Semiconductor Device Modeling
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Lecture - 31
Energy Band Diagrams

In the previous lecture, we have begun a discussion of the E-x diagram. We mentioned about the various levels in the E-x diagram with the help of a uniform semiconductor. So we considered a uniform semiconductor under equilibrium and under uniform volume generation. So with the help of these situations, we introduce the following levels of the E-x diagram.

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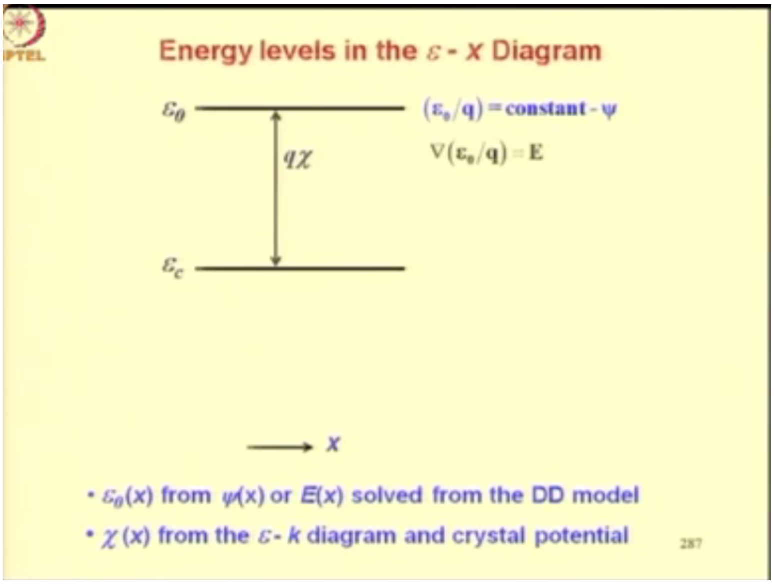

Energy levels in the ε - x Diagram

$(\varepsilon_0/q) = \text{constant} - \psi$

$\nabla(\varepsilon_0/q) = E$

- $\varepsilon_0(x)$ from $\psi(x)$ or $E(x)$ solved from the DD model
- $\chi(x)$ from the ε - k diagram and crystal potential

First we talked about the vacuum level E0. So E0 x can be obtained from psi x that is electrostatic potential distribution or Ex that is the field distribution solved from the drift-diffusion model. The equation is used for this purpose are E0/q = constant - psi or gradient of E0/q = E. Any one of the 2 equations can be used. Then we can locate the conduction bandage Ec.

The difference between E0 and Ec is equal to q times chi where chi is referred to as the electron affinity. So chi of x is obtained from the E-k diagram and crystal potential. Now in general in a non-uniform semiconductor, the electron affinity can be a function of position x if the crystal potential changes in this direction. In our case, the lines are flat, E0 is flat, Ec is flat because we introduce these levels considering a uniform semiconductor.

So all the levels in our case will be flat. The equations however will also give you the variation in the levels okay if they are not flat in some situation.

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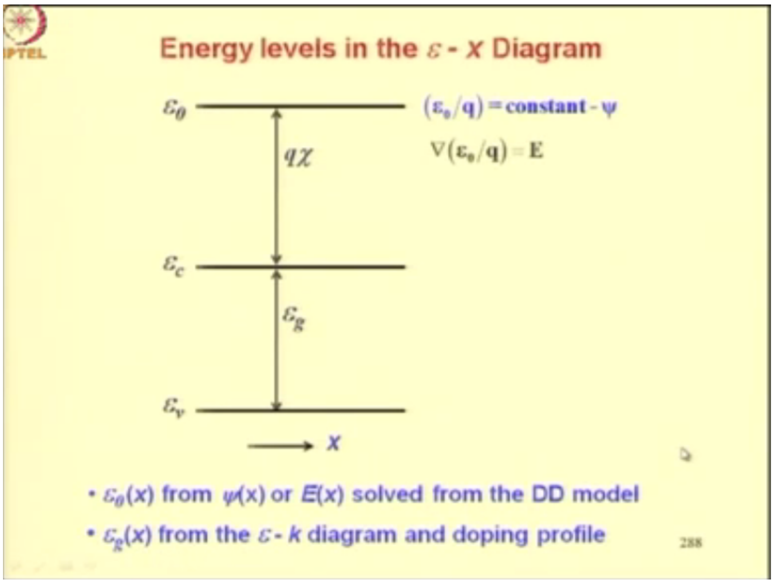

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- $\varepsilon_0(x)$ from $\psi(x)$ or $E(x)$ solved from the DD model
- $\varepsilon_g(x)$ from the ε - k diagram and doping profile

We can locate Ev that is a valence bandage the difference between Ec and Ev is energy gap and energy gap as a function of x is obtained from the E-k diagram and doping profile. So they have explained that the energy gap with the function of doping for heavy doping energy gap reduces. For example, if you have a situation where doping increases in this x direction then the energy gap will decrease in this direction. So that is why Eg can be a function of x in general.

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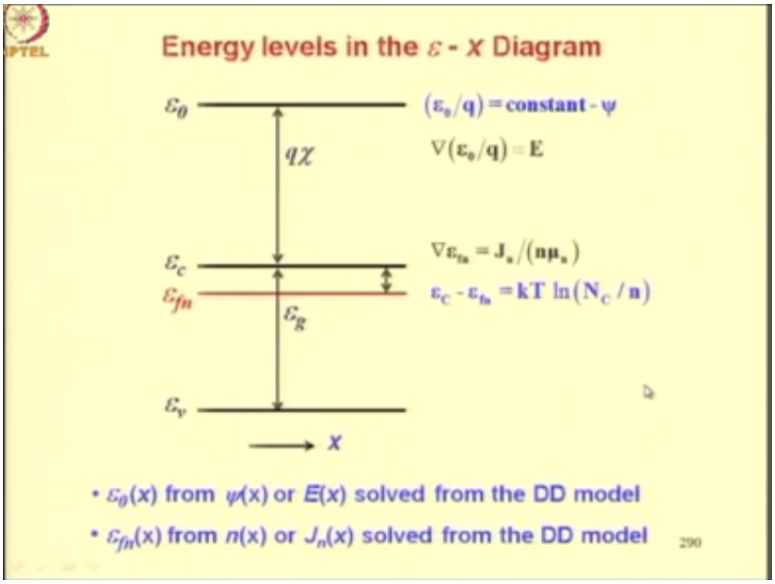

Energy levels in the ε - x Diagram

$(\varepsilon_0/q) = \text{constant} - \psi$

$\nabla(\varepsilon_0/q) = E$

$\nabla\varepsilon_{fn} = J_n/(n\mu_n)$

$\varepsilon_C - \varepsilon_{fn} = kT\ \ln(N_C/n)$

- $\varepsilon_0(x)$ from $\psi(x)$ or $E(x)$ solved from the DD model
- $\varepsilon_{fn}(x)$ from $n(x)$ or $J_n(x)$ solved from the DD model

The quasi Fermi level for electrons Efn, now this can be located from a knowledge of the electron concentration as a function of x or electron current density as a function of x solved from a drift-diffusion model. The relevant equations are gradient of Efn = Jn/n times Mu n or Ec-Efn=kT ln Nc/n. So this equation gives you the quasi Fermi level in terms of the electron concentration.

This equation gives you gradient of the quasi Fermi level in terms of the electron current density and electron concentration.

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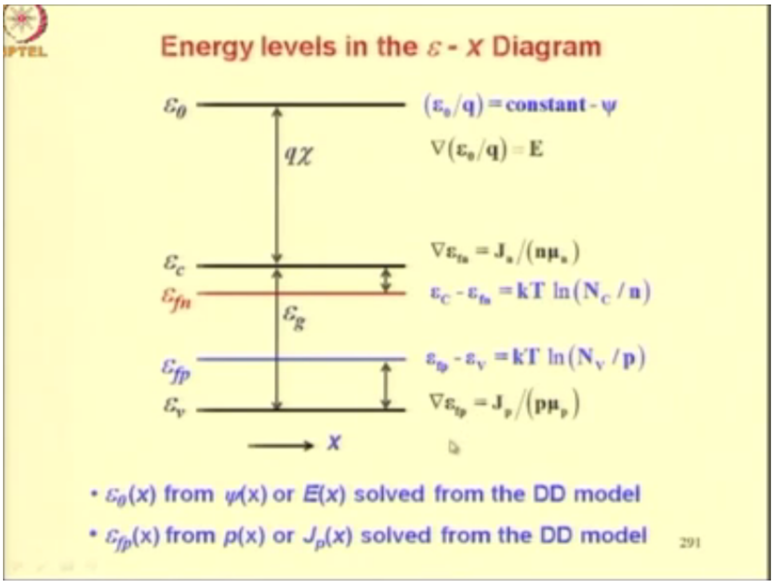

Energy levels in the $\mathcal{E}$ - x Diagram

$(\mathcal{E}_0/q) = \text{constant} - \psi$

$\nabla(\mathcal{E}_0/q) = E$

$\nabla\mathcal{E}_{fn} = J_n/(n\mu_n)$

$\mathcal{E}_C - \mathcal{E}_{fn} = kT\ln(N_C/n)$

$\mathcal{E}_{fp} - \mathcal{E}_V = kT\ln(N_V/p)$

$\nabla\mathcal{E}_{fp} = J_p/(p\mu_p)$

- $\mathcal{E}_0(x)$ from $\psi(x)$ or $E(x)$ solved from the DD model
- $\mathcal{E}_{fp}(x)$ from $p(x)$ or $J_p(x)$ solved from the DD model

So similarly we get quasi Fermi level for holes. These are the equations analogous to the equations for electrons and Efp x is obtained from hole concentration or hole current density as a function x solved from the drift-diffusion model.

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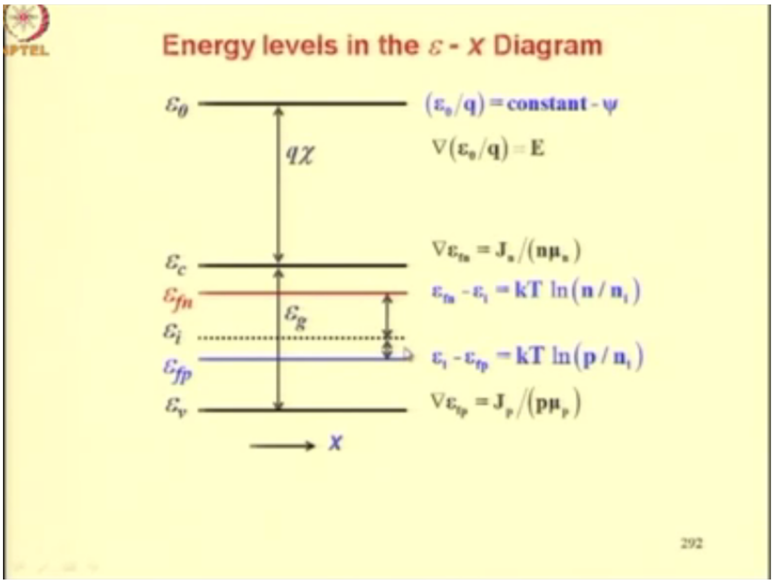

Energy levels in the ε - x Diagram

$(\varepsilon_0/q) = \text{constant} - \psi$

$\nabla(\varepsilon_0/q) = E$

$\nabla\varepsilon_{fn} = J_n/(n\mu_n)$

$\varepsilon_{fn} - \varepsilon_i = kT \ln(n/n_i)$

$\varepsilon_i - \varepsilon_{fp} = kT \ln(p/n_i)$

$\nabla\varepsilon_{fp} = J_p/(p\mu_p)$

You can also locate the quasi Fermi levels Efn and Efp with reference to the intrinsic level Ei. These are the relevant formulae.

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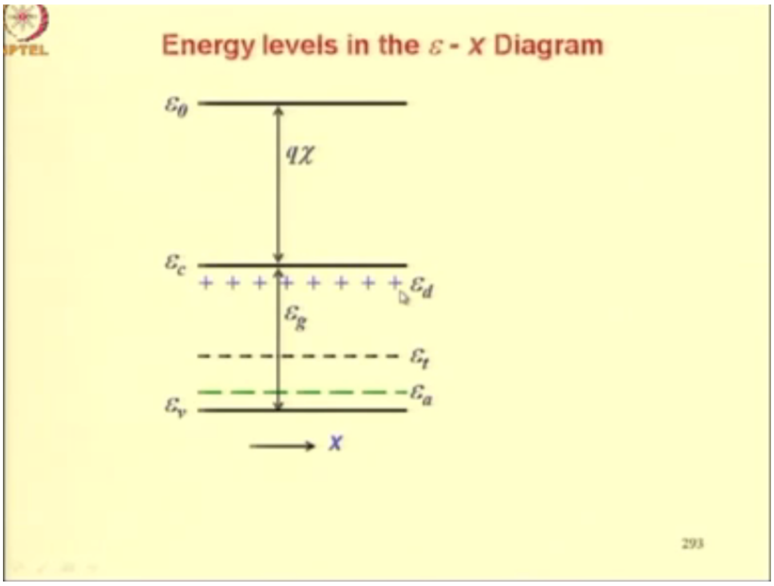

Energy levels in the ε - x Diagram

If you wish you could locate other levels within the energy gap for example the donor level, the acceptor level, the trap level etc. These are levels corresponding to impurities and defects. So this is how you can locate the various levels in an energy band diagram, which plots electron energies as a function of x.

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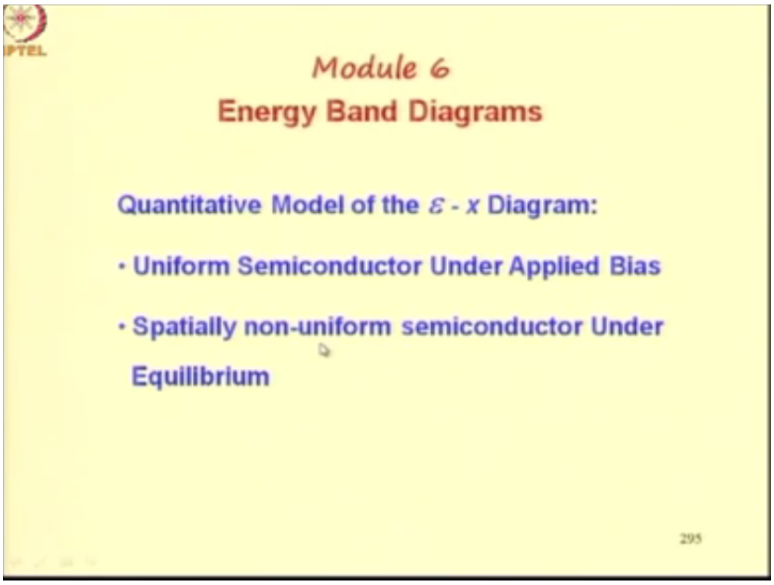
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Module 6

Energy Band Diagrams

Quantitative Model of the $\mathcal{E}$ - x Diagram:

- Uniform Semiconductor Under Applied Bias
- Spatially non-uniform semiconductor Under Equilibrium

Now in this lecture, we shall consider a uniform semiconductor under applied bias and then spatially non-uniform semiconductor under equilibrium. So spatially non-uniform means the doping may change as a function of x, the crystal structure or composition may change as a function of x.

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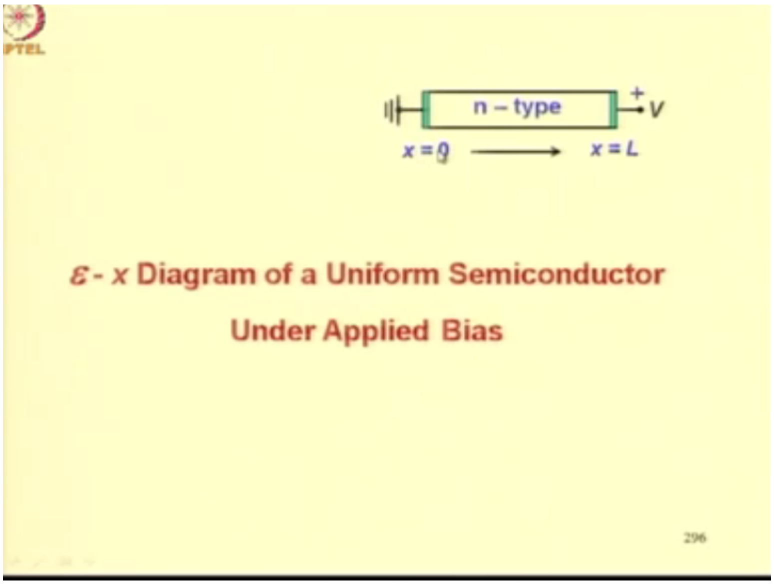

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$\mathcal{E}$ - x Diagram of a Uniform Semiconductor Under Applied Bias

Let us start with the E-x diagram of a uniform semiconductor under applied bias. So this is our diagram. Whenever you want to apply a bias you will have contacts. So here at x=0 and x=L, we have shown the contacts. In practice, the contacts are such that at these contacts equilibrium conditions are maintained for electron concentrations and hole concentrations such contacts are called ohmic contacts.

So we will assume ohmic contacts in our case whenever we are applying a voltage to any of the devices that we are considering. Now the length of this semiconductor for us is equal to L. We will be concentrating only on the semiconductor portion and we will ignore the variations in energy levels near the contacts for the present. We can always sketch the energy levels at the contacts using the E-x diagram that we draw for junctions later on.

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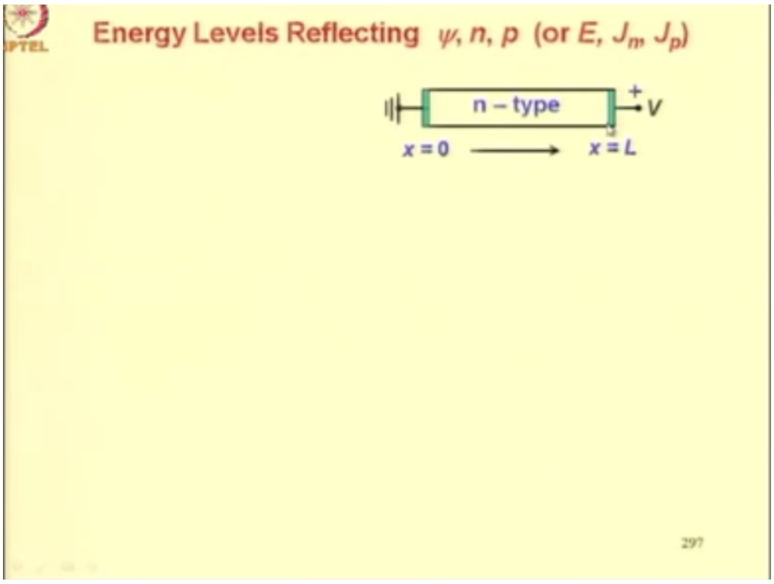

Energy Levels Reflecting ψ, n, p (or E, J_n, J_p)

Let us sketch the energy levels reflecting psi, n, p or E, Jn, and Jp inside the n-type semiconductor. So our x=0 point would be this edge and x=L would be this edge okay and we will ignore any space-charge regions associated with this contacts.

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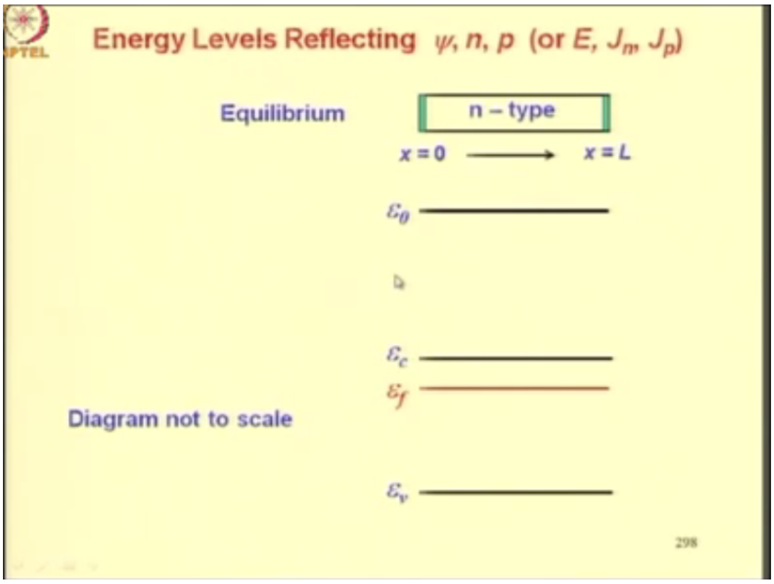

Energy Levels Reflecting ψ, n, p (or E, J_n, J_p)

Equilibrium

Diagram not to scale

The diagram under equilibrium conditions, which we have already drawn in the previous class is something like this which shows E0, Ec, Ef and Ev.

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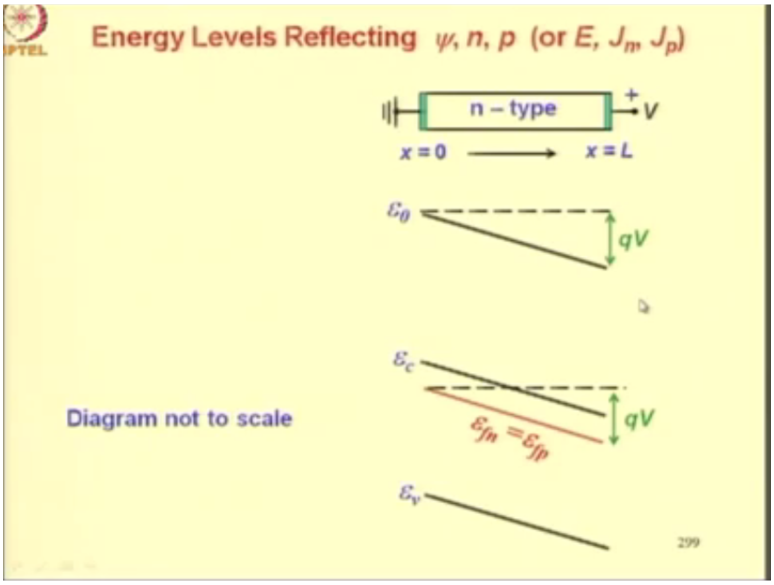

Energy Levels Reflecting ψ, n, p (or E, J_n, J_p)

Diagram not to scale

The moment you apply a voltage in this case we are applying a positive voltage to the right hand contact. All your levels tilt okay downwards to the right in this way. Let us develop this energy band picture. Now in principle you can start from any of the levels we will start from E0 in this case. Later on, we are going to lay out a procedure for drawing the levels and there we will show that although in principle we can start from any of the levels in most of the devices particularly when conditions are non-uniform inside the semiconductor, it is most efficient to start with the Fermi level.

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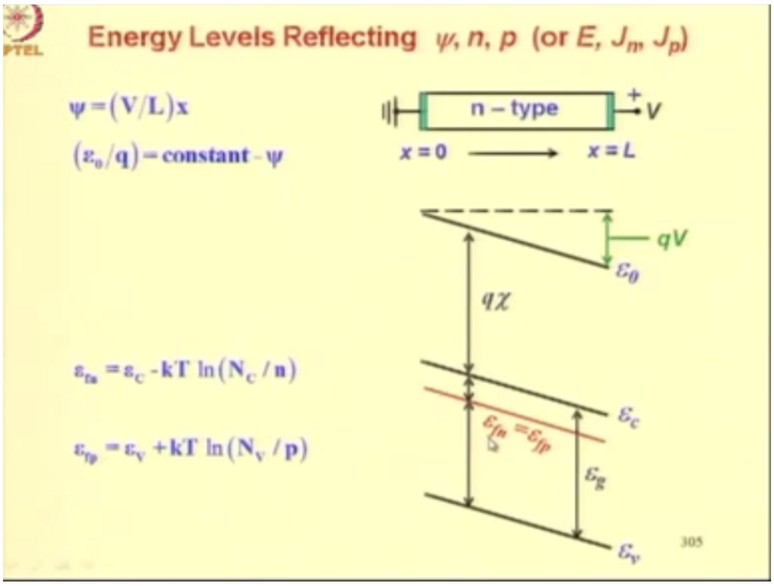

Energy Levels Reflecting ψ, n, p (or E, J_n, J_p)

$\psi = (V/L)x$

$(\varepsilon_0/q) = \text{constant} - \psi$

$\varepsilon_{fn} = \varepsilon_C - kT \ln(N_C/n)$

$\varepsilon_{fp} = \varepsilon_V + kT \ln(N_V/p)$

In this case however we will start with the E0 because we are not considering a non-uniform semiconductor. So our starting point is psi = V/L into x because we have applied a voltage V and the semiconductor is uniform, your potential variation in the semiconductor is linear. So potential increases from x = 0 to x = L in a linear fashion. This is what this equation shows.

For x=0, psi=0 that is what we have assumed as a reference. Now the E0/q is given by this formula constant - psi where psi will be this equation and if you sketch this equation on a graph this is how it looks E0 goes down linearly as a function of x. The difference between the values of E0 at x=L and x=0 is = q times the applied voltage.

This follows from this equation. Now you can locate Ec a distance q times chi below E0. Since our semiconductor is uniform chi is constant with x and therefore Ec line is parallel to E0 line. You can locate Efn at a distance below Ec given by this formula okay. So the distance marked here = kT ln Nc/n. Again since our semiconductor is uniform, n is uniform with x therefore the Efn line is parallel to Ec line.

Then we locate Ev at a distance Eg below Ec and then locate Efp it turns out since the electrons and hole concentrations are equal to the values under equilibrium, the quasi Fermi level for electrons and holes in this case will turn out to be the same. So when you apply this relation and locate Efp with respect to Ev, it will turn out to be at the same point as Efn located with respect to Ec using this formula.

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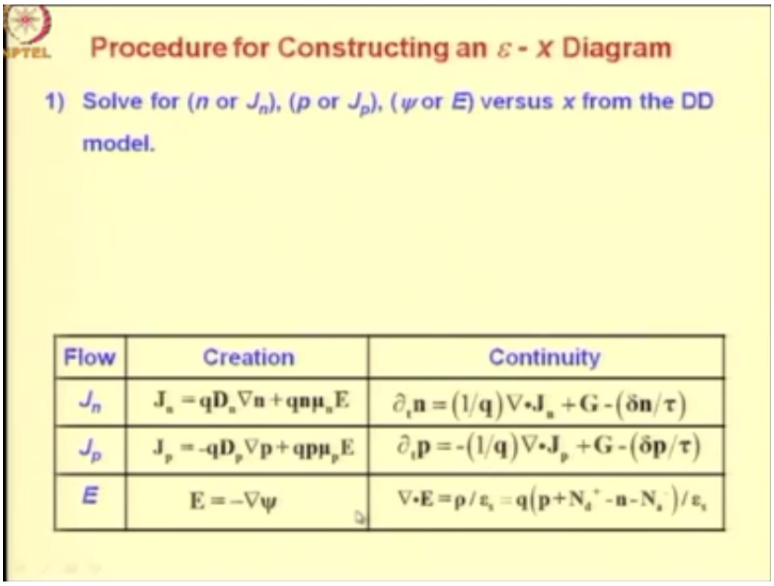

Procedure for Constructing an ε - x Diagram

1) Solve for (n or J_n), (p or J_p), (ψ or E) versus x from the DD model.

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

Now since we are going to move on to more complicated E-x diagrams, it is important to lay down the various steps that should be used to draw the E-x diagram for any general situation. So the first step is solve for electron concentration or electron current density, hole concentration or the hole current density and electrostatic potential or electric field versus x from the drift-diffusion model.

Now for the situations that we considered so far we actually did not go through all the equations of the drift-diffusion model to get n, p and psi. We seem to have obtained n, p and psi directly by (()) (10:23). This was alright because we were considering a uniform semiconductor right where the conditions are very, very simple. In general, however one will have to go through all these 6 equations to solve for n, Jn, p, Jp, psi and E.

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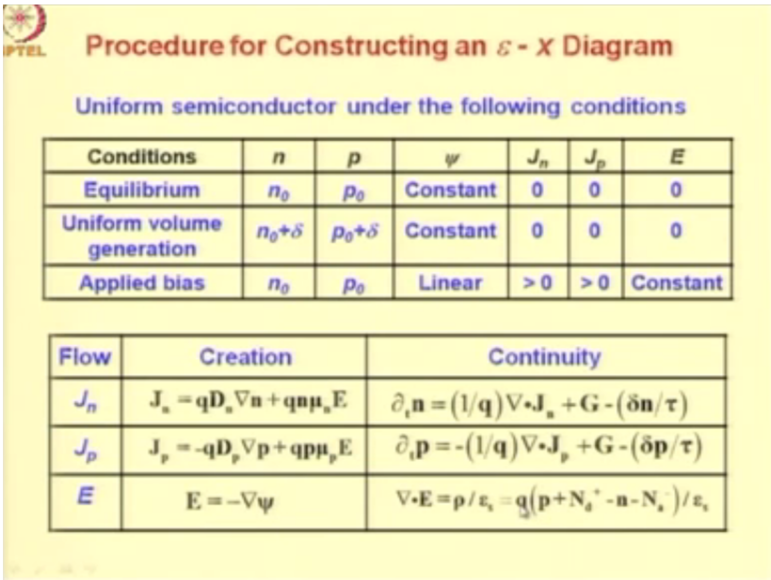

Procedure for Constructing an ε - x Diagram

Uniform semiconductor under the following conditions

Conditions	n	p	ψ	J_n	J_p	E
Equilibrium	n_0	p_0	Constant	0	0	0
Uniform volume generation	$n_0+\delta$	$p_0+\delta$	Constant	0	0	0
Applied bias	n_0	p_0	Linear	> 0	> 0	Constant

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

Just by example let us consider the situation that we discussed so far. So uniform semiconductor under following conditions is what we have discussed equilibrium, uniform volume generation and applied bias. Now for equilibrium n = n0, p is equal p0, psi is constant, Jn is 0, Jp is 0, E is 0. Now we did not specify how we used all these equations to get these 6 quantities.

So there are 6 equations here and there are 6 quantities. This is because equilibrium says that electron and hole concentration should be equilibrium value and since it is a uniform semiconductor, potential is uniform right or constant. This did not require us to go through these equations. So equilibrium means Jn=0, Jp=0 and say if psi is constant E has to be 0. You can however check by substituting these quantities in these equations that these solutions satisfy all these equations.

For uniform volume generation again n and p are uniform though you do have excess carriers here that is why you have this delta; however, uniform semiconductor means size going to be constant and E is going to be 0. Since there is no electric field and concentrations are uniform, there are no diffusion currents or drift currents. So Jn=0 and Jp=0. So that is what is given here.

Now in this particular case, you actually have to solve the continuity equations to get this delta. So for example look at this continuity equation, if n is varying with time, then you can solve this equation to get n or delta. So here since Jn is 0, this term will vanish, your equation would simply be dou n/dou t = G this is the volume generation because of light - delta n/tau where tau is the lifetime.

So you can solve these equations and you will get an exponential solution as a function of time for electron concentration and for delta. Now similarly one can solve the hole continuity equation to get this delta; however, delta is the same for both because the sample is neutral. Therefore, we solve any one of these continuity equations only. As far as electric field is concerned it is 0 and space-charge is also 0, so these equations are really not required.

So this is how you use these equations to get these conditions. Now let us also lay out the conditions for applied bias, which we discussed in today’s lecture. So here n and p are equal to equilibrium values even though you are applying a voltage the concentrations are not changing as compared to equilibrium; however, the psi is now a linear function of x instead of being constant because you applied a voltage and as a consequence you have an electric field and your Jn and Jp are not 0 okay.

So in terms of this equations if you see because carrier concentration is uniform, the different currents are absent however you do have drift currents because E is not 0 and you use E equal - grad psi to get a relation between the constant electric field and the linear potential. The space-charge is 0 so d/dx is 0 and E is constant.

As far as the continuity equations are concerned you find that since it is a steady state condition you applied a DC voltage dou n/dou t and dou p/dou t are 0, no excess carriers therefore these are 0, no excess volume generation and therefore these terms G are 0 and you get diversions of Jn is 0, diversions of Jp is 0 meaning Jn and Jp are constant with x. So that is how we use these equations to get Jn and Jp constant with x for this case.

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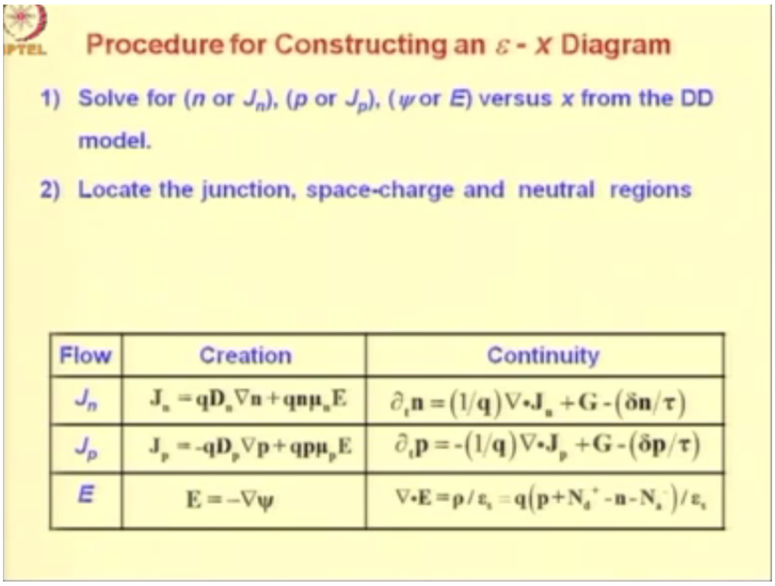

Procedure for Constructing an ε - x Diagram

1) Solve for (n or J_n), (p or J_p), (ψ or E) versus x from the DD model.
2) Locate the junction, space-charge and neutral regions

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

So that is how the equations are being used. So this was our first step solve for n Jn, p Jp, psi E versus x from the drift-diffusion model. The second important step in constructing the E-x diagram is to locate the junction, space-charge, and neutral regions within the device. Now let us take examples of some devices okay and illustrate how do we locate these various regions and points.

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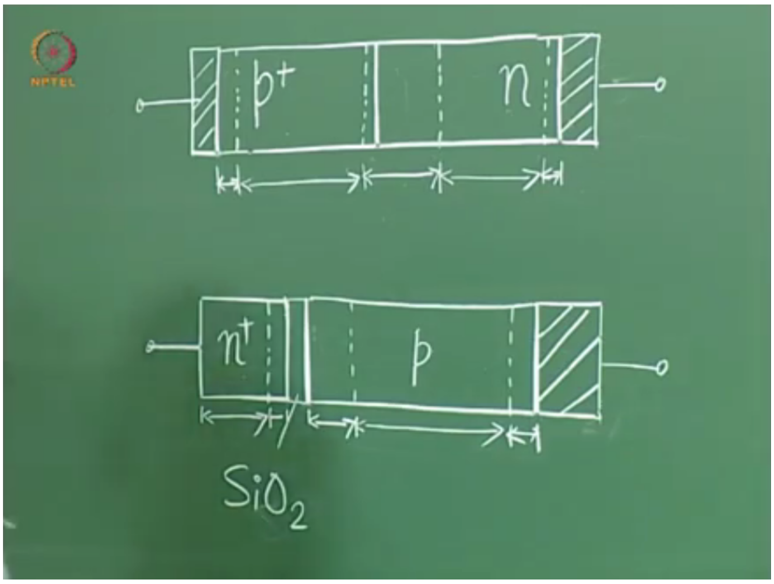

This is a p-n junction. This is an ohmic contact at the left end and an ohmic contact at the right end. Now for this device the junctions are at this location here between the contact and the p+ region, here between the contact and the n region and here between p+ and n regions.

Then this is a space-charge region near the p-n junction. This is the space-charge region near the ohmic contact.

We have not shown the region inside the contact because generally the contacts are made of metal and the space-charge you know is really very, very thin inside the metal. Similarly, this is the space-charge region near this junction. So near junctions in general you will have space-charge regions. Now between the space-charge regions you have the neutral regions so this is a neutral region, this is a neutral region.

Let us take another example. This is a capacitor right so called MOS capacitor. Here the gate is made of polysilicon. In this case, your junctions are located as follows. Now this is a junction between silicon dioxide and n+ region, this is the junction between silicone dioxide and p region, this is the junction between an ohmic contact and the p region okay. You have space-charge regions near the junctions.

This is a space-charge region; this is also a space-charge region. Similarly, you have a space-charge region near the contact and this region is the neutral region okay. Similarly, here this is neutral okay and here also this region is neutral. You can similarly show this region also to be neutral. So we are saying that when you want to draw the band diagram first you must identify these regions in the device.

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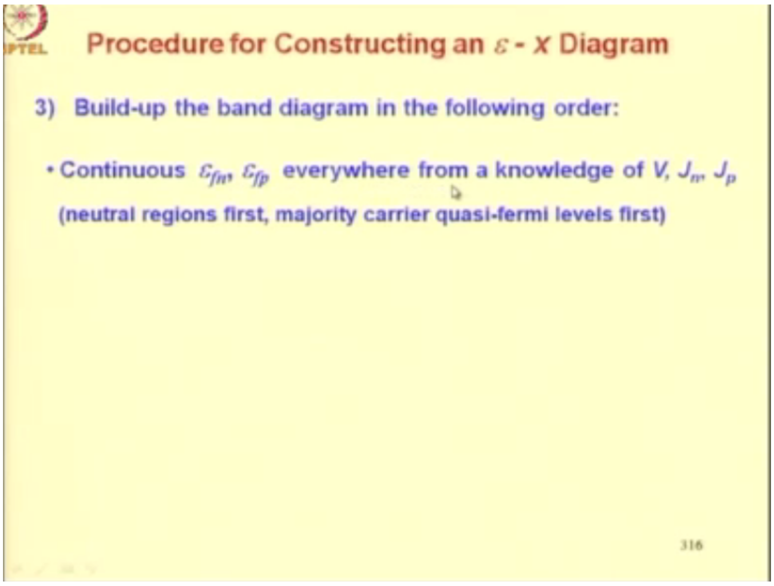

Procedure for Constructing an ε - x Diagram

3) Build-up the band diagram in the following order:

- Continuous ε_{fn}, ε_{fp} everywhere from a knowledge of V, J_n, J_p (neutral regions first, majority carrier quasi-fermi levels first)

316

The next step would be to build up the band diagram or the energy levels in the following order. The first we draw continuous quasi Fermi levels, Efn and Efp everywhere from a knowledge of the applied voltage and the current densities of electrons and holes. Now we may not have actually numerically solved all the equations of the drift-diffusion model to get exact distributions of n, p, Jn, Jp, E and psi okay.

So we may be doing this solution qualitatively even when we are doing it qualitatively, we must do a simultaneous solution that is if I am sketching qualitatively let us say n and p as a function of x I must remember how n and p as a function of x will be affected by psi as a function of x and how the psi will be affected by n and p. So mentally you have to do a simultaneous solution while plotting all these okay.

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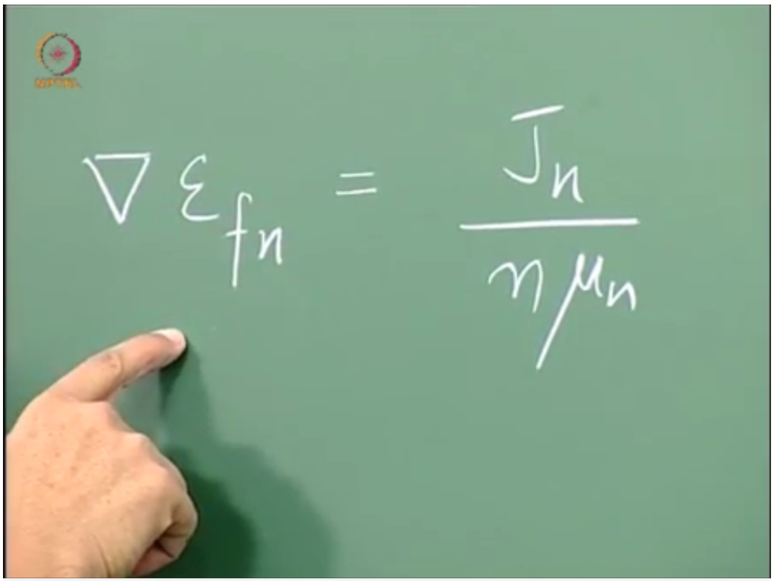

$$\nabla \mathcal{E}_{fn} = \frac{J_n}{n\mu_n}$$

Now after having done that you can use that information to locate the quasi Fermi levels. Now quasi Fermi levels should be drawn as a continuous line because if there is abrupt change in quasi Fermi level anywhere then we know from the equation, for example gradient of Efn = Jn/n mu n. So if there is an abrupt change in Efn, gradient of Efn goes to infinity, this would amount to infinite current density, which is not possible.

Therefore, Efn and Efp should always be continuous. Now since we are asking you to draw Efn and Efp everywhere this means in space-charge, neutral and junction regions, issue arises which region do you draw the levels first? So the guideline is first draw the levels in the neutral region and further since you are drawing both Efn and Efp, which one to draw first of these 2? So draw the majority carrier quasi Fermi levels first.

So neutral region first and majority carrier quasi Fermi level first. Will illustrate this with the help of some examples later on.

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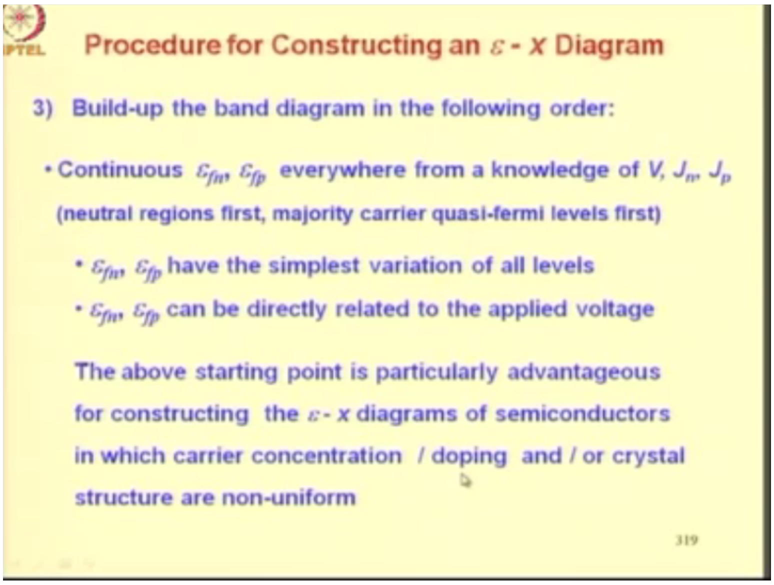

Procedure for Constructing an ε - x Diagram

3) Build-up the band diagram in the following order:

- Continuous ε_{fn}, ε_{fp} everywhere from a knowledge of V, J_n, J_p (neutral regions first, majority carrier quasi-fermi levels first)
  - ε_{fn}, ε_{fp} have the simplest variation of all levels
  - ε_{fn}, ε_{fp} can be directly related to the applied voltage

The above starting point is particularly advantageous for constructing the ε - x diagrams of semiconductors in which carrier concentration / doping and / or crystal structure are non-uniform

Now what is the reason that you start with Efn and Efp. The Efn and Efp have the simplest variation of all levels this is the reason. Another reason is Efn and Efp can be directly related to the applied voltage V. We will shortly explain why this is the case. Now before we do that let us make the point that the above starting point that is starting with the quasi Fermi levels for electrons and holes is particularly advantages for constructing the E-x diagrams of semiconductors in which carrier concentration or doping and/or crystal structure are non-uniform.

So in semiconductors where conditions are non-uniform lot of variations conditions are there, this starting point proves particularly advantages.

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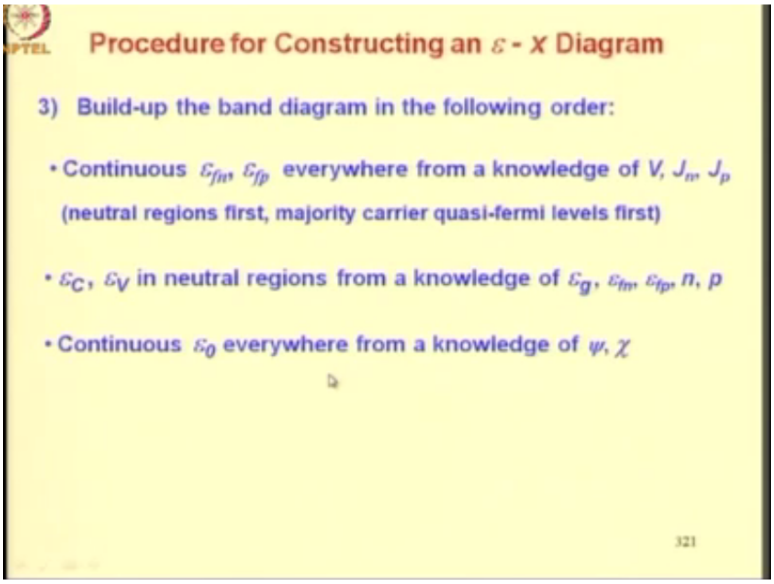

Procedure for Constructing an ε - x Diagram

3) Build-up the band diagram in the following order:

- Continuous ε_{fn}, ε_{fp} everywhere from a knowledge of V, J_n, J_p (neutral regions first, majority carrier quasi-fermi levels first)
- ε_C, ε_V in neutral regions from a knowledge of ε_g, ε_{fn}, ε_{fp}, n, p
- Continuous ε_0 everywhere from a knowledge of ψ, χ

The next step is Ec and Ev in neutral regions from the knowledge of the energy gap, quasi Fermi levels, electron concentrations and hole concentrations. Next we draw a continuous E0 everywhere from a knowledge of electrostatic potential psi and electron affinity chi okay. So because you have drawn Ec and Ev you can locate E0 in the neutral regions above a distance chi from Ec and Ev.

And then you can connect the E0 in the neutral regions why other space-charge region. So in the space-charge region then you can use the psi electrostatic potential. We will explain this point. Now why should E0 be continuous? As we have remarked the gradient of E0 actually reflects the electric field.

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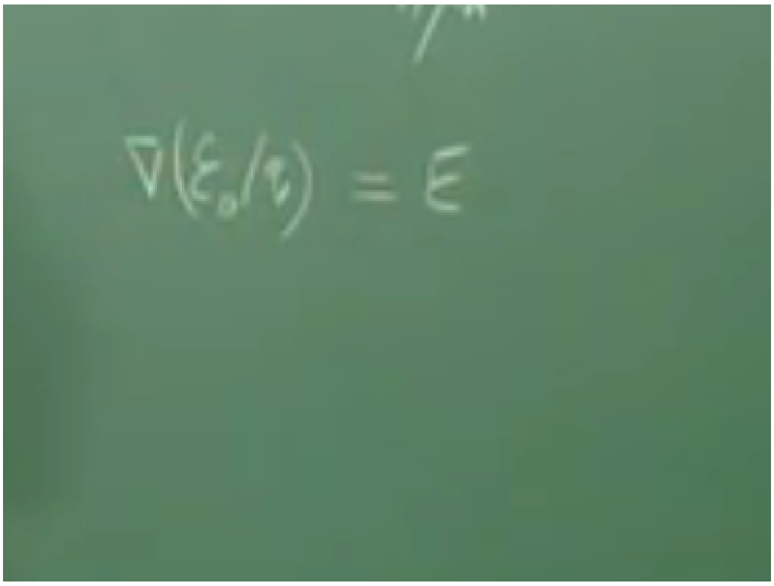

$$\nabla(\mathcal{E}_0/q) = \mathcal{E}$$

So this is E, so if E0 changes abruptly at any point it means gradient of E0/q is infinity it would amount to having an infinite electric field and this is not possible. That is why E0 should be continuous.

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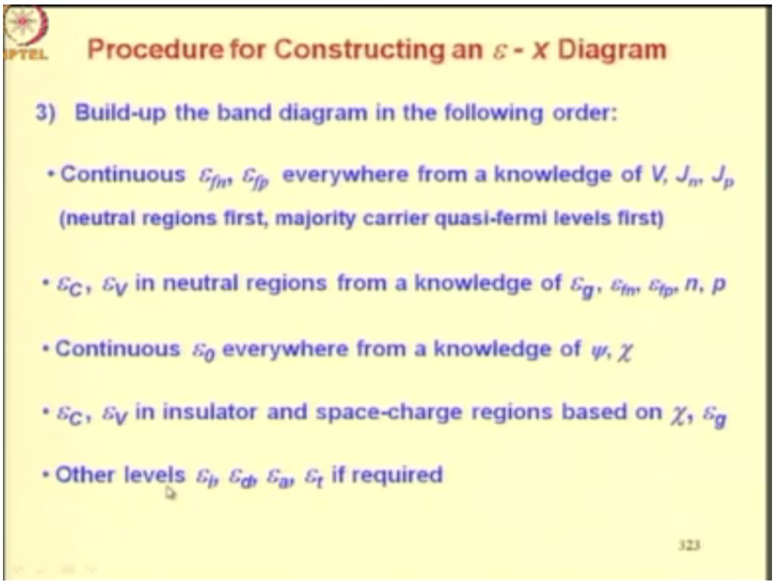

Procedure for Constructing an ε - x Diagram

3) Build-up the band diagram in the following order:

- Continuous ε_{fn}, ε_{fp} everywhere from a knowledge of V, J_n, J_p (neutral regions first, majority carrier quasi-fermi levels first)
- ε_C, ε_V in neutral regions from a knowledge of ε_g, ε_{fn}, ε_{fp}, n, p
- Continuous ε_0 everywhere from a knowledge of ψ, χ
- ε_C, ε_V in insulator and space-charge regions based on χ, ε_g
- Other levels ε_i, ε_d, ε_a, ε_t if required

323

After we have sketched E0 as a continuous line everywhere then sketch Ec and Ev in the insulator and space-charge regions based on knowledge of electron affinity chi and Eg. So based on chi you can locate Ec as E0 - chi into q of course and you can locate Ev at a distance energy gap below Ec. Then you can show other levels such as intrinsic level, donor level, acceptor level, trap level and so on if required.

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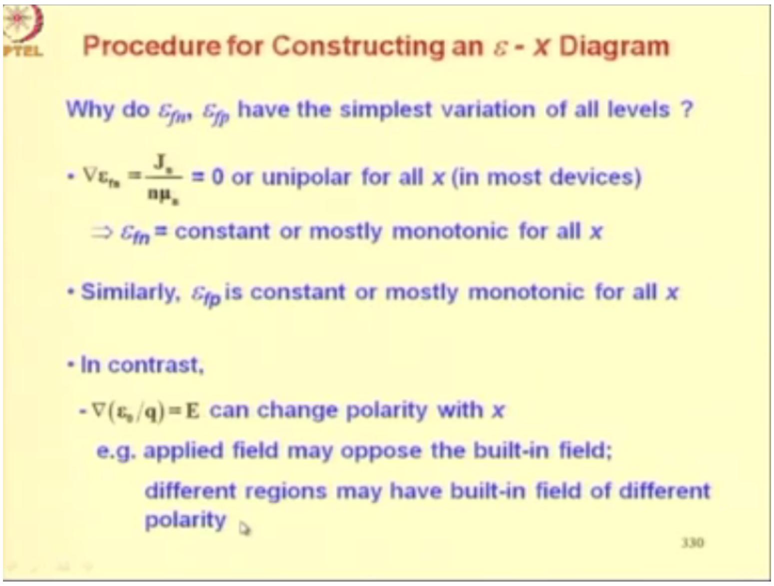

Procedure for Constructing an ε - x Diagram

Why do ε_{fn}, ε_{fp} have the simplest variation of all levels ?

- $\nabla \varepsilon_{fn} = \frac{J_n}{n\mu_n}$ = 0 or unipolar for all x (in most devices)
  $\Rightarrow \varepsilon_{fn}$ = constant or mostly monotonic for all x
- Similarly, ε_{fp} is constant or mostly monotonic for all x
- In contrast,
  - $\nabla(\varepsilon_0/q) = E$ can change polarity with x
    e.g. applied field may oppose the built-in field;
    different regions may have built-in field of different polarity

330

Now let us explain why do Efn and Efp have the simplest variation of all levels? If you take this equation gradient of Efn = Jn/n mu n. Now gradient of Efn is either 0 in case of equilibrium or unipolar for all x in most devices. Now why is it unipolar? Because the Jn has to be in a particular direction throughout the device it has to be in the same direction. Jp also similarly has to be in the same direction.

So this means that gradient of Efn should have the same sign throughout the device. This is a non-equilibrium case so either gradient of Efn is 0 or unipolar. This means that Efn is either constant or mostly monotonic for all x. So when you say mostly it is because in most devices the current Jn is in the same direction throughout the device. In a similar way, we can show that Efp is either constant or monotonic for all x.

Now if you contrast this situation with for example E0, now gradient of E0/q = E it can change polarity with x. So while gradient of Efn has to remain unipolar for all x in a device, the gradient of E0 can change polarity with x. Examples, applied field may oppose the built-in field.

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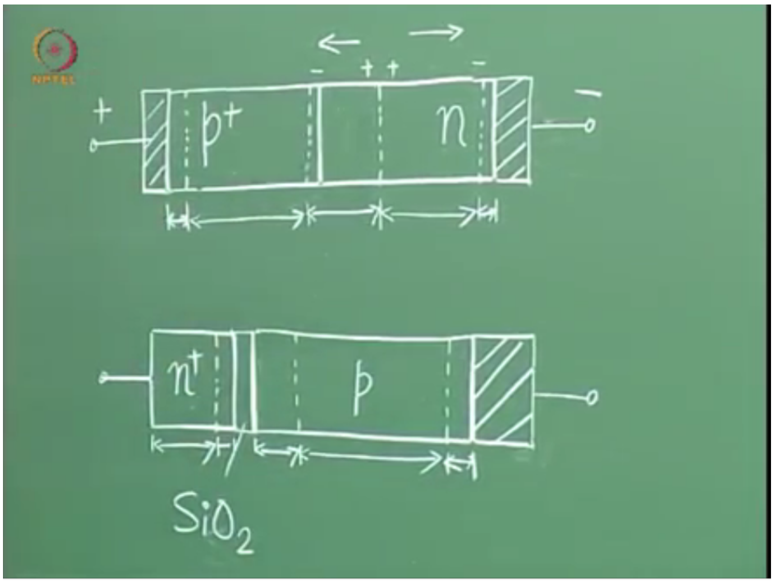

So suppose you take this p-n junction, the built-in field here is directed from n to p, so built-in potential positive at this end, negative at this end, but when you apply a forward bias, p is positive with respect to n and when the part of this forward bias falls across say n region, then the potential drop in this direction. So you can see that this potential drop opposes this potential drop right.

So therefore the field E here is like this, but the space-charge region it is like this so it is changing sign you can similarly have potential drops here okay. So this is an example where applied voltage opposes the built-in voltage. So applied field opposes the building field. Another example is different regions may have built-in field of different polarity.

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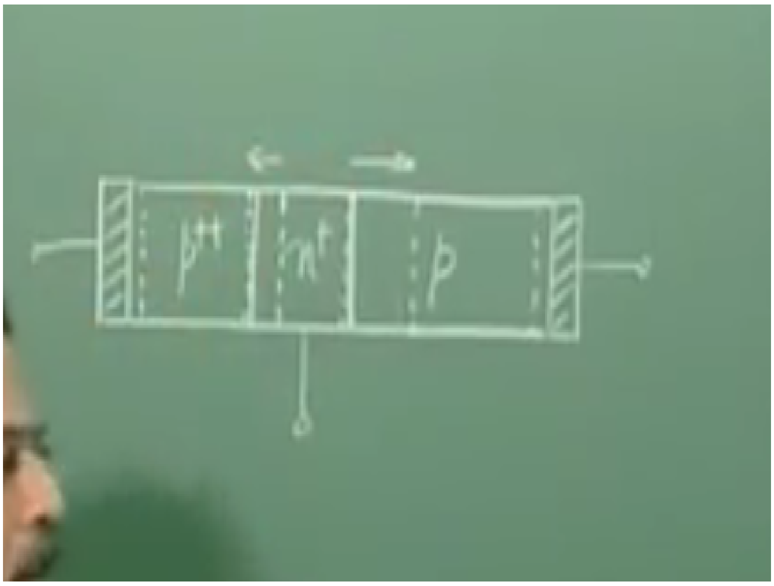

Take this bipolar transistor, now here if I take the space-charge region associated with the emitter base junction, the built-in electric field is like this whereas if I take the built-in field associated with this space-charge region, base collector it is directed from n to p. So you can see that the field is changing polarity.

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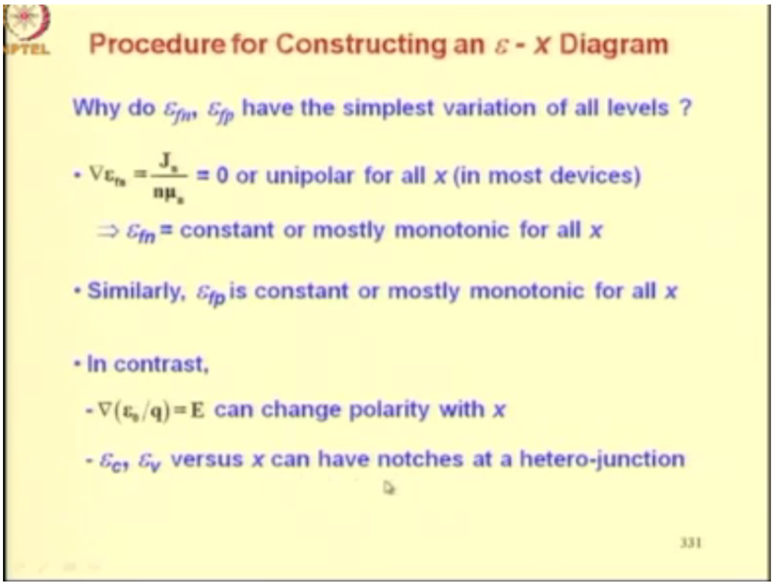

Procedure for Constructing an $\mathcal{E}$ - x Diagram

Why do $\mathcal{E}_{fn}$, $\mathcal{E}_{fp}$ have the simplest variation of all levels ?

- $\nabla \mathcal{E}_{fn} = \frac{J_n}{n\mu_n}$ = 0 or unipolar for all x (in most devices)
  - $\Rightarrow \mathcal{E}_{fn}$ = constant or mostly monotonic for all x
- Similarly, $\mathcal{E}_{fp}$ is constant or mostly monotonic for all x
- In contrast,
  - $\nabla(\mathcal{E}_s/q) = E$ can change polarity with x
  - $\mathcal{E}_c$, $\mathcal{E}_v$ versus x can have notches at a hetero-junction

If you consider Ec and Ev variations then Ec Ev versus x can have notches at a hetero-junction so you can have sharp peaks or troughs. Now this point will become clear when we actually draw the band diagram of a hetero-junction, which we are going to do later in this lecture.

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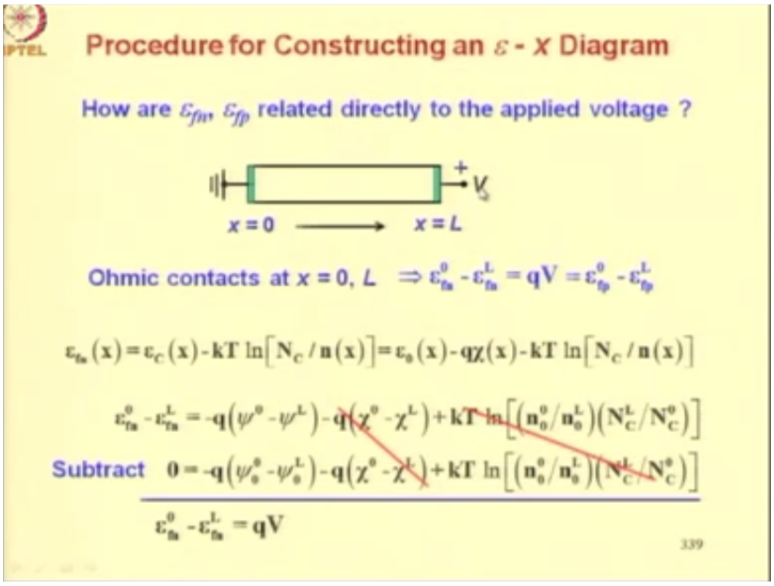

Procedure for Constructing an ε - x Diagram

How are ε_{fn}, ε_{fp} related directly to the applied voltage ?

Ohmic contacts at $x = 0, L$ $\Rightarrow \varepsilon_{fn}^{0} - \varepsilon_{fn}^{L} = qV = \varepsilon_{fp}^{0} - \varepsilon_{fp}^{L}$

$$\varepsilon_{fn}(x) = \varepsilon_C(x) - kT\ln\left[N_C/n(x)\right] = \varepsilon_0(x) - q\chi(x) - kT\ln\left[N_C/n(x)\right]$$

$$\varepsilon_{fn}^{0} - \varepsilon_{fn}^{L} = -q\left(\psi^{0} - \psi^{L}\right) \cancel{- q\left(\chi^{0} - \chi^{L}\right)} + kT\ln\left[\left(n_0^{0}/n_0^{L}\right)\cancel{\left(N_C^{L}/N_C^{0}\right)}\right]$$

Subtract $0 = -q\left(\psi_0^{0} - \psi_0^{L}\right) \cancel{- q\left(\chi^{0} - \chi^{L}\right)} + kT\ln\left[\left(n_0^{0}/n_0^{L}\right)\cancel{\left(N_C^{L}/N_C^{0}\right)}\right]$

$$\varepsilon_{fn}^{0} - \varepsilon_{fn}^{L} = qV$$

339

How are Efn and Efp related directly to the applied voltage? That is the next question we need to answer related to the statement that Efn and Efp should be used as a starting point for drawing the energy band diagram. Now consider any general device like this where this region may contain junctions, non-uniform conditions and so on. So we make no particular assumptions regarding the nature of variation in this region.

The device has 2 contacts at x=0 and x=L. Will assume that the contacts are ohmic. This means that carrier concentrations will be at equilibrium even when you apply a voltage at these contacts. So ohmic contacts at x = 0 and L. Now we can show that if this is the case if your ohmic contacts then Efn at x = 0 - Efn at x = L = q times V and the same thing applies even for the difference between the quasi Fermi level for holes at x=0 and x=l.

Let us see how we can show this. Now we know that Efn as a function of x is nothing but Ec as a function of x - kT ln Nc/n as a function of x. Now you write Ec x in terms of E0 x and electron affinity so this is the relation. Now I can take the Efn at 0 and Efn at L in terms of E0 at x = 0 and L, chi at x = 0 and L and so on, n0 x = 0 and L.

So I will get this relation Efn at x = 0 - Efn at x = L = - of q times psi at 0 - psi at L - q times electron affinity at 0 - electron affinity at L+kT into logarithm of n at 0 divided by n at L. We are using the equilibrium values because we have ohmic contacts at x = 0 and L and multiplied by the conduction band effective density of states Nc at L divided by Nc at 0.

So we are taking a general situation where conditions may change within this region okay. So that is why electron affinity has been assumed to be different in general at x = 0 and L. Nc is assumed to be different at x equal L and x = 0. Now one point, how do you get psi here whereas you had E0? Here what we have done is we have used the relation for E0 in terms of psi. So they are linearly related E0 and psi we know that we have just seen.

So this fact has been used here except that there is a negative sign because E0 is electronic potential energy whereas psi is potential of a positive charge. If I write the same equation under equilibrium, we know that Efn at 0 and Efn at L will have to be the same under equilibrium because Efn has to be constant because there can be no current Jn at equilibrium so Jn is 0 means gradient of Efn is 0 this means Efn at 0 = Efn at L.

Right hand side is potential at x = 0 correspond to equilibrium potential at L corresponding to equilibrium therefore you have the suffix 0 and the remaining part of the equation remains the same both under equilibrium and applied bias. So now if you subtract this equilibrium equation from this equation for applied bias, then these terms will cancel and one can easily show that right hand side will become q times V.

Now this is seen easily because suppose I assume x = 0 as a reference potential then at x = 0 the psi remains = 0 both under equilibrium and under applied bias so this quantity let us assume to be 0 for reference then all that we have to show is psi of L - psi of L under applied bias - psi of L under equilibrium is applied voltage now which is straight forward to see.

So at x=L, the potential under applied bias and potential under equilibrium the difference between the 2 will have to be equal to applied voltage if you take x=0 as a reference.

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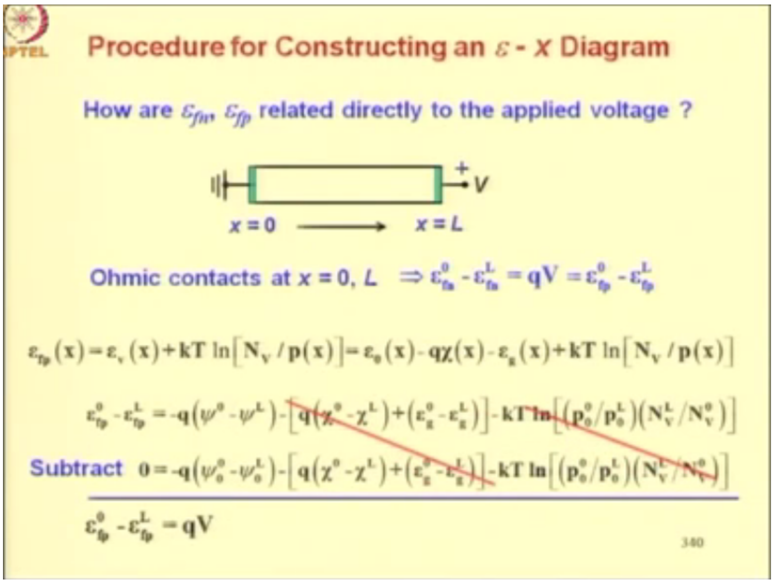

Procedure for Constructing an ε - x Diagram

How are ε_{fn}, ε_{fp} related directly to the applied voltage ?

Ohmic contacts at $x = 0, L$ $\Rightarrow \varepsilon_{fn}^{0} - \varepsilon_{fn}^{L} = qV = \varepsilon_{fp}^{0} - \varepsilon_{fp}^{L}$

$$\varepsilon_{fp}(x) = \varepsilon_{v}(x) + kT\ln\left[N_V/p(x)\right] = \varepsilon_{0}(x) - q\chi(x) - \varepsilon_{g}(x) + kT\ln\left[N_V/p(x)\right]$$

$$\varepsilon_{fp}^{0} - \varepsilon_{fp}^{L} = -q\left(\psi^{0} - \psi^{L}\right) - \cancel{\left[q\left(\chi^{0} - \chi^{L}\right) + \left(\varepsilon_{g}^{0} - \varepsilon_{g}^{L}\right)\right]} - kT\cancel{\ln\left[\left(p_{0}^{0}/p_{0}^{L}\right)\left(N_V^{L}/N_V^{0}\right)\right]}$$

Subtract $0 = -q\left(\psi_{0}^{0} - \psi_{0}^{L}\right) - \cancel{\left[q\left(\chi^{0} - \chi^{L}\right) + \left(\varepsilon_{g}^{0} - \varepsilon_{g}^{L}\right)\right]} - kT\cancel{\ln\left[\left(p_{0}^{0}/p_{0}^{L}\right)\left(N_V^{L}/N_V^{0}\right)\right]}$

$$\varepsilon_{fp}^{0} - \varepsilon_{fp}^{L} = qV$$

Exactly similar approach can be used to show that Efp at x = 0 - Efp at x = L is q times V. The only difference here is that in your equation for Efp you have Ev and you have a positive sign here when you have hole sensitive of electrons here and this is effective density of states at the valence bandage and when you want to write Ev in terms of E0 then you will have apart from electron affinity also the energy gap coming in.

Then this E0 is converted into electrostatic potential just the way we did for quasi Fermi levels for electrons and you end up with this relation. Now note that the quasi Fermi level at 0 will be higher than the quasi Fermi level at L for both electrons and holes when you apply a positive voltage to x = L. Now this is because E represents electronic energies whereas V represents the voltage or potential corresponding to positive charge.

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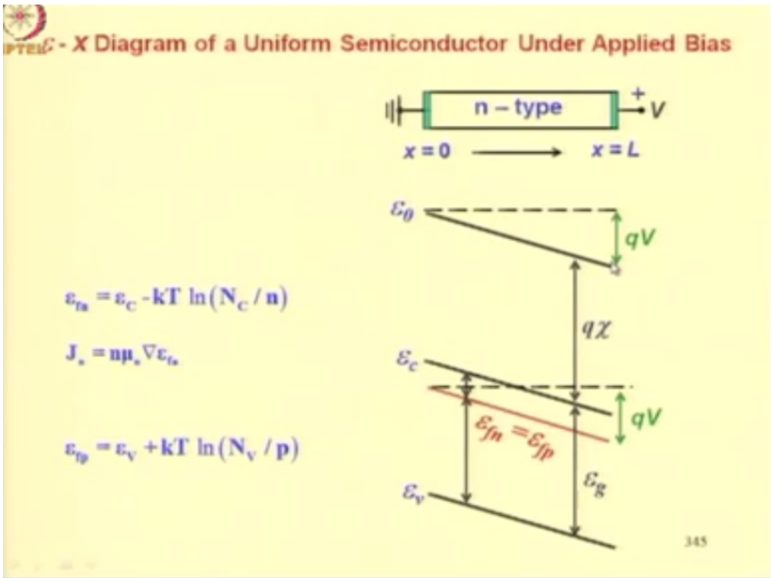

ε - x Diagram of a Uniform Semiconductor Under Applied Bias

$\varepsilon_{fn} = \varepsilon_{C} - kT\ln\left(N_C/n\right)$

$J_n = n\mu_n\nabla\varepsilon_{fn}$

$\varepsilon_{fp} = \varepsilon_{V} + kT\ln\left(N_V/p\right)$

Now let us redraw the E-x diagram of a uniform semiconductor under applied bias using the procedure that we have just outlined meaning we start from the quasi Fermi level first and then build up all the levels. So in this case you start from Efn now you know that Efn will be varying linearly as a function of x and it will go down in this fashion because this is the relevant equation.

We know that Jn is constant with x therefore gradient of Efn is constant. The Jn is in the negative x direction because it is from right hand side to left hand side. Therefore, gradient of Efn is negative. Now you can locate Ec above Efn using this formula in terms of the electron concentration. You locate Ev as a distance Eg below Ec and when you locate quasi Fermi level for holes it will turn out to be the same as quasi Fermi level for electron when you use this formula.

Then you can locate E0 at a distance q times chi above Ec. The E0 will turn out to be linear in this whole procedure because it simply follows the Efn, which was linear because of the conditions in the device. So this is how you get the E0 variation over the length to be equal to q times V. Now you might wonder last time you had used an equation for psi what happened to that? Why have we not used it in this case?

Well as we have said in our procedure we have to first solve for n, p and psi simultaneously from the drift-diffusion model so moment we have made some assumption about electron concentration, hole concentration and psi as a function of x in the device, we have in some way utilized all the equations of the drift-diffusion model okay. So when I used this equation to locate for example Ec as a straight line above Efn have used information about electron concentration and in principle since the equations of drift-diffusion model are coupled to get the electron concentration, I have used the equation for the potential also.

So this is how we actually use all the equations of the drift-diffusion model okay. For instance, when we drift the energy levels starting from E0 we did not write this equation for current density in terms of gradient of Efn explicitly; however, indirectly one can show this equation was used in that case.

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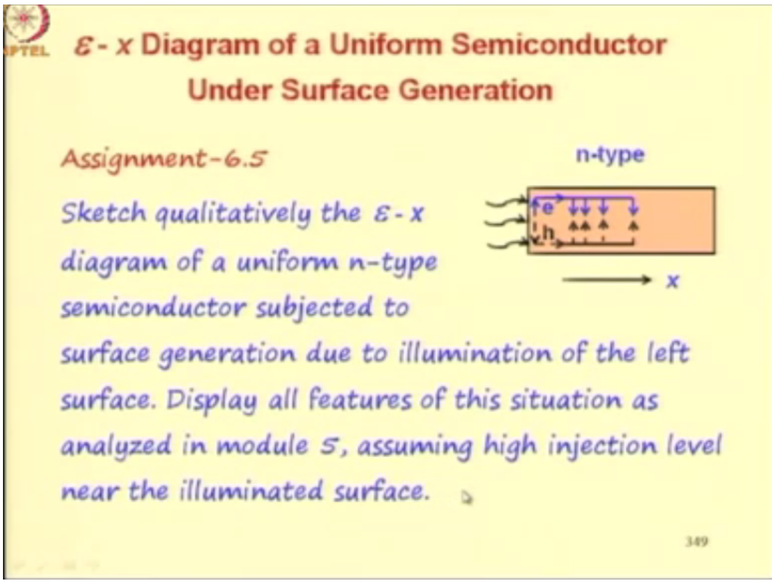

$\mathcal{E}$ - x Diagram of a Uniform Semiconductor Under Surface Generation

Assignment-6.5

Sketch qualitatively the $\mathcal{E}$ - x diagram of a uniform n-type semiconductor subjected to surface generation due to illumination of the left surface. Display all features of this situation as analyzed in module 5, assuming high injection level near the illuminated surface.

Now here is an assignment E-x diagram of a uniform semiconductor under surface generation. Sketch qualitatively the E-x diagram of a uniform n-type semiconductor subjected to surface generation due to illumination of the left surface. So here the surface is illuminated. Electron hole pairs are generated at this end, they move in and then recombine. Display all features of this situation as analyzed in module 5 assuming high injection level near the illuminated surface.

In module 5, we analyzed this situation completely assuming low injection level so the only difference now is that you must assume high injection level near the illuminated surface. So from the analysis you will get n, p, Jn, Jp and psi and electric field as a function of x and use that information to draw the energy band diagram.

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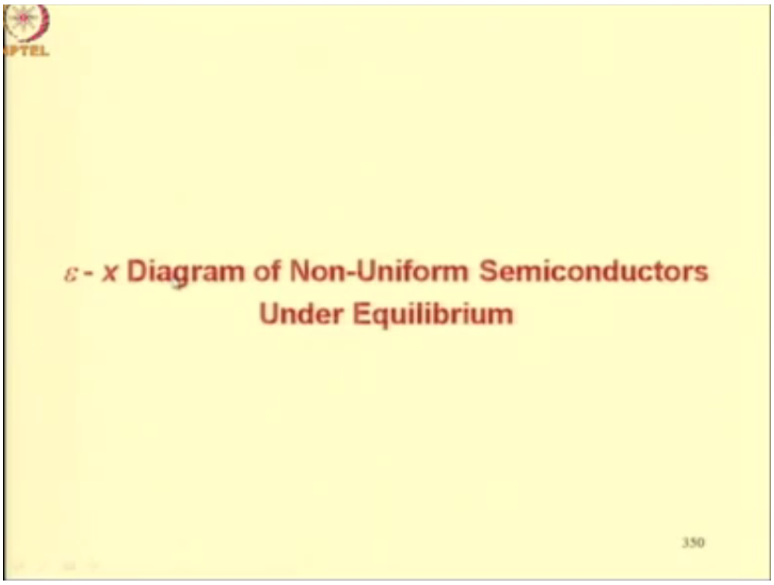

$\mathcal{E}$ - x Diagram of Non-Uniform Semiconductors Under Equilibrium

Let us discuss now E-x diagram of non-uniform semiconductors under equilibrium. So there are several kinds of non-uniformities that can arise in semiconductors such as non-uniform doping, non-uniform composition of crystal structure, combination of these and so on.

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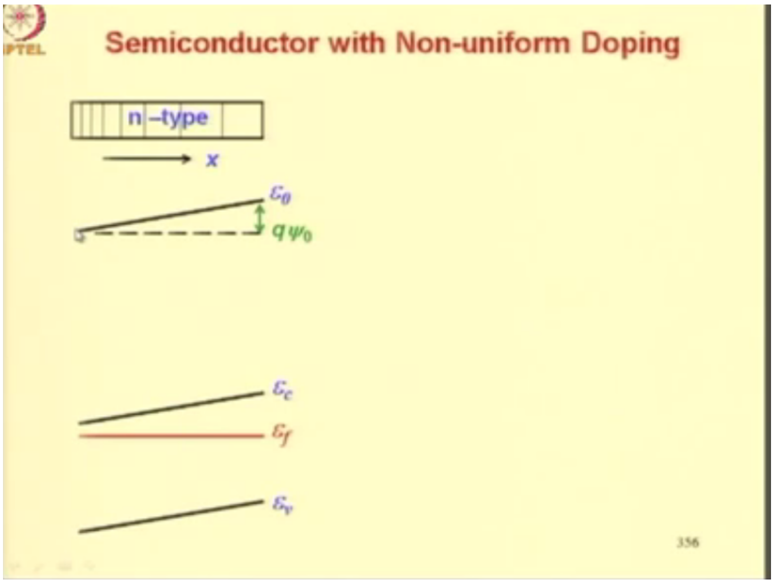

Semiconductor with Non-uniform Doping

Let us say semiconductor with non-uniform doping okay. Crystal structure remains the same, but doping is varying as a function of x. So here for instance the n-type doping is more on the left hand side than on the right hand side that is the meaning of these vertical lines. How do you draw the band diagram? So you start with a constant Fermi level because it is equilibrium Jn and Jp both are 0 and Efn = Efp = Ef and it is drawn as a constant line.

Then I draw Ec as a function of x. Here I have drawn Ec as a straight line why it should be straight? Let us come to that in a moment. First let us explain why is the line sloping up when you move in the positive x direction? This difference is related to the electron concentration we know that and electron concentration is decreasing as you go from left end to right end because our doping is decreasing from left to right.

Now the reason the line is drawn straight is that we have assumed an exponential doping so the doping decreases exponentially from left to right something like this.

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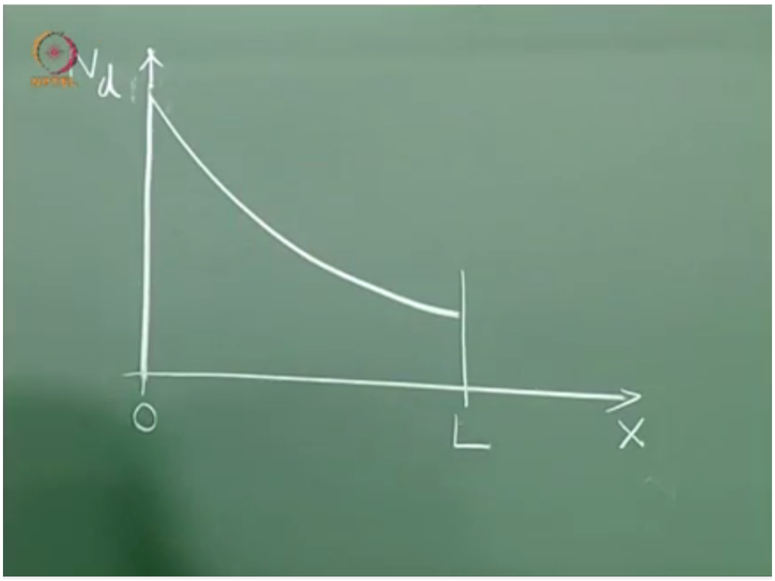

Now as a result your electron concentration if we assume it to be approximately equal to the doping that would also decrease exponentially okay. This is L, if there is exponential variation as a function of x then because of the logarithmic dependence of Ec-Ef on the electron concentration the variation in Ec-Ef would be linear that is why Ec is drawn as a straight line.

Then we draw Ev below Ec at a distance equal to energy gap and then we draw E0 above Ec at a distance of the electron affinity. This difference between E0 at the right end and left end = q times psi 0 where psi 0 is the built-in potential. So this is how you get a built-in potential when you have non-uniform doping.

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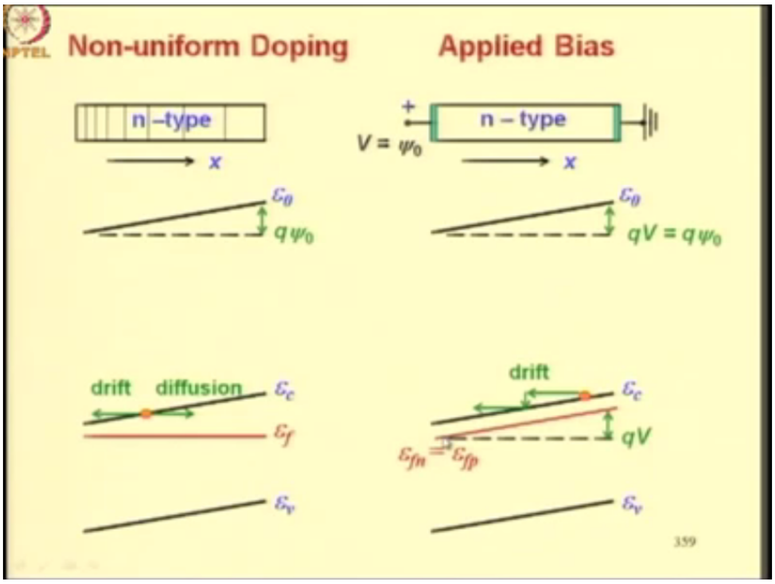

Non-uniform Doping

Applied Bias

It will be of interest to compare this non-uniform doping with the applied bias case where also we had energy level slanting in this fashion right. So what was the difference? The Fermi level however was not constant in that case so here is the reproduction of the diagram for applied bias. Specifically, in this case, we have assumed that the applied voltage q times V = the q times the built-in voltage that we have got here.

So the difference between these 2 diagrams is that the quasi Fermi level is not a constant because there is a non-zero current flow. Further other differences are constant Fermi level and a slanting Ec. A slanting Ec means there is an electric field, which influences the conduction electrons and this means there is a tendency for drift in this direction. However, since this is equilibrium there can be no net current.

And this is because the tendency for drift is balanced by the tendency for diffusion. Because an increasing distance between Ec and Ef from left to right means the electron concentration is decreasing from left to right and there is a tendency for diffusion. So at each point the drift is being balanced by diffusion. Now this is what is brought out by a combination of the variations of Ec and Ef, a constant Ef and an increasing Ec.

On the other hand, here, the same Ec variation implies electric field and therefore a drift current in this direction right. So this movement of the electron in the conduction band shows the drift so electron is moving between 2 collisions it has a constant energy, at this point it undergoes scattering so its velocity is randomized and then it again starts accelerating right so against the direction of the electric field.

So this is what is shown by this variation Ec. Here however there is no diffusion current because distance between Ec and Ef and Efp is constant throughout electron concentration and hole concentrations of the constant, so no diffusion current, only drift current.

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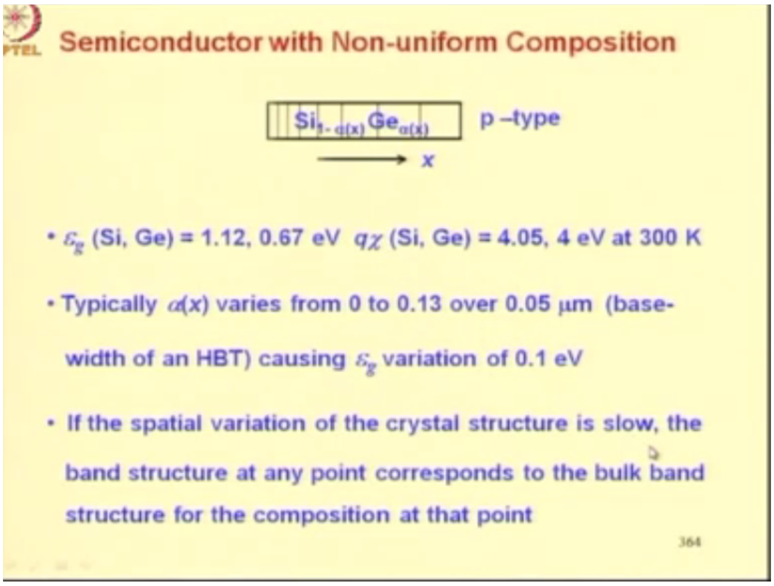

Semiconductor with Non-uniform Composition

$Si_{1-\alpha(x)}Ge_{\alpha(x)}$ p –type

- $\mathcal{E}_g$ (Si, Ge) = 1.12, 0.67 eV $q\chi$ (Si, Ge) = 4.05, 4 eV at 300 K
- Typically $\alpha(x)$ varies from 0 to 0.13 over 0.05 μm (base-width of an HBT) causing $\mathcal{E}_g$ variation of 0.1 eV
- If the spatial variation of the crystal structure is slow, the band structure at any point corresponds to the bulk band structure for the composition at that point

Towards the end of the lecture, let us discuss semiconductor with non-uniform composition. Specifically let us take an example, assume that this is a compound semiconductor silicon germanium. So you are adding more and more atoms of germanium to silicon, left end is let us say pure silicon, high concentration of silicon atoms therefore and as you move to the right the silicon is being replaced by germanium progressively.

Let us assume that this is a p-type semiconductor. Let me give you a feel for numbers in this situation. The energy gap of silicon and germanium are 1.12 and 0.67 electron volt at 300 K. The electron affinity of silicon and germanium is 4.05 and 4 so not very much different mostly the same. Therefore, as a composition changes from left to right there would be not much change in the electron affinity though the energy gap will change significantly as brought out by these numbers.

Now typically in a device alpha x varies from say 0 to 0.13 that means 13% germanium at this end over 0.05 micron. So the width of this sample here this is 0.05 microns, so this example is related to base width of hetero-junction bipolar transistor causing an Eg variation of 0.1 electron volt from left end to right end.

Now the important point to note while drawing the band diagram is that if the spatial variation of the crystal structure is slow as it happens in most cases such as this, the band structure at any point that means at any x corresponds to the bulk band structure for the composition at that point. So now this is important approximation that we made to draw the band picture. So let us draw the band picture. How do we draw it?

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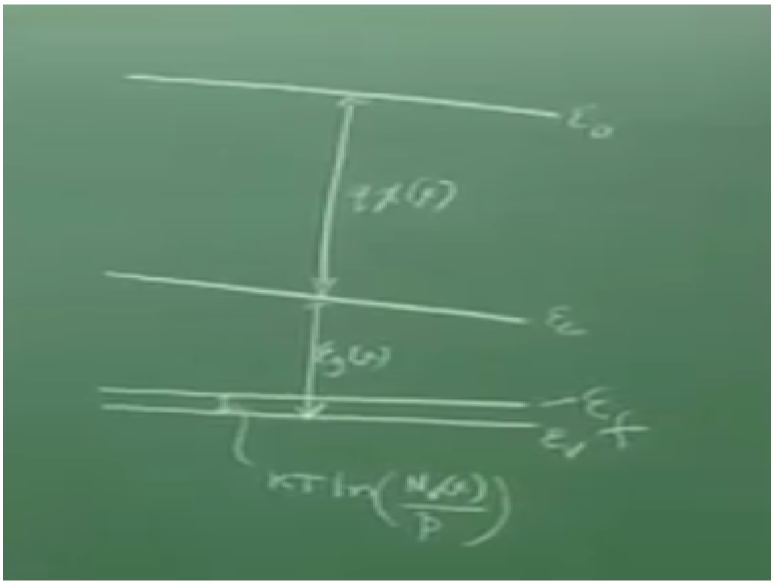

So going by the procedure that we have outlined, first I draw the Fermi level now that is drawn on the constant line because it is equilibrium then I can locate either the Ec or the Ev. In this case, since it is a p-type semiconductor and doping is uniform, I prefer to locate the Ev at a constant distance from Ef. Now you might say if the composition is varying, the effective density of states in the valence band would also vary yes.

However, since in the formula which gives you the difference between these 2, which is = kT ln Nv x by hole concentration p, this Nv x appears in the logarithm so any variation in Nv does not have that much impact on the difference. Now we sketch Ec at a distance Eg above. Now left end is silicon, right end is germanium therefore the energy gap is decreasing from left to right.

So this is energy gap at any x the value of energy gap is obtained from the value of alpha x okay. So here this is the alpha x okay from the value of alpha. Now we are assuming a linear grading therefore the energy gap also varies linearly. I have exaggerated the variation in the energy gap just to make points clear.

So this is your Ec then I take electron affinity above this and then draw E0 so this is electron affinity as a function of x. Now we have just remarked that the electron affinity does not change significantly therefore E0 will be parallel to Ec though Ec is not parallel to Ev because Eg x is varying with distance. So that is how you can draw this band diagram for non–uniform composition.

Now in fact it will not be very difficult for you to draw a band diagram for the situation where doping also is varying with x because even then you would start with the constant Ef and then the distance between Ef and Ev would vary right, but you will go in this order.

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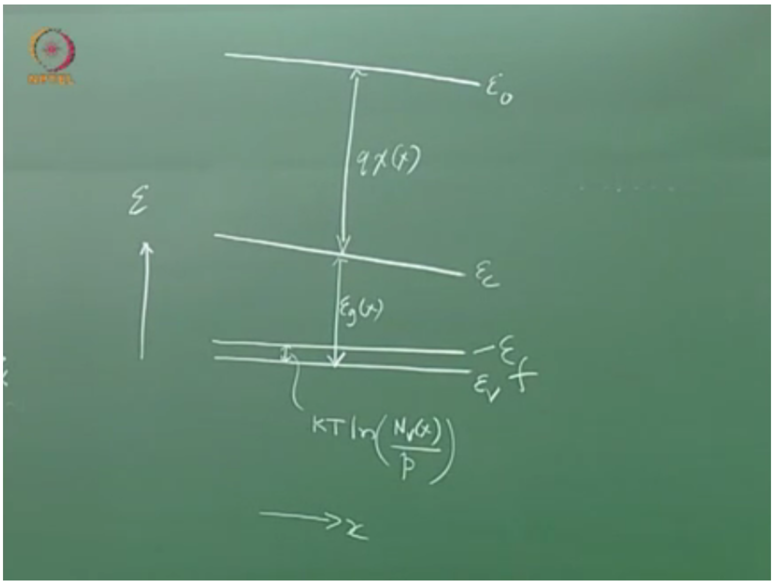

Here this is x and this is electronic energy now let us give you an assignment related to composition graded semiconductors.

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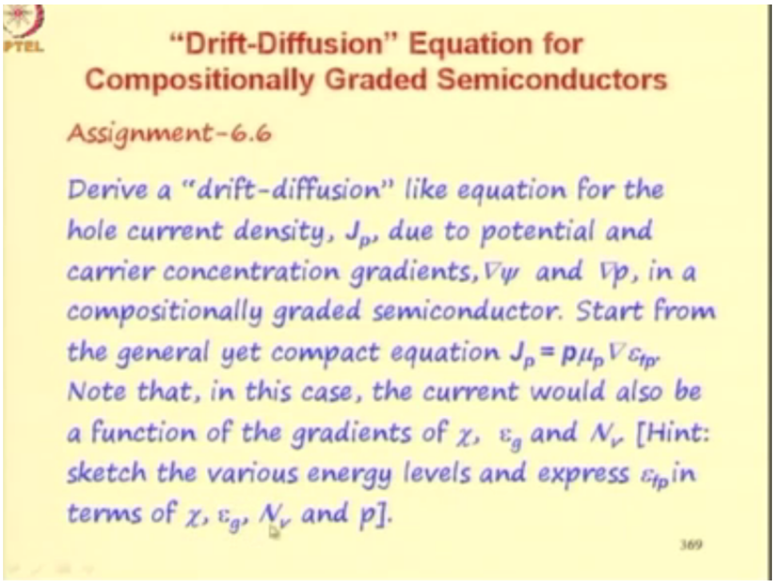

"Drift-Diffusion" Equation for Compositionally Graded Semiconductors

Assignment-6.6

Derive a "drift-diffusion" like equation for the hole current density, J_p, due to potential and carrier concentration gradients, $\nabla\psi$ and ∇p, in a compositionally graded semiconductor. Start from the general yet compact equation $J_p = p\mu_p \nabla \varepsilon_{fp}$. Note that, in this case, the current would also be a function of the gradients of χ, ε_g and N_v [Hint: sketch the various energy levels and express ε_{fp} in terms of χ, ε_g, N_v and p].

Derive a drift-diffusion like equation for the hole current density Jp due to potential and carrier concentration gradients grad psi and grad p in a compositionally graded semiconductor. Start from the general yet compact equation Jp = p times mu p into gradient of Efp. Note that in this case, the current would also be a function of the gradients of chi, Eg and Nv.

So a hint is given, sketch the various energy levels and express Efp in terms of the electron affinity Eg, Nv and hole concentration and then you can apply this equation and substitute it in this formula to derive the transport equation.

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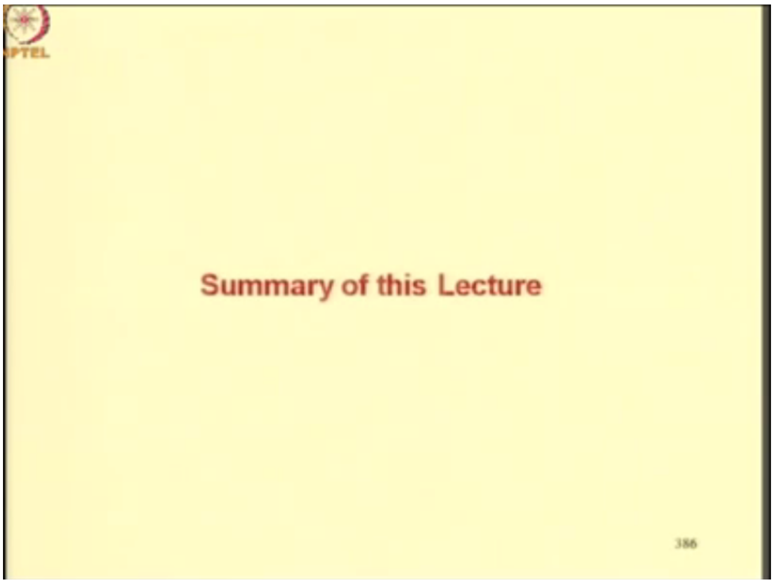

Summary of this Lecture

386

Now we have come to the end of this lecture. Let us make a summary of the important points. So in this lecture, we continued to discuss the E-x diagram for semiconductors and devices. Specifically, we considered the E-x diagram of a uniform semiconductor and applied bias and then we considered energy band diagram of non-uniform semiconductors under equilibrium. We considered 2 types of non-uniformities, doping non-uniformity and compositional non-uniformity.

Another thing we did in this lecture is that we laid out a step-by-step procedure to draw the energy band diagram of any device. The 3 steps in this were first solve the drift-diffusion model to get n, p and psi, next step is located in the device junctions, space-charge and neutral regions, third step is to draw the various levels in a specific sequence in which the quasi Fermi levels are drawn first.

Because the variation in these levels is least complex of all the levels and also because the difference in Fermi levels at the 2 contacts of the device is equal to the applied voltage if the contacts are ohmic. The next step after drawing the quasi Fermi levels is to draw the band diagram in neutral regions.

Then you draw the E0 as a continuous line everywhere. Finally, you construct the Ec and Ev levels in the space-charge region following the E0 variation and then you can draw other levels of interest such as impurity levels and so on. In the next lecture, we will draw the energy band diagram of a hetero-junction under equilibrium and we shall also consider energy band diagrams of p-n junction under high bias and then some other topics related to the energy band diagram.