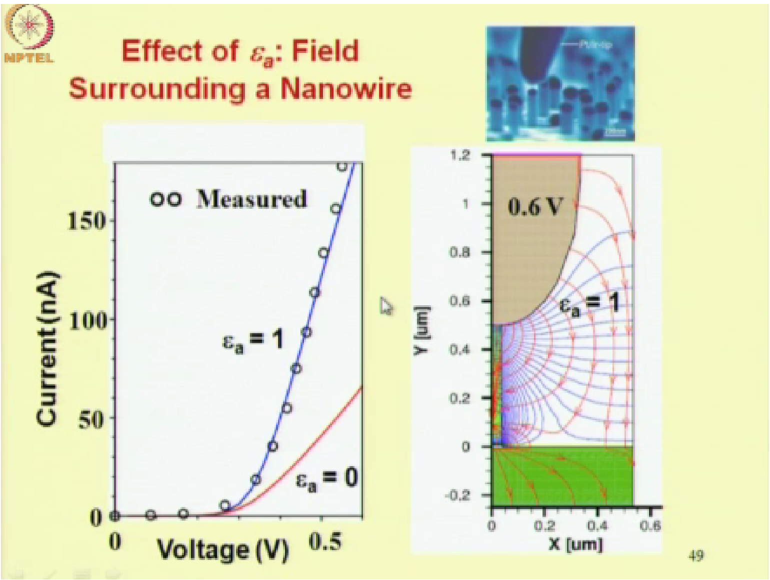

Effect of ε_a: Field Surrounding a Nanowire

Now, that conductivity modulation you are going to ignore if you remove this ambient dielectric constant and effect that shown here the simulated results if you put epsilon a = 0 you get this current as a function of voltage and if you put epsilon a = 1 as it is because you have air outside then you get this blue line and as you can see the blue line passes through the measured data very nicely. Whereas, if you did a simulation setting epsilon a = 0 you would get the red line which is grossly inaccurate as compare to the real condition.

So this should explain to you while the boundary conditions should be appropriately imposed to get the correct results. And in particular one must be careful while neglecting the electric field in the ambient. So ideal boundary conditions should be used with lot of care while they simplify your modeling problem and calculations they may give you grossly inaccurate results particularly for small devices.

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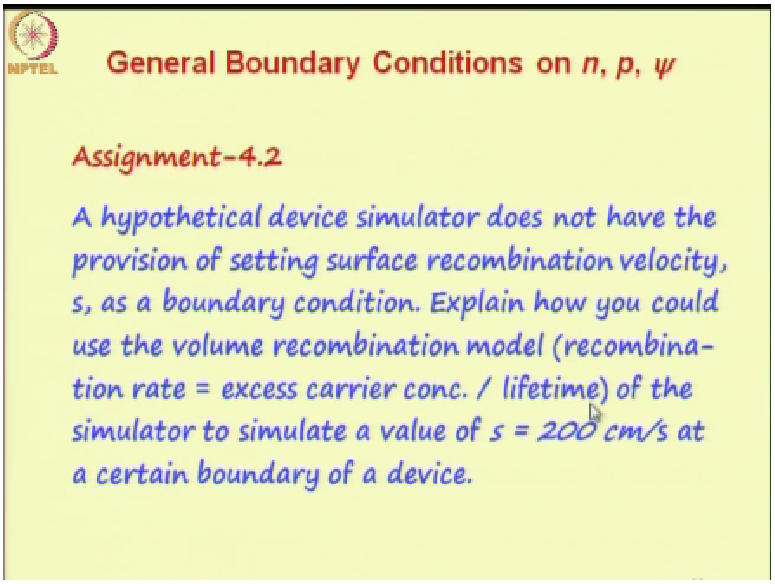

General Boundary Conditions on n, p, ψ

Assignment-4.2

A hypothetical device simulator does not have the provision of setting surface recombination velocity, s, as a boundary condition. Explain how you could use the volume recombination model (recombination rate = excess carrier conc. / lifetime) of the simulator to simulate a value of $s = 200$ cm/s at a certain boundary of a device.

So we are towards the end of the lecture, a couple of assignments related to the boundary conditions. A hypothetical device simulator does not have the provision of setting surface recombination velocity, s as a boundary condition. Explain how you could the volume recombination model that is the recombination rate = excess carrier concentration by lifetime. This is the model of volume recombination.

So how you are going to use them volume recombination model of the simulator to simulate a value of s equals to centimeters per second at a certain boundary of a device. So actually want to simulate surface recombination at a boundary. But you have simulated does not have a provision for. So can you use the model for the volume recombination around this surface and simulate the surface recombination that is the question.

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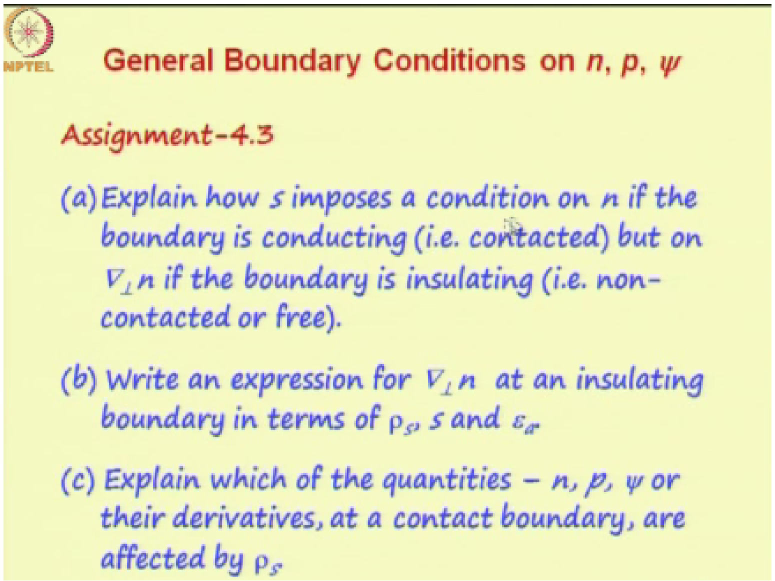

General Boundary Conditions on n, p, ψ

Assignment-4.3

(a) Explain how s imposes a condition on n if the boundary is conducting (i.e. contacted) but on $\nabla_\perp n$ if the boundary is insulating (i.e. non-contacted or free).

(b) Write an expression for $\nabla_\perp n$ at an insulating boundary in terms of ρ_s, s and ε_a

(c) Explain which of the quantities – n, p, ψ or their derivatives, at a contact boundary, are affected by ρ_s

Another one, explain how s imposes a condition on n if the boundary is conducting that is contacted but on perpendicular gradient of n the boundary insulting that is non-contacted or free. Write an expression for perpendicular gradient of carrier concentration at an insulating boundary in terms of surface charge s and epsilon a. So assume surface recombination is present, surface charge is present and the ambient dielectric constant is also there.

So the field in ambient also to be considered, take all these into account and write an expression. Explain which of the quantities n, p, Psi or their derivatives at a contact boundary are affected by the surface charge.

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Summary of this lecture

Now with that we have come to the end of the lecture, so let us make a summary of the important points. So in this lecture we begin detail discussion of the Drift-Diffusion model involving the Drift-Diffusion current equation and other equations such as the continuity equations or carrier balance equations, the heat flux equation and the Gauss' Law and an equation for electric field in terms of the potential gradient.

Now if you leave out the expression for the heat flux you have 6 equations in the Drift-Diffusion model and we showed that these 6 equations can be reduced to just 3 equations in terms of n, p and Psi and therefore to solve these equations you need 3 boundary condition 1 on n, 1 on p and 1 on Psi. Now we explained how the boundary conditions can be imposed either on the value of the quantity or on the gradient of the quantity and on the derivative of the quantity.

So we discussed about ideal boundary conditions and real boundary conditions. The ideal boundary conditions were that the carrier concentration, and the potential are uniform at a contacted boundary; the carrier concentration being equal to the equilibrium concentration. And the gradients of the carrier concentrations and potential are all 0 at non-contacted boundaries.

And we explain that in general the condition the conditions—the boundary condition at the contacted or non-contacted boundaries a derived in terms of the information about current at these boundaries. For example, at a non-contacted boundary the net current either leaving the device or entering the device perpendicular to the surface is 0. Okay. And similarly for contacted boundaries one can derive the boundary conditions based on information about the current density.

“Professor and Student conversation starts”, Sir for the Nanowire characteristic can you give some reference for the measure and simulated data. Yes, I think I should have provided the reference, thank you for point that out. “Professor and Student conversation ends”.

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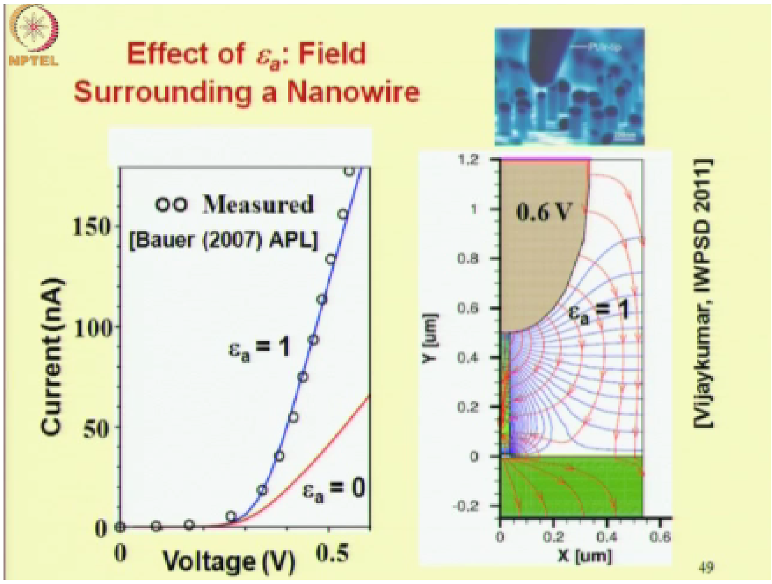

Effect of ε_a: Field Surrounding a Nanowire

[Vijaykumar, IWPSD 2011]

So this data is now given here on the slide. So the measured data has been picked up from a paper by Bauer APL published in Applied Physic Letters in 2007. You can do a Google search with this name and this year in Applied Physic Letters and you will get the reference. The simulation is our own and this study was published—presented in a conference International Workshop on Physics of semiconductor devices conducted in IIT-Kanpur in 2011. Presentation was by myself and my students namely Vijaykumar and Jayanand.