Semiconductor Device Modeling

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Lecture - 30
Energy Band Diagrams

In the previous lecture, we have discussed the utility of the E-K relation, we showed how from this relation we can obtain the crystal momentum of the electron by differentiating it we can obtain the electron velocity called the group velocity and by double differentiating it we can obtain the effective mass of the electron. We discussed the concept of crystal momentum in detail. Now in this lecture we are going to start a discussion of the energy versus distance diagram.

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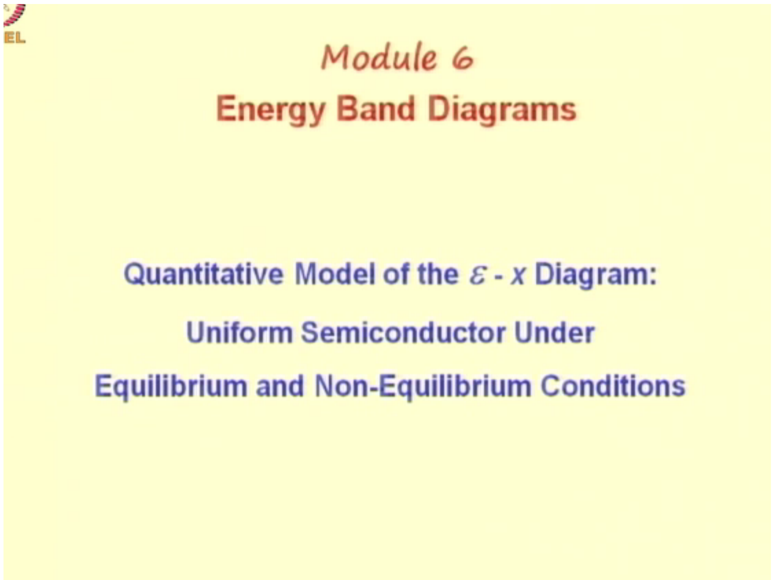

Module 6

Energy Band Diagrams

Quantitative Model of the ε - x Diagram:

Uniform Semiconductor Under

Equilibrium and Non-Equilibrium Conditions

Specifically, we will discuss a quantitative model of a uniform semiconductor under equilibrium and non-equilibrium conditions, so we are going to discuss the E-X diagrams or energy distance diagrams for various conditions. In this lecture we are starting with uniform semiconductor because this is simplest case that one can think of and discussion of the energy levels in this semiconductor will give you a good foundation for drawing the band diagrams for other more complicated cases.

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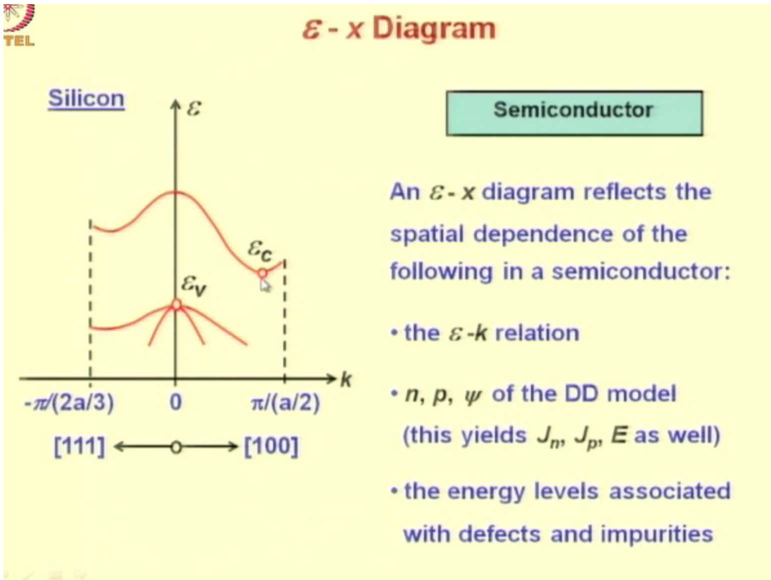

$\mathcal{E}$ - x Diagram

Semiconductor

An $\mathcal{E}$ - x diagram reflects the spatial dependence of the following in a semiconductor:

- the $\mathcal{E}$-k relation
- n, p, ψ of the DD model (this yields J_n, J_p, E as well)
- the energy levels associated with defects and impurities

Let us look at some features of the E-X diagram, an E-X diagram reflects the spatial dependence of the following in a semiconductor, so when we are talking of a semiconductor we are talking of semiconductor volume and actually the energy levels E can change as a function of x, y, z, however in this course we will concentrate for most part on the one dimensional band diagram.

We will have approximately introduced you to 2 dimensional band diagrams but that will be only a small part of the course, so an E-X diagram reflects the spatial dependence of the following firstly the E-K relation, in the previously lecture you have come across this E-K diagram okay, now we would like to see how this particular E-K relation shown on this graph varies throughout the volume of the semiconductor as a function of position.

Next the E-X diagram reflects the spatial dependence of electron concentration, hole concentration and electrostatic potential which are the parameters of the drift diffusion model, now you already know that once you know n, p and psi you can also derive information about Jn, Jp and E as well, so although there are 6 equations in the drift diffusion model these can be reduced to 3 coupled equations in n, p and psi.

So Jn, Jp and E are quantities that can be derived from n, p and psi, thirdly the E-X diagram reflects spatial dependence of the energy levels associated with defects and impurities, now when we talk of the spatial dependence of the E-K relation it is sufficient if you focus on these 2 energies namely Ec and Ev, Ec is the bottom of the conduction band E-K relation and Ev is the top of the valence band E-K relation.

Once you know the variation of Ec and Ev as a function of position in the semiconductor volume we can always build up the complete E-K relation around these points. Let us begin with the E-X diagram of a uniform semiconductor under equilibrium.

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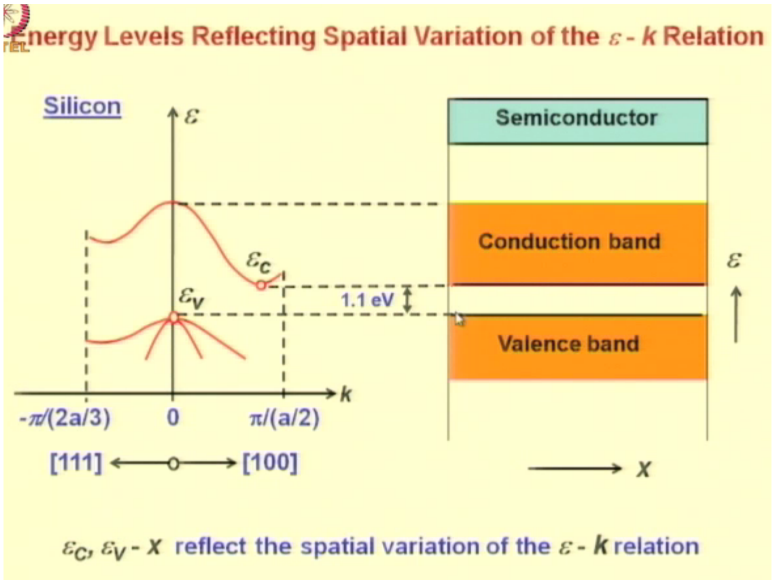

Energy Levels Reflecting Spatial Variation of the ε - k Relation

ε_C, ε_V - x reflect the spatial variation of the ε - k relation

So first we talk about the energy levels, reflecting spatial variation of the E-K relation, here is the E-K relation with the critical energies namely Ec and Ev we want to plot Ec and Ev as a function of X in the semiconductor, so within the semiconductor Ec and Ev will be constant because the semiconductor is uniform and it is under equilibrium and therefore isolated from all other influences point

So no electric field is applied across the semiconductor and no other fields in fact there is no electromagnetic field applied to the semiconductor and therefore you expect the E-K relation to be uniform and therefore the Ec and Ev are constant with X, now you can also show the entire conduction band energy width and valence band energy width, because the top of the conduction band is obtained from the top of the conduction band E-K relation on this diagram here point

Similarly, you can take the E-K line correspond to the valence band it will have a bottom and you can use that bottom point to get this energy and then get the bottom of the valence band, so Ec and Ev as a function of X reflects the spatial variation of the E-K relation, we do not bother about the top of the conduction band or bottom of the valence band because once you know Ec and Ev you can always build up all other quantities.

Now let us look at the energy level reflecting spatial variation of electrostatic potential psi or the electric field E.

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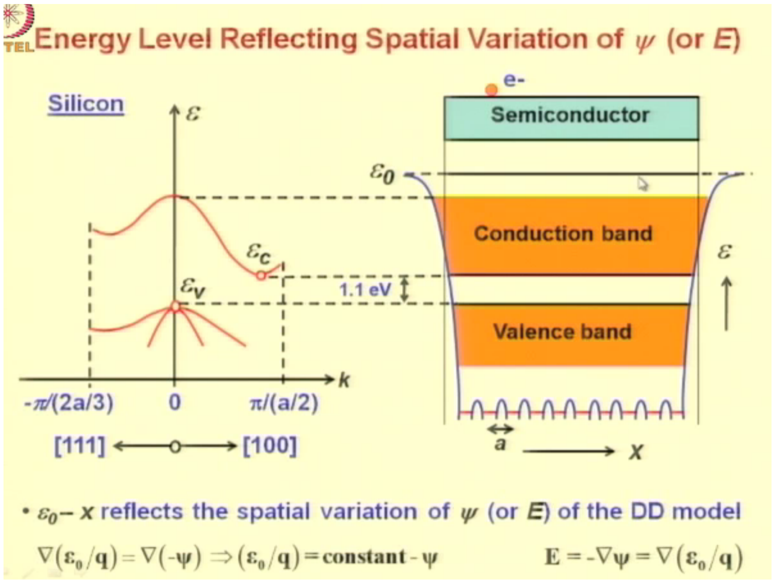

Energy Level Reflecting Spatial Variation of ψ (or E)

- $\varepsilon_0 - x$ reflects the spatial variation of ψ (or E) of the DD model

$\nabla(\varepsilon_0/q) = \nabla(-\psi) \Rightarrow (\varepsilon_0/q) = \text{constant} - \psi$ $\quad$ $E = -\nabla\psi = \nabla(\varepsilon_0/q)$

This energy level happens to be E0 which is present in the crystal potential diagram, this crystal potential diagram actually contributes to these allowed bands and energy gaps, there is also allowed band shown here which is very thin because this band is associated with electrons which are located close to the crystal atom.

So this E0 you recall from the previous lectures is the vacuum level that means it corresponds to an electron which has been moved from semiconductor outside into the vacuum but it is touching the semiconductor surface, so that is the energy level E0, so this E0 is shown as a constant line and this E0 as a function of X reflects the spatial variation of psi or E of the drift diffusion model.

It is shown as a constant line because there is no electric field apply to the semiconductor it is under equilibrium, therefore there is no potential variation and therefore the E0 does not change, so if I move the electron on the surface along the this line it will not experience any change in the potential because there are no fields within the semiconductor, now why should the energy of an electron touching the semiconductor surface from outside in vacuum reflect the electrostatic potential.

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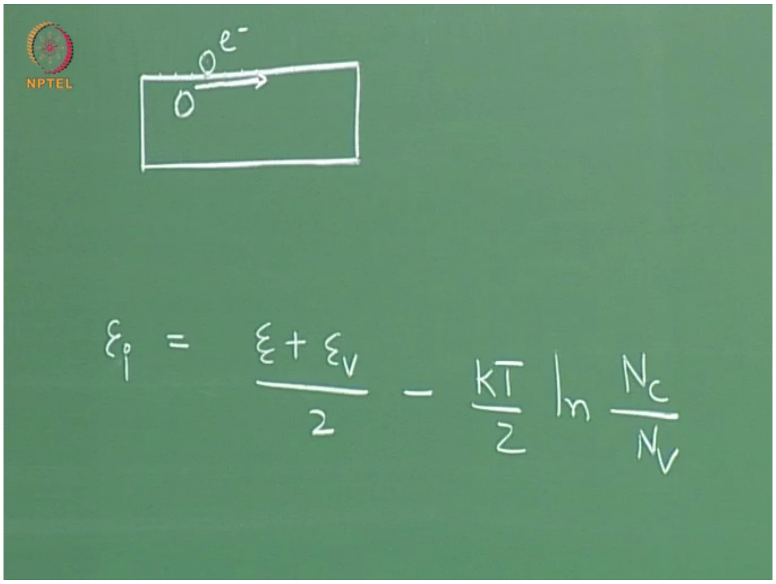

$$\mathcal{E}_i = \frac{\mathcal{E} + \mathcal{E}_V}{2} - \frac{kT}{2} \ln \frac{N_c}{N_V}$$

So suppose you have a semiconductor like this and there is an electric field inside then this electric field will cause a potential variation on the surface and this potential variation can be sensed by the electron which is present here, you might ask why not an electron inside will that not experience this electric field yes this electron will also experience this electric field, however this electron will also experience the effect of the atomic potentials.

Therefore, we prefer to use an electron which is touching the semiconductor surface from outside, so that it experiences the electrostatic field alone because of space charges and so on and not any electric field because of the atoms, the relation between the vacuum level E0 which is an energy and the electrostatic potential psi of the drift diffusion model is given here, so gradient of E0/q = gradient of - psi.

So in fact what this means is E0/q = constant - psi, the negative sign comes about here because psi is the potential associate with positive charge whereas E0/q is the potential associate with an electron which has a negative charge, so this relation is obtained just by integrating this, now you can get the electric field as negative gradient of psi which is nothing but gradient of E0/q.

So if you take the slope of this line that should give you the electric field in this case the slope is 0 because there is no electric field because the semiconductor is in equilibrium, so no external fields are applied and since it is uniform there are no built-in fields either.

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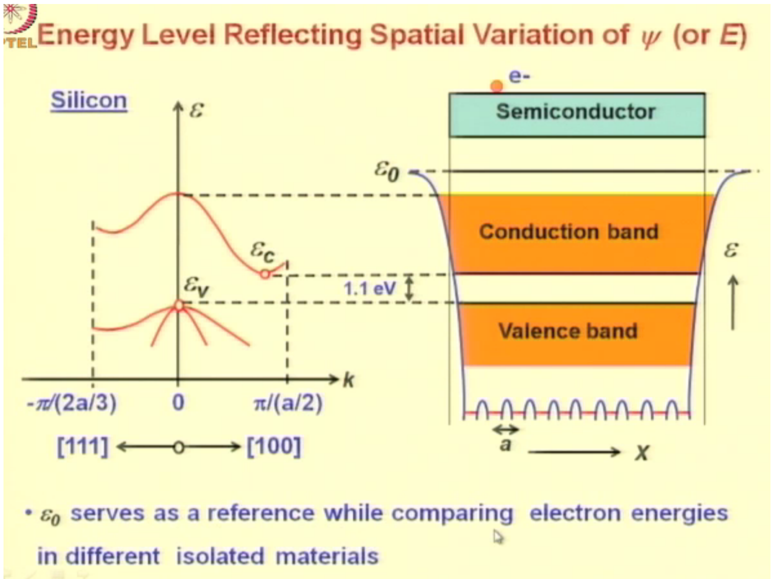

Energy Level Reflecting Spatial Variation of ψ (or E)

- ε_0 serves as a reference while comparing electron energies in different isolated materials

The E0 is an important energy which also serves as a reference while comparing electron energies in different isolated materials.

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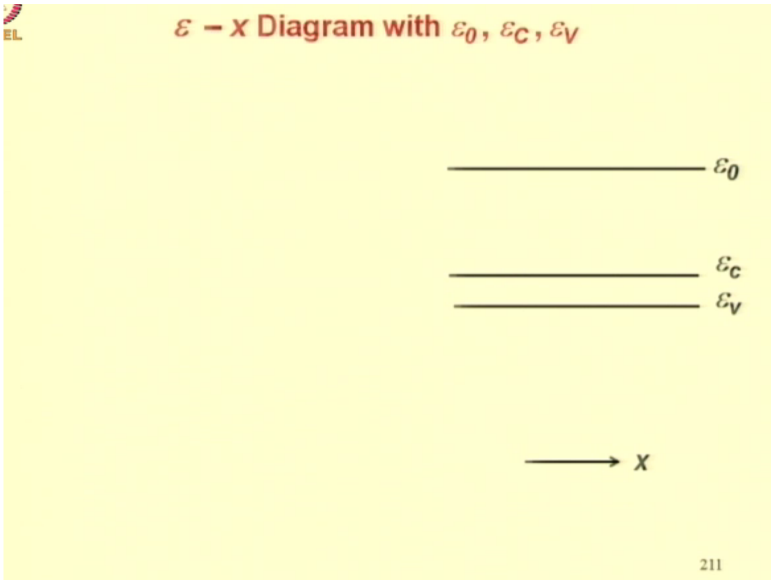

$\varepsilon - x$ Diagram with $\varepsilon_0, \varepsilon_C, \varepsilon_V$

Normally, we do not show the conduction, valence bands and the crystal potential etc. because it complicates the diagram, so what we do is we simply extract these 3 levels E0, Ec and Ev in an E-X diagram. Once we know the variation of these 3 levels as a function of X we can always build up the other details about what happens to the energy conduction band, what happens to the valence band, what happens to the crystal potential as a function of X, what happens to the E-K a relation those can always be build up around these energy levels.

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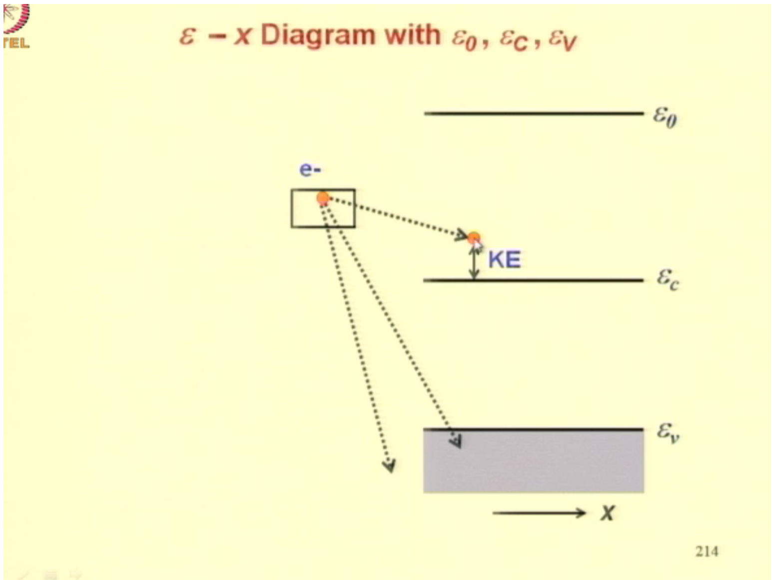

$\varepsilon - x$ Diagram with $\varepsilon_0, \varepsilon_C, \varepsilon_V$

Let us increase the distance between E0, Ec and Ev because we want to show many more energy levels within these levels, so now the diagram is not to scale, let us familiarize ourselves with these 3 levels E0, Ec and Ev a little more consider an electron inside a semiconductor what would be the energy associated with this electron, now this electron in terms of its energy could be anywhere as shown here.

For example, it could be in the conduction band, it could be in the valence band or it could be in any of the lower bands which are present, suppose electron is in the conduction band and its total energy is as shown here with this particular location, then the distance between the energy of the electron and Ec the energy level Ec is actually the kinetic energy therefore Ec is the potential energy of a conduction electron any energy higher than Ec would imply presence of a kinetic energy.

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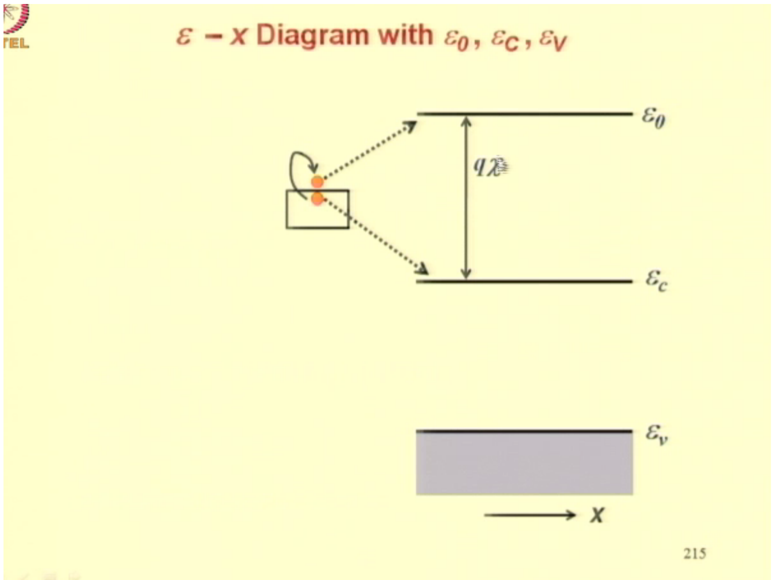

$\varepsilon - x$ Diagram with $\varepsilon_0, \varepsilon_C, \varepsilon_V$

The difference in E0 - Ec is normally represented using the symbol q times chi, so chi is an potential dimension q chi is an energy and this is called electrons affinity, now what is the physical significance of this difference if there is an electron inside the semiconductor that is at the conduction band edge and it is just moved out into the vacuum touching the semiconductor surface then its energy would change by a magnitude = q times chi.

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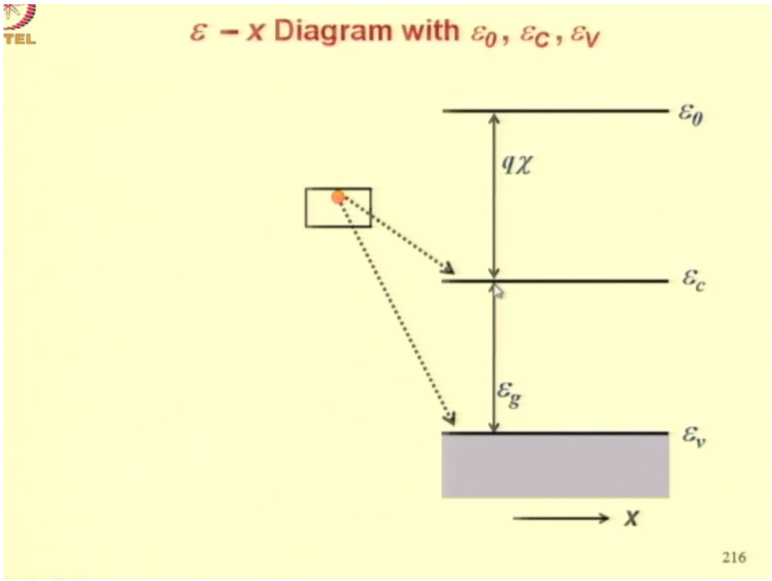
$\varepsilon - x$ Diagram with $\varepsilon_0, \varepsilon_C, \varepsilon_V$

An electron inside the semiconductor if it changes the energy from the conduction band edge to the valence band edge then it would undergo a change in energy equal to the energy gap, so Ec – Ev referred to as energy gap

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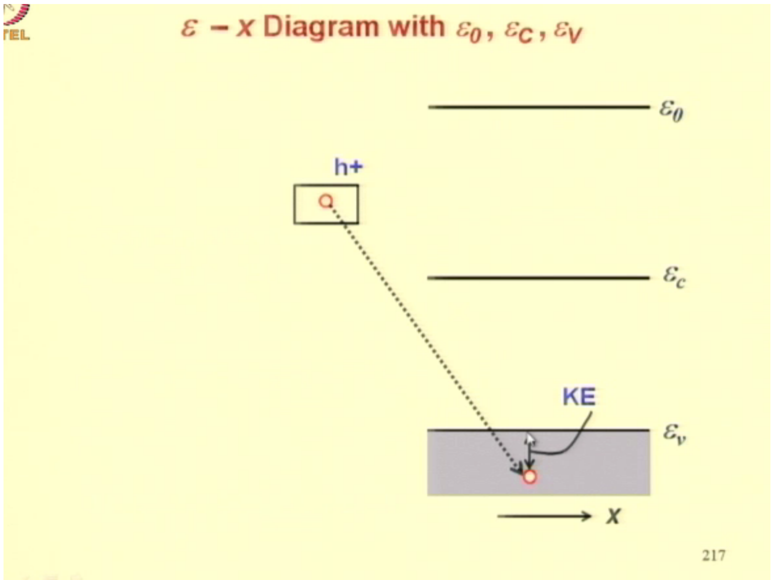
$\varepsilon - x$ Diagram with $\varepsilon_0, \varepsilon_C, \varepsilon_V$

A hole inside a semiconductor will we located in the valence band, so the kinetic energy of the hole = the energy level Ev which is the potential energy of a hole - the energy of the hole, so this difference is the kinetic energy, so as the hole gains more and more kinetic energy it moves down from Ev.

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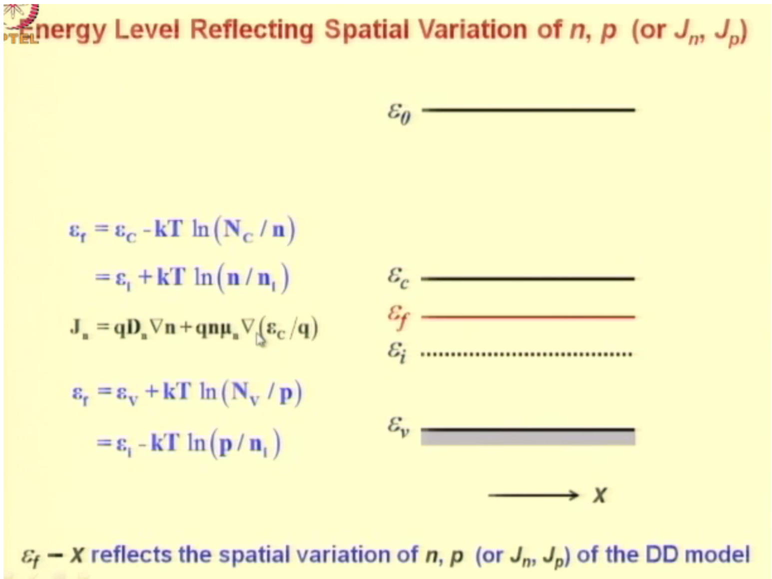

Energy Level Reflecting Spatial Variation of n, p (or J_n, J_p)

$$\varepsilon_f = \varepsilon_C - kT \ln(N_C / n)$$
$$= \varepsilon_i + kT \ln(n / n_i)$$
$$J_n = qD_n \nabla n + qn\mu_n \nabla(\varepsilon_C / q)$$
$$\varepsilon_f = \varepsilon_V + kT \ln(N_V / p)$$
$$= \varepsilon_i - kT \ln(p / n_i)$$

$\varepsilon_f - x$ reflects the spatial variation of n, p (or J_n, J_p) of the DD model

Now once we are familiarized with these levels E0, Ec and Ev, let us now at more energy levels, first we consider energy level reflecting spatial variation of electron and hole concentrations are equivalently electron and hole current densities under equilibrium this energy level is the fermi level, Ef is the function of X reflects the spatial variation of n, p or Jn, Jp of the drift diffusion model, now let us see how does it reflect this information.

Now these are the relations for fermi level in terms of the electron and hole concentrations, so in terms of electron concentration Ef = Ec - kT ln Nc/n, where Nc is called the effective density of states in the conduction band and similarly the same Ef can also be written as Ev+kT in to ln of effective density of states in the valence band divided by the hole concentration, so here we are reflecting this different Ef – Ev in terms of the hole concentration.

And we are reflecting the difference Ec – Ef in terms of the electron concentration, these relations you would have come across already in the first level course, under equilibrium normally the symbol for electron concentration n suffix 0 and for hole concentration it is p suffix 0, so these are the 2 relations which connect the electron and hole concentrations to Ef, note that the same Ef is representing both electrons and holes.

Because this is the situation of equilibrium we will see later that in general in non-equilibrium the Ef associated with electron concentration called the Ef suffix n are quasi fermi level for electrons is different from Ef suffix p that is the quasi-fermi level for holes which reflects the non-equilibrium hole concentration, we also have another energy level E suffix i, E suffix i is the energy level corresponding to the fermi level in an intrinsic semiconductor.

So you are already know what is the intrinsic semiconductor, it is a semiconductor which has no doping okay, now you can say why not call it pure semiconductor, so the difference between pure semiconductor intrinsic semiconductor is that a pure semiconductor has no defects or doping whereas the intrinsic semiconductor may have some defects and doping but if it has doping then its n type and p type doping will cancel each other.

So that the carrier concentration of this particular semiconductor which is not pure will be equal to the carrier concentration in a pure semiconductor, so an intrinsic semiconductor can be a pure semiconductor or an impure semiconductor whose carrier concentration = the concentration in a pure semiconductor, because the acceptor and donor type doping's cancel each other, so in an intrinsic semiconductor the fermi level will be close to the middle of the energy gap.

The reason why it is not in the middle of energy gap is because Nc and N v are different in general, so from your first level course you would have known that Ei is given by Ec+Ev upon 2 - kT upon 2 ln Nc/Nv, for silicon since Nc is more than N v it means a fermi level in intrinsic semiconductor is a little below the middle of the energy gap Ec+Ev/2 is the middle of energy gap okay.

Now the Ei has the following utility you can express the fermi level as fermi level with reference to Ei, so in n type semiconductor as for example the semiconductor shown here Ef is above Ei and therefore Ef is given by Ei+kT ln n/n i and the same Ef can be written in terms of hole concentration as Ei - kT ln p/n i, now how does the fermi level reflect the current density.

Now the formula for current density drift diffusion model is Jn = q Dn grad n+q n mu n into E, now since it is a uniform semiconductor Ef is shown as flat line and the semiconductor is under equilibrium therefore there is no electric field, so E0, Ec and Ev are all flat there no slope because no electric field and therefore uniform difference between Ec and Ef as a function of X reflects a constant electron concentration and therefore grade n is 0.

Similarly, we are already remarked that the electric field is 0 because E0 is flat, Ec is flat and so on, therefore Jn = 0 so that is how flat Ec and flat Ef together imply a 0 electron current, now the electric field acting on the electrons is given by gradient of Ec/q, so it is the gradient of Ec/q that reflects the electric field, now you might say why not gradient of a E0 just now we had mentioned that the gradient of E0 is related to the electric field electrostatic field. Now the point is the gradient of Ec and gradient of E0 are same in this particular case.

Because this is the semiconductor whose atomic structure is not changing with distance and therefore even if you were to replace Ec/q/E0/q your electric field would have been the same. However strictly speaking the electric field that comes into this location here for the expression for the electron current is the electric field experienced by the conduction electron it is not the electric field experienced by an electron which is touching the semiconductor from outside right?

So E0 corresponds to the energy of this electron which is touching semiconductor from outside. Whereas the electric field in the J n expression is the electric field acting on the electron in the conduction band that is the electron inside the semiconductor but in the conduction band, therefore the correct expression is, accurate expression is in terms of gradient of the Ec/q which is the potential energy which is the potential of a conduction electrons, when we go to the heterostructures where the composition changes with distance.

The atomic structure changes with distance then E0 and Ec in general would not be parallel and therefore a conflict will arise has to should you take the slope of E0 or should you take the slope of Ec for the electric field on an electron in a semiconductor, so for a conduction electron you must use Ec/q,

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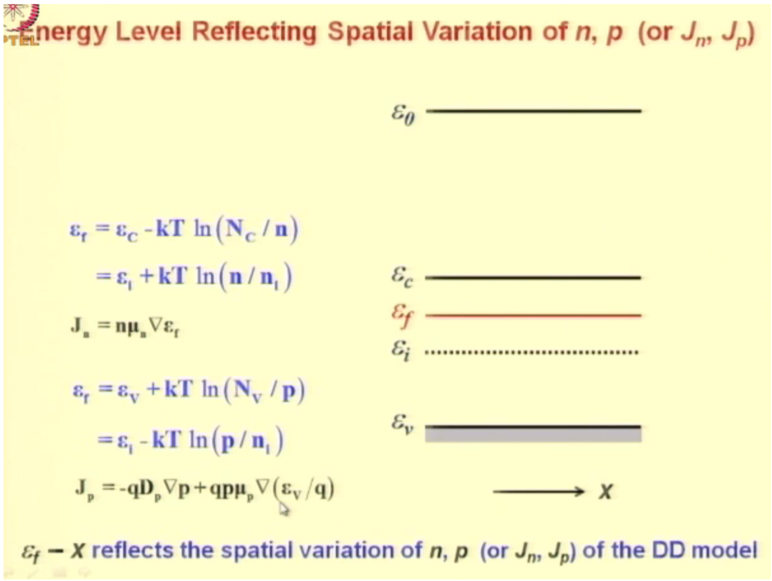

Energy Level Reflecting Spatial Variation of *n*, *p* (or J_n, J_p)

$$\varepsilon_f = \varepsilon_C - kT \ln(N_C / n)$$
$$= \varepsilon_i + kT \ln(n / n_i)$$
$$J_n = n\mu_n \nabla \varepsilon_f$$
$$\varepsilon_f = \varepsilon_V + kT \ln(N_V / p)$$
$$= \varepsilon_i - kT \ln(p / n_i)$$
$$J_p = -qD_p \nabla p + qp\mu_p \nabla(\varepsilon_V / q)$$

$\varepsilon_f - x$ reflects the spatial variation of *n*, *p* (or J_n, J_p) of the DD model

Now we are shortly going to give you an assignment in which you can show that drift+diffusion current both the terms can be compressed in the compact form as shown in this relation n into mu n into gradient of Ef, so the gradient of Ef reflects both the drift as well as diffusion currents together, this compact form is very useful because it directly tells you how, it tells you how directly Ef or gradient of Ef reflects the electron current.

Assignment will be given in a short time okay, now let us discuss the current of holes current density for holes following the same approach this is the expression for hole current density which you can write as shown here where the electric field acting on the holes is represented by gradient of Ev/q, because of arguments which are similar to the arguments given for the case of electron the electric field acting on holes should be related to the gradient of the valence band edge.

In heterostructures the valence band edge may not be parallel to the conduction band edge and may not be parallel to the vacuum level E0 and therefore in such a situation it is important to note that the electric field in the hole current expression is given by the gradient of Ev/q and you cannot use E0 here nor can you use Ec.

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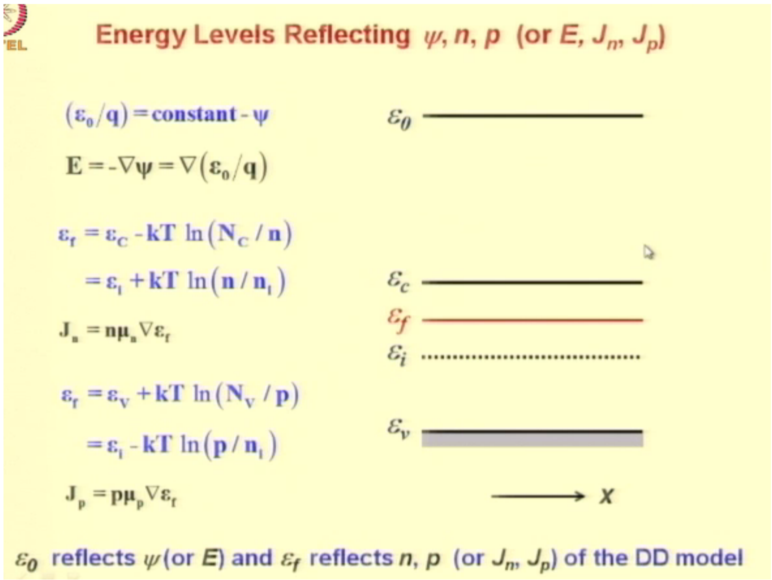

Energy Levels Reflecting ψ, n, p (or E, J_n, J_p)

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

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

$$\varepsilon_f = \varepsilon_C - kT\ \ln(N_C/n)$$
$$= \varepsilon_i + kT\ \ln(n/n_i)$$

$$J_n = n\mu_n\nabla\varepsilon_f$$

$$\varepsilon_f = \varepsilon_V + kT\ \ln(N_V/p)$$
$$= \varepsilon_i - kT\ \ln(p/n_i)$$

$$J_p = p\mu_p\nabla\varepsilon_f$$

ε_0 reflects ψ (or E) and ε_f reflects n, p (or J_n, J_p) of the DD model

Once again in analogy to the case of electron current density, the hole current density can be expressed in terms of gradient of the fermi level, since it is in equilibrium case the same fermi level is entering into the expression for holes as well as for electrons, otherwise as the assignment will show what you will have in the expression for current density of electrons would be the quasi-fermi level electrons Efn.

And what you will have in the expression for Jp would be quasi-fermi level for holes that is E suffix fp, you can see here that seems the fermi level is flat, the hole current is 0 and similarly electron current is 0, so this is very straight forward reasoning based on the gradient of the fermi level for deriving the information about the electron and hole current densities, now let us complete the picture let us show all the energy levels which reflects psi n and p or E, Jn, Jp.

So reproducing from our previous discussion the E0 reflects the electrostatic potential psi, it also reflects the electric field E according to this relation, so we summarize by saying E0 reflects psi or E and Ef reflects n or p or equivalently Jn or Jp of the drift diffusion model, so this is how the levels E0, Ec, Ef and Ev together represent the conditions in a semiconductor device those conditions which are used in a drift diffusion model and these levels are also useful to give you the spatial variation of the E-K relation.

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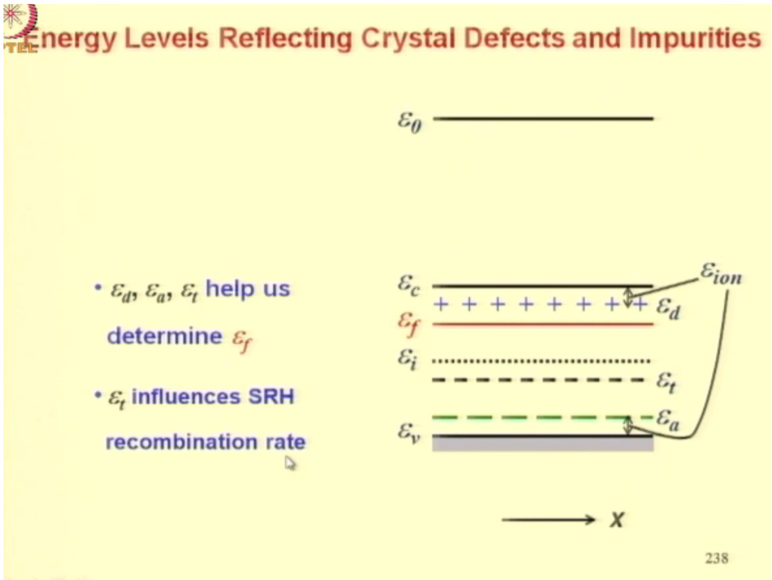

Energy Levels Reflecting Crystal Defects and Impurities

- ε_d, ε_a, ε_t help us determine ε_f
- ε_t influences SRH recombination rate

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Let us add now to this diagram energy levels reflecting crystal defects and impurities, the donor level corresponding to a shallow donor would be somewhere here close to the in energy gap close to the conduction band edge, now it is not necessary at a donor level should always be close to the conduction band edge only a shallow donor that is that kind of a donor which gives you a large number of electrons in a semiconductor.

And converts the semiconductor into n type would be a shallow donor its energy level will be close to the conduction band edge, example of this is phosphorus or antimony or arsenic in silicon, the positive sign here indicates donors because it means that when this impurity loses its electron it is positively ionized so donor is one which gives an electron right and in process becomes positively charged so that is why positive signs are used to indicate the donor level.

Similar way one can show the acceptor level with negative signs this is the shallow acceptor such as boron or aluminium in silicon, so it is located close to the valence band edge, once again in acceptor level would lie anywhere in the energy gap a shallow acceptor would be close to the valence band edge, a trap level apart from donors and acceptors you can also have defects.

And you can also have apart from shallow donors and acceptors other types of impurities which create energies near the middle of energy gap, so either defects or impurities both can give us to the energies near the middle of the energy gap and these are reflected here by this energy level call the trap level it is called a trap because these impurities can actually physically trap electrons or holes.

The distance between the conduction band edge and the donor level is referred to as ionization energy of the donor and the distance between the valence band edge and the acceptor level is referred to as ionization energy of the acceptor, for example if you take this trap level if it is acceptor type as it is shown here with negative signs then its ionization energy would be the difference between Et and Ev.

If the same trap level was donor type the ionization energy would be Ec – Et, the donor level the acceptor level and the trap level help us determine Ef, so this levels are useful in determination of Ef, the trap level Et influences the Shockley Read Hall recombination rate, in our early lectures we have discussed about Shockley Read Hall recombination and there you would recall we had used an energy level called this trap level.

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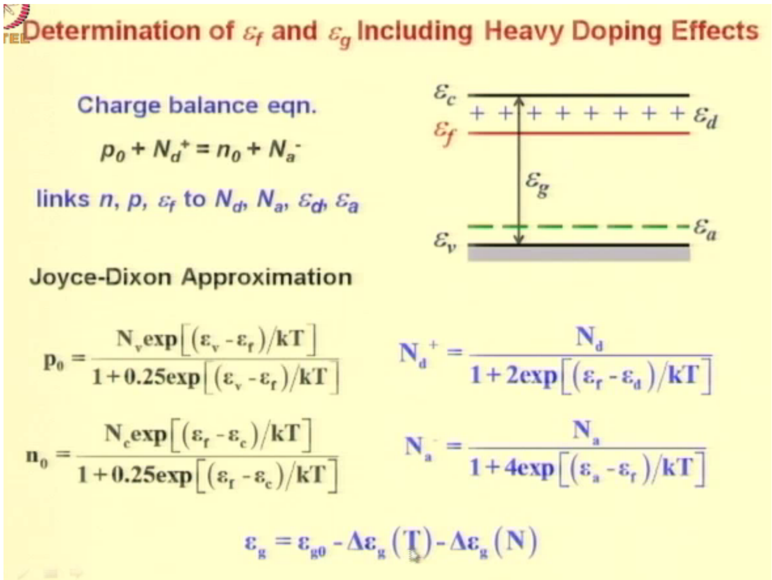

Determination of ε_f and ε_g Including Heavy Doping Effects

Charge balance eqn.

$$p_0 + N_d^+ = n_0 + N_a^-$$

links n, p, ε_f to N_d, N_a, ε_d, ε_a

Joyce-Dixon Approximation

$$p_0 = \frac{N_v \exp\left[(\varepsilon_v - \varepsilon_f)/kT\right]}{1 + 0.25\exp\left[(\varepsilon_v - \varepsilon_f)/kT\right]} \qquad N_d^+ = \frac{N_d}{1 + 2\exp\left[(\varepsilon_f - \varepsilon_d)/kT\right]}$$

$$n_0 = \frac{N_c \exp\left[(\varepsilon_f - \varepsilon_c)/kT\right]}{1 + 0.25\exp\left[(\varepsilon_f - \varepsilon_c)/kT\right]} \qquad N_a^- = \frac{N_a}{1 + 4\exp\left[(\varepsilon_a - \varepsilon_f)/kT\right]}$$

$$\varepsilon_g = \varepsilon_{g0} - \Delta\varepsilon_g(T) - \Delta\varepsilon_g(N)$$

Now let us discuss how you determine the Ef and Eg in a uniform semiconductor under equilibrium including heavy doping effects, in the first level course you would have determined Ef in a dope semiconductor, what we want to do here is to so slightly improve upon the formula and include heavy dropping effects when the energy gap can decrease as compared to low doping.

And Fermi Dirac statistics sorry the Boltzmann statistics for electrons may not be valid and you will have to use Fermi Dirac statistics, so this is your energy level diagram relevant to this problem, the determination of Ef starts from the charge balance equation that is p0+Nd+= n0+Na -, you have come across this equation in the first level course, the suffix 0 indicates the fact that we are considering equilibrium condition Nd+is a concentration of ionized donors

And Na - is the concentration of ionized acceptors, now this charge balance equation links electron concentration, hole concentration and fermi level to the donor doping, acceptor doping the donor level and the acceptor level, let us see how now we discuss the Joyce-Dixon approximation to the Fermi Dirac statistics.

According to this approximation the hole concentration is given by Nv which is the effective density of states in the valence band into exponential of Ev– Ef/kT divided by 1+0.25 exponential Ev– Ef/kT, the Boltzmann approximation is p0 = the numerator part of this expression, so this expression tells you that as your doping becomes heavy acceptor doping’s becomes heavy the Ef will start moving closer and closer to the valence band and in such a case this Ev- Ef can become smaller in magnitude.

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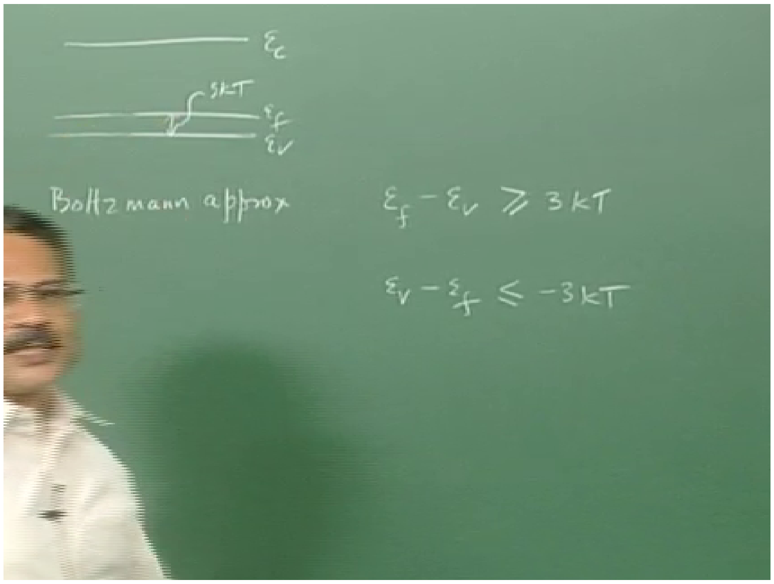

Boltzmann approx

$$\mathcal{E}_f - \mathcal{E}_v \geqslant 3kT$$

$$\mathcal{E}_v - \mathcal{E}_f \leqslant -3kT$$

Now Boltzmann approximation is valid when Ev– Ef is >= to 3 times kT or Ev- Ef <= - 3 time kT, so this is your band diagram and this is your Ef, this is Ev, this Ec, so as your doping becomes heavy this starts coming closer and closer if the Ef gets closer than 3 times kT then you know that the Boltzmann approximation fails now that is where the Joyce-Dixon approximation becomes important okay.

So the Joyce-Dixon is such that for low doping it will be reduced to Boltzmann approximation you can see from when the doping is low Ev– Ef is really a large negative quantity and therefore this denominator term simply becomes about 1 and you have only the numerator term, whereas for example when Ef becomes = Ev for heavy doping in such a case p 0 becomes = Nv/1.25 whereas the Boltzmann approximation will only give you N v okay.

So there is 25% error almost due to expression based on Boltzmann approximation when the doping is a heavy and Ef is at Ev, a similar approximation exists for electron concentration and it is given by n 0 = Nc exponential Ef - Ec/kT divided by 1+0.25 exponential Ef - Ec/kT, so when Ef = Ec the Joyce-Dixon approximation predicts n 0 = Nc/1.25 whereas the Boltzmann approximation which is simply the numerator part of this expression predicts only N c.

So there is a 25% error due to Boltzmann approximation when Ef = Ec, the expression for Nd+in this equation is given by N d/1+2 times exponential Ef – E d/kT.

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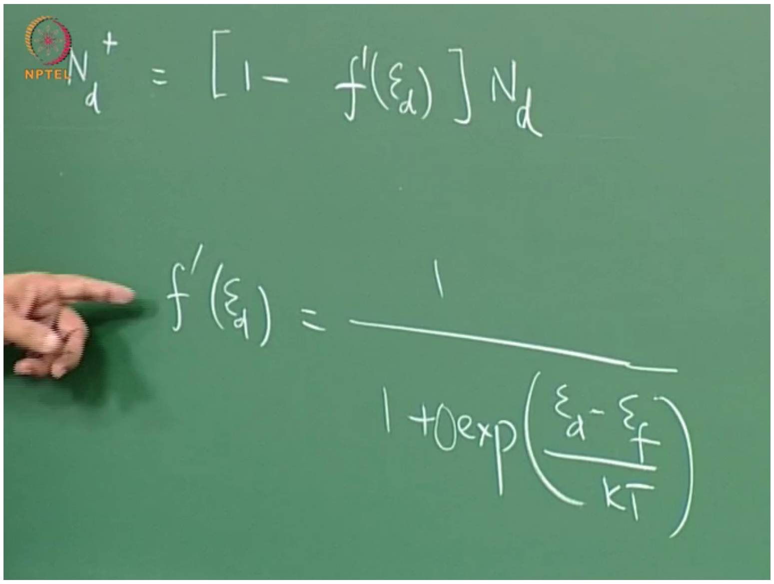

$$N_d^+ = [1 - f'(\varepsilon_d)]\, N_d$$

$$f'(\varepsilon_d) = \frac{1}{1 + \bigcirc \exp\left(\frac{\varepsilon_d - \varepsilon_f}{kT}\right)}$$

This you would have come across in the first level course Nd+= 1 - the fraction of occupied states at Ed into the total concentration of donors, now this fraction is not given by the Fermi Dirac function exactly so that is why you put a dash so Fermi Dirac function would be 1/1+exponential of E d – Ef/kT but when you are applying the function to impurity level there is always a constant coming here it is called degeneracy factor.

And that is why you use a different function than the Fermi Dirac function and because of this factor that you have 2 coming in here Na - is similarly given by Na/1+ 4 times exponential E a – Ef/kT, again this 4 is because of the degeneracy factor, so Na – is nothing but Na into the fraction of occupied states at Ea.

Finally, the energy gap is given by the energy gap for low doping and low temperature - a change as a function of temperature - a change as a function of doping this is really referred to as the band gap narrowing because of heavy doping effects.

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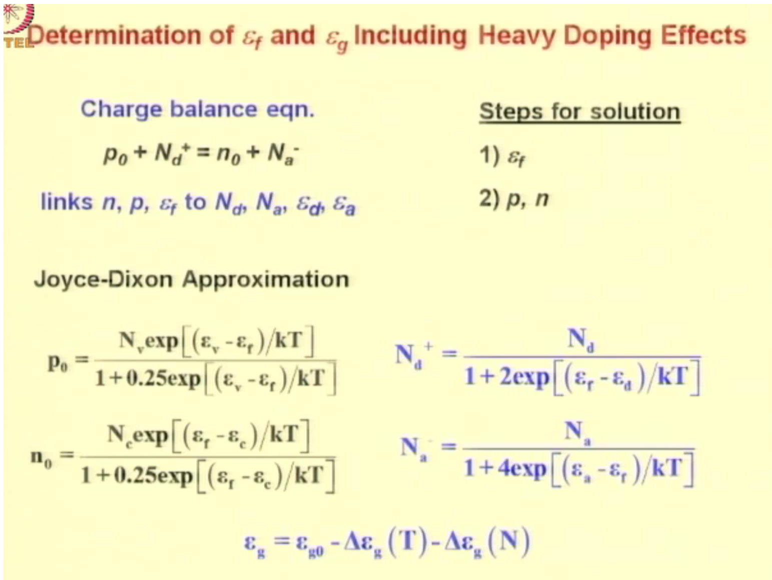

Determination of ε_f and ε_g Including Heavy Doping Effects

Charge balance eqn.

$p_0 + N_d^+ = n_0 + N_a^-$

links n, p, ε_f to N_d, N_a, ε_d, ε_a

Steps for solution

1) ε_f

2) p, n

Joyce-Dixon Approximation

$$p_0 = \frac{N_v \exp\left[(\varepsilon_v - \varepsilon_f)/kT\right]}{1 + 0.25\exp\left[(\varepsilon_v - \varepsilon_f)/kT\right]} \qquad N_d^+ = \frac{N_d}{1 + 2\exp\left[(\varepsilon_f - \varepsilon_d)/kT\right]}$$

$$n_0 = \frac{N_c \exp\left[(\varepsilon_f - \varepsilon_c)/kT\right]}{1 + 0.25\exp\left[(\varepsilon_f - \varepsilon_c)/kT\right]} \qquad N_a^- = \frac{N_a}{1 + 4\exp\left[(\varepsilon_a - \varepsilon_f)/kT\right]}$$

$$\varepsilon_g = \varepsilon_{g0} - \Delta\varepsilon_g(T) - \Delta\varepsilon_g(N)$$

Now the way this equation is solved is that first you solve for Ef and then you solve for electron and hole concentrations okay, so what you do is you take this expressions substitute for p0 take this expression substitute for n0, similarly substitute these 2 things here for Nd +and Na - and then solve for Ef, now you might wonder how do you solve for Ef when you have Ev and Ec, Ed and Ea also present there.

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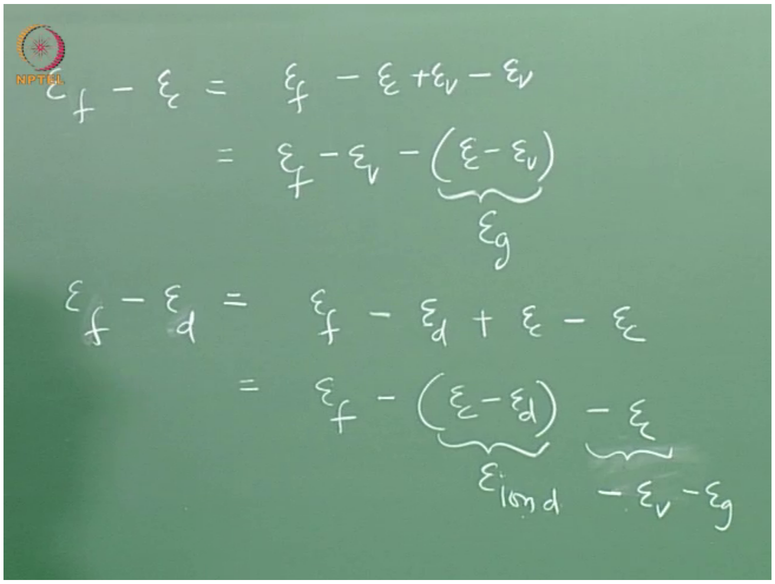

$$\varepsilon_f - \varepsilon_c = \varepsilon_f - \varepsilon_c + \varepsilon_v - \varepsilon_v$$
$$= \varepsilon_f - \varepsilon_v - \underbrace{(\varepsilon_c - \varepsilon_v)}_{\varepsilon_g}$$

$$\varepsilon_f - \varepsilon_d = \varepsilon_f - \varepsilon_d + \varepsilon_c - \varepsilon_c$$
$$= \varepsilon_f - \underbrace{(\varepsilon_c - \varepsilon_d)}_{\varepsilon_{ion\,d}} \underbrace{- \varepsilon_c}_{-\varepsilon_v - \varepsilon_g}$$

So here what you need to do is you take anyone energy as a reference let us see if I choose to take Ev as reference, so in another words all expressions which are in terms of other energy levels like Ec, Ea, Ed should be converted to energy level in terms of Ev, let us see how supposing you have for example this expression Ef – Ec, so you can write Ef – Ec = Ef - Ec+Ev– Ev, so add and subtract Ev because this is your reference.

Now what will happen is this can be written as Ef - Ev- Ec – Ev and this is nothing but energy gap and you have an expression for energy gap in fact we are shortly going to give you expression for energy gap, so that is how Ef - Ec can be converted into Ef - Ev, similarly supposing you want to convert Ed - Ec sorry you want to convert Ef – Ed into an expression consisting of the valence band.

So Ef – Ed so you can write this as Ef – Ed+Ec – Ec that = Ef - Ec – Ed which you can identify as ionization energy of the donor so that is why I put a suffix d because ionization energy of the donor can be different from ionization energy of the acceptor, so - Ec now this - Ec you can always convert it to Ev as shown here, so you can see Ef – Ec was Ef – Ev– this, so I can write this part as - Ev- Eg so your Ef – Ed is Ef - ionization energy of the donor - Ev- Eg.

So like that you can convert each expression into an expression containing Ef and Ev, then you can solve for Ev– Ef.

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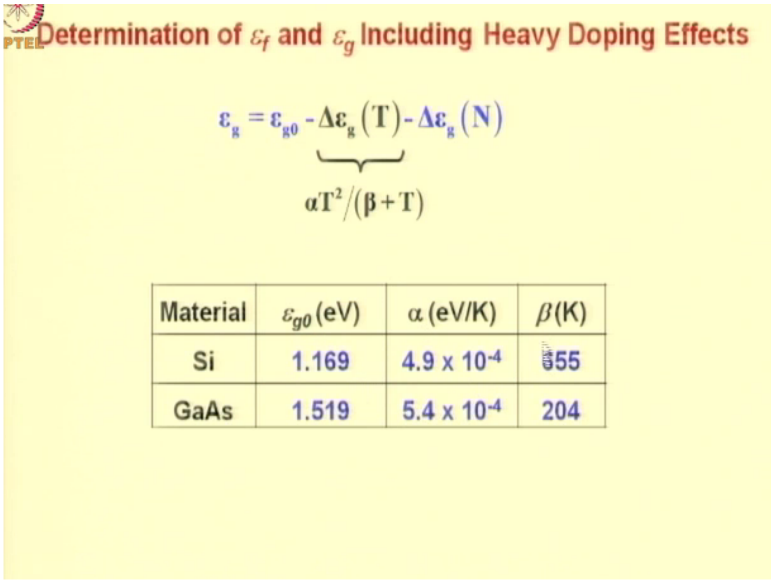

Determination of ε_f and ε_g Including Heavy Doping Effects

$$\varepsilon_g = \varepsilon_{g0} - \underbrace{\Delta\varepsilon_g(T)}_{\alpha T^2/(\beta + T)} - \Delta\varepsilon_g(N)$$

Material	ε_{g0} (eV)	α (eV/K)	β (K)
Si	1.169	4.9×10^{-4}	655
GaAs	1.519	5.4×10^{-4}	204

Now the expression for energy gap is as follows, let us look at the term that depends on the temperature is given by alpha times T square/beta+T were for different materials the constants have different values, so for silicon the E g0 that is this term is 1.169 electron volts alpha its units are electron volt per kelvin it is 4.9 10 power - 4 and beta has the unit kelvin at 655, for gallium arsenide the values are 1.519 for E g0, 5.4 into 10 power - 4 for alpha and 204 for beta, so alpha is of the order of 10 power - 4 electron volt per kelvin.

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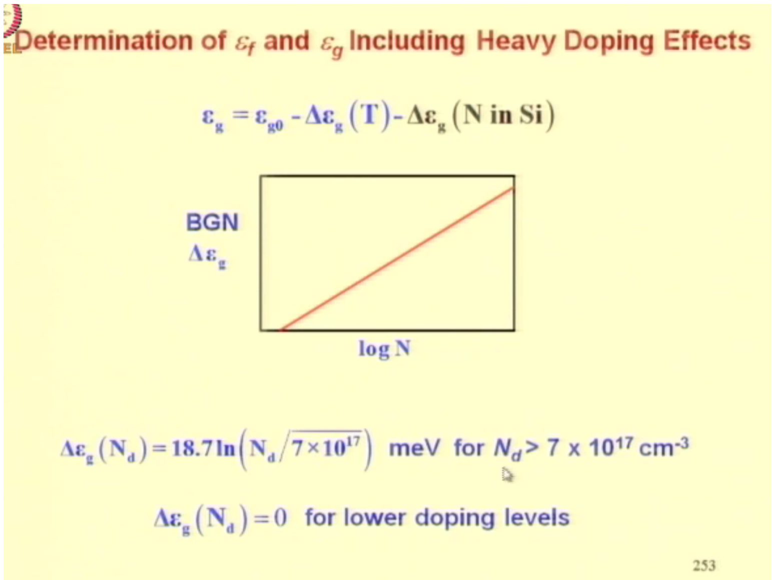

Determination of ε_f and ε_g Including Heavy Doping Effects

$$\varepsilon_g = \varepsilon_{g0} - \Delta\varepsilon_g(T) - \Delta\varepsilon_g(\text{N in Si})$$

$\Delta\varepsilon_g(N_d) = 18.7\ln\left(N_d/7\times10^{17}\right)$ meV for $N_d > 7 \times 10^{17}$ cm^{-3}

$\Delta\varepsilon_g(N_d) = 0$ for lower doping levels

Let us look at the band gap narrowing term for silicon, so N stands for doping it could be donor or acceptor you have different expression for donor and acceptor it turns out that for both donor and acceptor delta Eg as a function of log N is close to a straight line. And therefore the form of expression is as follows delta Eg as a function of Nd if you have donors then it = 18.7 into logarithm of Nd divided by 7 into 10 power 17 where this quantity or Nd is in per centimeter cube so milli-electron volts for Nd > 7 into 10 power 17, now for Nd < 7 and 10 power 17.

This logarithmic term will be negative it might give you a feel that the delta Eg becomes negative which is not correct. So for lower doping levels we assume delta Eg is 0, so this formula is valid only for Nd > 7 into 10 power 17, so this means in silicon for donor doping >7 into 10 power 17 band gap will start narrowing.

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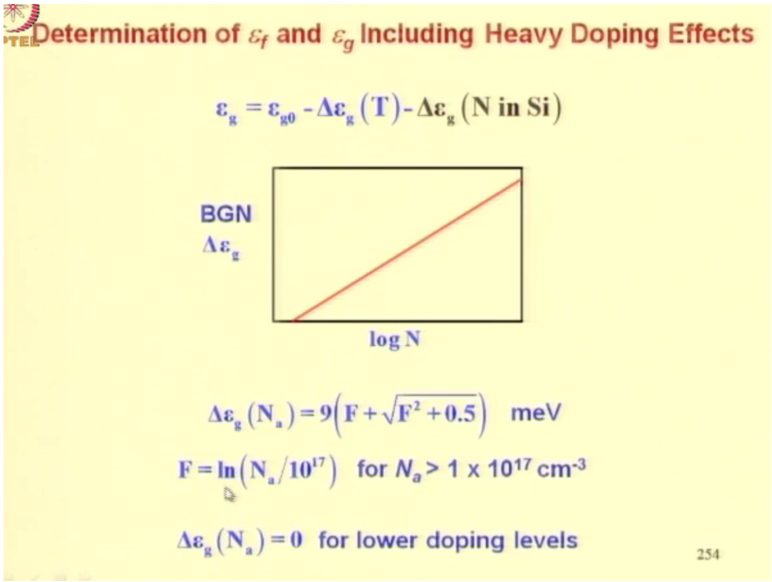

Determination of ε_f and ε_g Including Heavy Doping Effects

$$\varepsilon_g = \varepsilon_{g0} - \Delta\varepsilon_g(T) - \Delta\varepsilon_g(N \text{ in Si})$$

$$\Delta\varepsilon_g(N_a) = 9\left(F + \sqrt{F^2 + 0.5}\right) \quad \text{meV}$$

$F = \ln(N_a/10^{17})$ for $N_a > 1 \times 10^{17}$ cm^{-3}

$\Delta\varepsilon_g(N_a) = 0$ for lower doping levels

The formula for acceptor type case has given here delta Eg as the function of Na = 9 times F+square root of F square+0.5 milli-electron volt where F is logarithm of Na divided by 10 power 17 where Na is in per centimeter cube, so evidently this formula is valid for Na > 1 into 10 power 17 centimeter cube and for lower doping levels delta Eg is assumed to be 0, because then logarithmic becomes negative which is not physical correct.

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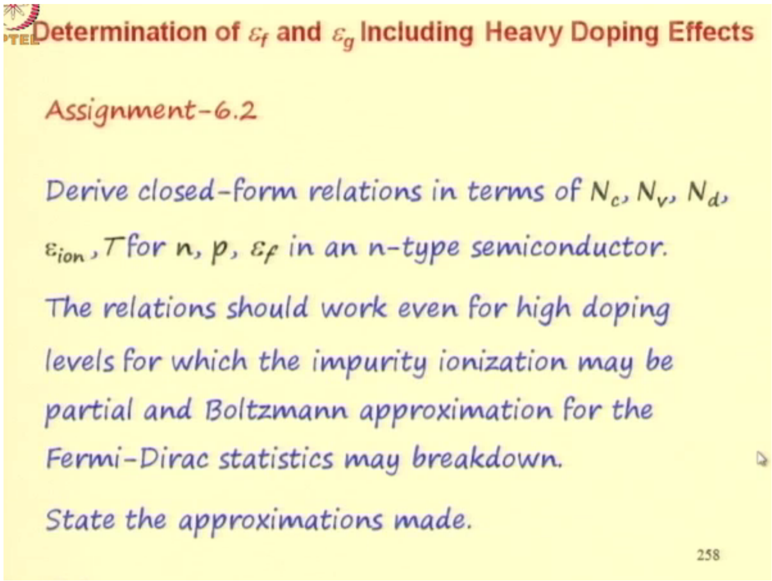

Determination of ε_f and ε_g Including Heavy Doping Effects

Assignment-6.2

Derive closed-form relations in terms of N_c, N_v, N_d, ε_{ion}, T for n, p, ε_f in an n-type semiconductor.

The relations should work even for high doping levels for which the impurity ionization may be partial and Boltzmann approximation for the Fermi-Dirac statistics may breakdown.

State the approximations made.

So here is an assignment for you derive closed form relations in terms of Nc, Nv, Nd and E ion and temperature for electron concentration, hole concentration and fermi level in an n-type semiconductor, so you have do the charge balance equation the Joyce-Dixon approximation and the equation for concentration of ionized impurities.

The simplification that will result here is that this is an n-type semiconductor therefore you do not have to bother about hole concentration and ionized acceptor impurities that is simplifies the expression a lot and it allows you to derive an analytical expression if you want to do a calculation including Nd and Na in a general case then you will have to resolve to numerical calculations.

The relations should work even for high doping levels for which impurity ionization maybe partial and Boltzmann approximation for the Fermi Dirac statistics may breakdown, state the approximations made.

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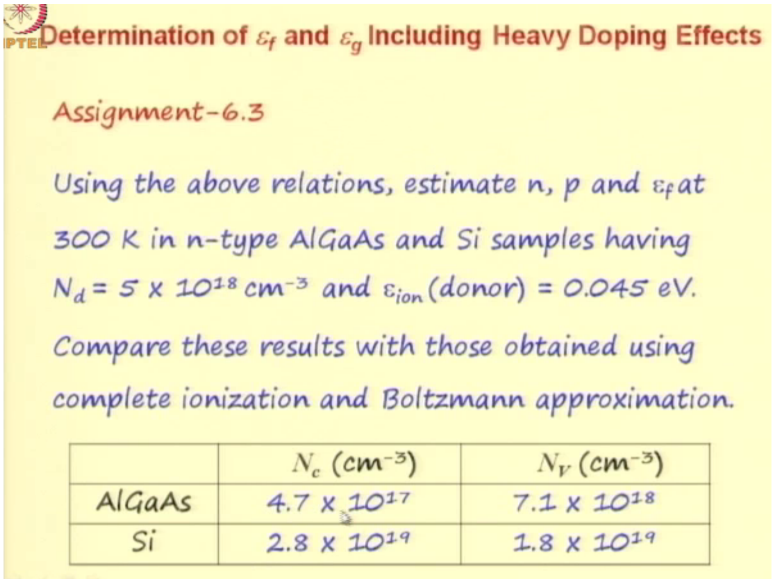

Determination of ε_f and ε_g Including Heavy Doping Effects

Assignment-6.3

Using the above relations, estimate n, p and ε_f at 300 K in n-type AlGaAs and Si samples having $N_d = 5 \times 10^{18}$ cm^{-3} and ε_{ion}(donor) = 0.045 eV.

Compare these results with those obtained using complete ionization and Boltzmann approximation.

	N_c (cm^{-3})	N_V (cm^{-3})
AlGaAs	4.7×10^{17}	7.1×10^{18}
Si	2.8×10^{19}	1.8×10^{19}

There is the another assignment where you use the derived the expression for calculations, using the above relations estimate n p and Ef at 300 kelvin in n-type aluminium gallium arsenide and silicon samples having Nd = 5 into 10 power 18 per centimeter cube and ionization energy of donor = 0.045 electron volts, compare these results with those obtained using complete ionization and Boltzmann approximation.

Here are the values of Nc and N v for aluminium gallium arsenide and silicon, for aluminium gallium arsenide 4.7 into 10 power 17 per centimeter cube and for silicon 2.8 into 10 power 19 per centimeter cube, for Nc and similarly for N v the values are 7.1 into 10 power 18 per centimeter cube for aluminium gallium arsenide and 1.8 into 10 power 19 per centimeter cube for silicon.

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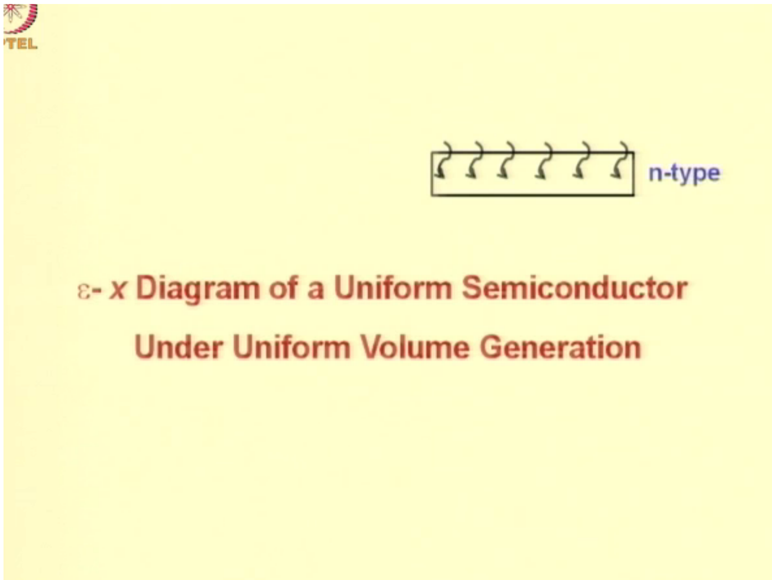

ε- x Diagram of a Uniform Semiconductor Under Uniform Volume Generation

Finally, let us discuss the E-X diagram of a uniform semiconductor under uniform volume generation.

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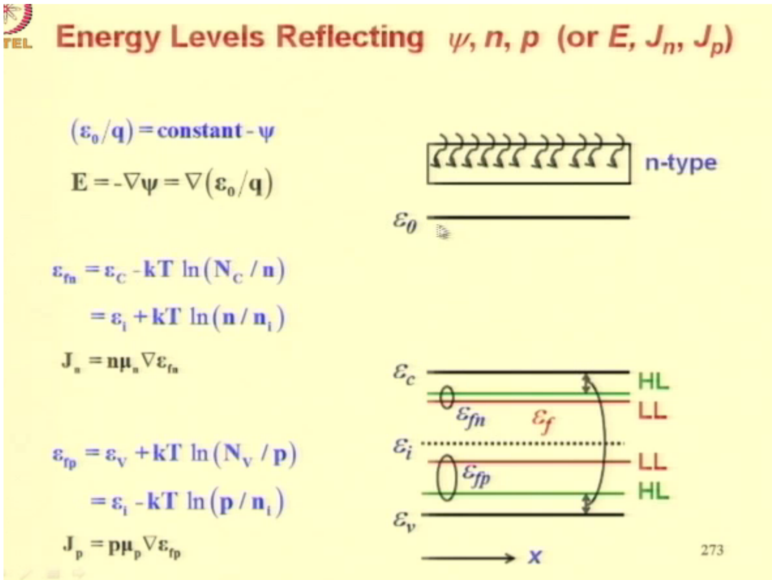

Energy Levels Reflecting ψ, n, p (or E, J_n, J_p)

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

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

$$\varepsilon_{fn} = \varepsilon_C - kT\ln(N_C/n)$$
$$= \varepsilon_i + kT\ln(n/n_i)$$
$$J_n = n\mu_n\nabla\varepsilon_{fn}$$

$$\varepsilon_{fp} = \varepsilon_V + kT\ln(N_V/p)$$
$$= \varepsilon_i - kT\ln(p/n_i)$$
$$J_p = p\mu_p\nabla\varepsilon_{fp}$$

So we want to show energy levels reflecting psi n and p of the drift diffusion model which will also reflect E, Jn and Jp, let us begin from the equilibrium condition for which we already know the band diagram it contains E0, Ec, Ef, Ei and Ev, Ef is above Ei because the semiconductor is n type, now when you shine light and there is a uniform volume generation in this semiconductor then everywhere there is success electrons and holes.

And situation is depicted in an energy diagram by splitting of fermi level into electron quasi fermi level and hole quasi fermi level it turns out that when the injection level is low LL stands for low level when the injection level is low the quasi fermi level for electrons is same as or almost the same as the equilibrium fermi level the fermi level under equilibrium, whereas the quasi fermi level for holes moves significantly away from the equilibrium fermi level, now let us understand why?

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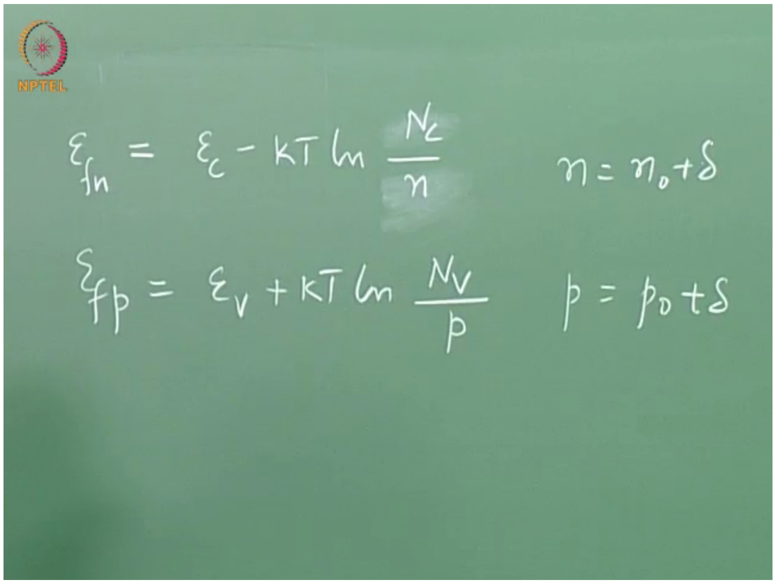

$$\mathcal{E}_{fn} = \mathcal{E}_c - kT \ln \frac{N_c}{n} \qquad n = n_0 + \delta$$

$$\mathcal{E}_{fp} = \mathcal{E}_v + kT \ln \frac{N_v}{p} \qquad p = p_0 + \delta$$

So using the concept of quasi fermi level Efn = Ec - kT Nc upon n and n = n0+delta and similarly for holes it is Ev+kT into ln Nv upon p, p = p0+delta excess carrier concentration is the same for electrons and holes, now you can see from here if n increases this term reduces which means the fermi level goes closer to Ec, on the other hand if p increase compared to p0 this term decreases and according to this formula the quasi fermi level for holes goes close to Ev.

So the same fermi level now cannot represent both electrons and holes because quasi fermi level for electron should go to closer to Ec whereas the fermi level for holes should go closer to Ev.

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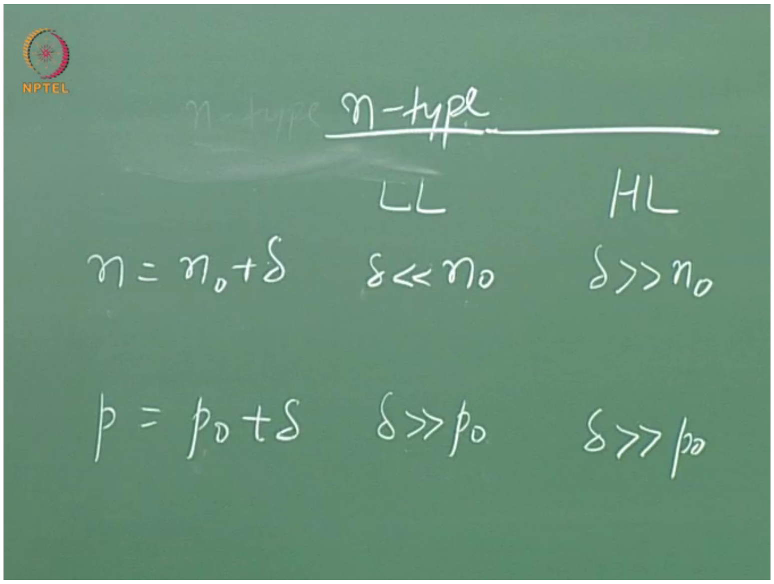

n-type

	LL	HL
$n = n_0 + \delta$	$\delta \ll n_0$	$\delta \gg n_0$
$p = p_0 + \delta$	$\delta \gg p_0$	$\delta \gg p_0$

Low level conditions delta is much < n0 however delta is always > p0 because p0 is the minority carrier concentration in n type semiconductor, so this very, very small so generally delta will be much > p0 and therefore this quantity will significantly deviate from Ev because p changes significantly from p0, whereas n remains close to n0 because if the delta is much < n0, n is n0 itself and therefore this remains close to the equilibrium fermi level.

Now, the carrier concentration are therefore represented these 2 formulae which we just now wrote down on the board they could also be represented using an equation in which the reference is Ei for electrons and holes rather than Ec for electrons and Ev for holes, now if you increase the intensity of light you can have high level conditions, high level conditions there is a small change in the electron fermi level so it moves closer to the Ec as compared to equilibrium.

And the hole quasi fermi level moves closer to Ev also in a similar way, now what happens in high level is that if I write expression for high level for the same n type then here delta is becoming much more than n0 and anyway it is much more than p0, so therefore in this case you have n approximately = delta and p approximately = delta both n and p are almost the same and = delta.

And therefore if you put delta here and here the difference between Ec and Efn and difference between Ev and Efp would be almost the same they are not exactly the same because Nc is slightly different from Nv okay otherwise they are almost the same, so therefore the high-level condition is depicted by this situation so this difference equal to this difference approximately, now let us complete the picture because we want to show psi also.

So the electrostatic potential psi is reflected by E0/q and from these levels E0, Ef and Efp you can also get electric field, the electron current density and hole current density, so these expressions are repeated from the previous slide, so in this case for example Efn and Efp both are flat which means that electron current is 0 and hole current is 0 it is expected because electron and hole concentration are uniform throughout the volume.

Therefore, there cannot be any diffusion current and there are there is no electric field between the semiconductor because it is uniform and no external electric field is applied therefore drift current is also 0, so that is how Jn and Jp are 0 we can derive the information directly from slope of a Efn and Efp, the electric field is obtained from the slope of E0.

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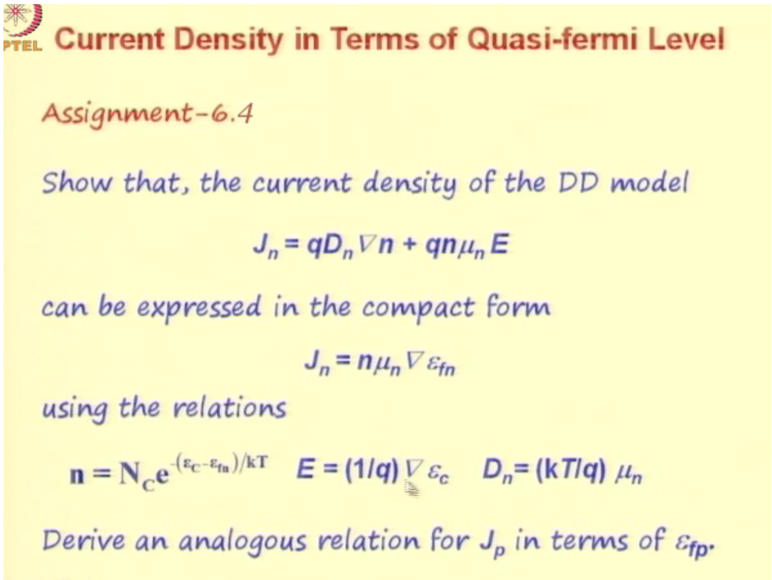

Current Density in Terms of Quasi-fermi Level

Assignment-6.4

Show that, the current density of the DD model

$$J_n = qD_n \nabla n + qn\mu_n E$$

can be expressed in the compact form

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

using the relations

$$n = N_C e^{-(\varepsilon_C - \varepsilon_{fn})/kT} \quad E = (1/q) \nabla \varepsilon_c \quad D_n = (kT/q)\, \mu_n$$

Derive an analogous relation for J_p in terms of ε_{fp}.

Here is an assignment current density in terms of quasi fermi level, show that the current density of the drift diffusion model Jn = q Dn grad n+q n mu n E can be expressed in the compact form Jn = n mu n grad Efn using the relations n = Nc into exponential of - Ec - Efn/kT and E = 1/q gradient of Ec, Dn = kT/q into mu n this is an Einstein relation.

So you use these 3 facts and substitute this here and you should show by algebraic manipulation that this equation containing 2 terms drift and diffusion reduce as to a single term in terms of gradient of Efn, derive an analogous expression for Jp in terms of Efp, when you derive the expression for Jp you must use gradient of Ev here instead of gradient of Ec, we have already explained why you should not use gradient of E0.

Because for using for the electric field term in the current density expressions because in general in heterostructures E0, Ec and Ev all may not be parallel, so for conduction electrons you must use gradient of Ec as electric field acting on electrons, for holes you must use gradient of Ev acting as the electric field acting on holes, with that we have come to the end of the lecture.

Let us make a summary of the important points, so in this lecture we have begun a discussion of the energy versus distance diagram we explained that this energy versus distance diagram contains following critical energy levels these E0 the vacuum level, Ec the conduction band edge, Ev the valence band edge and quasi fermi level for electrons and holes Efn and Efp which reduced to a single fermi level Ef in equilibrium.

We also show the intrinsic fermi level or fermi level in intrinsic semiconductor in the energy band diagram because it proves as a convenient reference, we also showed how the energies associated with impurities can be shown on the energy band diagram basically impurities and defects add additional energy levels within the energy gap the E0 reflects the electrostatic potential.

And the slope of E0 reflects the electrostatic field experienced by an electron touching the semiconductor surface from outside, the fermi level the quasi fermi level for electrons reflects the electron concentration as well as the electron current density, the quasi fermi level for holes reflects the hole concentration and current density for holes, this is how the levels E0, Efn and Efp together represent psi, n and p or E, Jn and Jp of the drift diffusion model, Ec and Ev represents the variation of the E-K relation throughout the semiconductor volume.

Finally, we have mentioned that the electric field in the expression for current density for electrons should be expressed in terms of the gradient of the conduction band edge because conduction band edge which is the potential of electrons in the conduction band and the electric field term in the expression for hole current density should be expressed in terms of gradient of the valence band edge because valence band edge is the potential energy of holes.