Optoelectronic Materials and Devices
Prof. Dr. Monica Katiyar
Department of Materials Science and Engineering
Indian Institute of Technology, Kanpur

Module - 3
Optoelectronic Materials Device Physics
Lecture - 29
Diffusion

Today, we are going to talk about diffusion.

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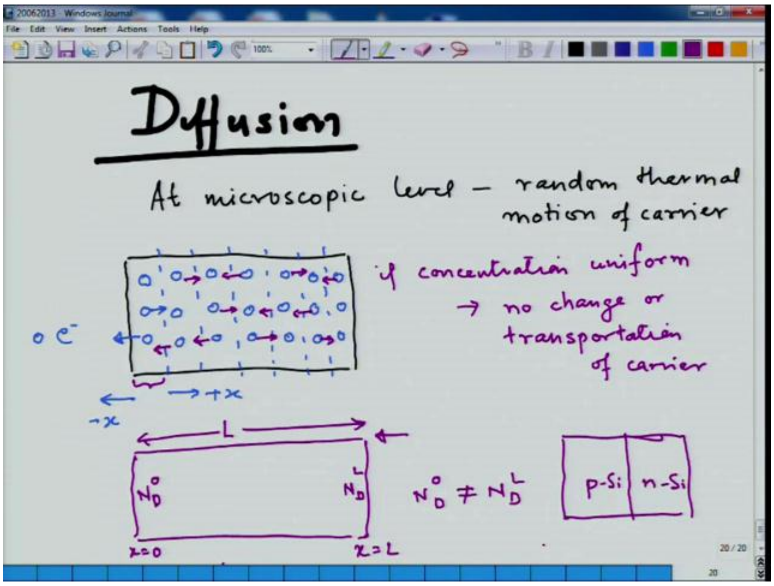

What is diffusion? Diffusion is basically at microscopic level, it is random thermal motion of carriers. So, if I if we look at microscopic level, it is random thermal motion of carriers. If you recall, we discuss this when we started discussing about drift of carriers. We said that at in the classical picture, if we look at the thermal motion of carriers then, there they are always moving around. But their net motion is 0.

So, this random motion of the carriers is what leads to diffusion. But, earlier we said that if we have this motion then, you do not have any effective transport of carriers. So, what is happening if basically? What we are saying is if we have a semiconductor. In this semiconductor, if I divide it by; let us say this material in different sections just to illustrate. I am going to look at only motion in one dimension. Although we know that charge particles are going to move in any random direction but it makes it easier to show.

What we want to display here? Let us say, let us look at behavior of electrons in this material. So, there are electrons in different sections. The material is homogeneously doped. So, we have sort of homogeneous concentration of electrons in these uniform sections that I have drawn of the material at any point. What we are saying is that due to random motion these particles are always moving around. So, at any given point, if the motion is completely random that is; half of probability that will be go in the plus x direction. Half probability that it will go in the minus x direction, which means I can represent it in this manner.

Now, this is going to be true for all other layers, which means I am going to have this interaction between particles in different sections. But, as you can see overall this will not lead to any change because my concentration is homogeneous. It means that the number of particles that I am taking out from a given section is equal to the number of charge carriers, which are coming in that section. So because of this thermal motion, if concentration is uniform for charge carriers and when will that be? It will be when you have uniform doping of the semiconductor.

Then, due to diffusion due to this thermal random motion, you have no change in the or transportation of carrier. So, when does it become important? So, diffusion becomes important when we have non homogeneous carrier concentration in the material or in the device structure, which could be a heterostructure or multilayer. So, why is that possible? Because, we have seen that it is possible for us. When we will look at the devices that we can make a material such that the concentration of, let us say donors at point x is equal to 0 may be at some value.

The concentration of donors at point L x is equal to L. It is not the same. We can always process a material such that these two are not the same. You may wonder how that is possible. It is possible because when we try to dope a material; normally what we do is we start with the uniformly doped intrinsic material of length L. Then, we are going to start diffusion from one end. It basically means that the material will always have a different concentration at this end versus at the opposite end.

Hence, in the processing of semiconductor, it is very common to have non-uniform concentration gradient in the material. Hence, the diffusion becomes an important process. There can be other situation when we often make devices. We put two different kinds of materials adjacent to each other, which mean I may be having a p n junction. I put in close contact metallurgical contact, a p junction, a p semiconductor and a n semiconductor.

Let us say, p silicon and n silicon. For obvious reason, it is clear that the carrier concentration of hole here is going to be very different from here and vice a versa. Carrier concentration of electrons here is going to be very different from n to p. so, there are several situations, which we will deal with later. Also, in the lectures where you have concentration gradient in the device structure or in the material, that would lead to diffusion. So, what will happen in that case if you do have a concentration gradient? You can; one can visualize this process of diffusion.

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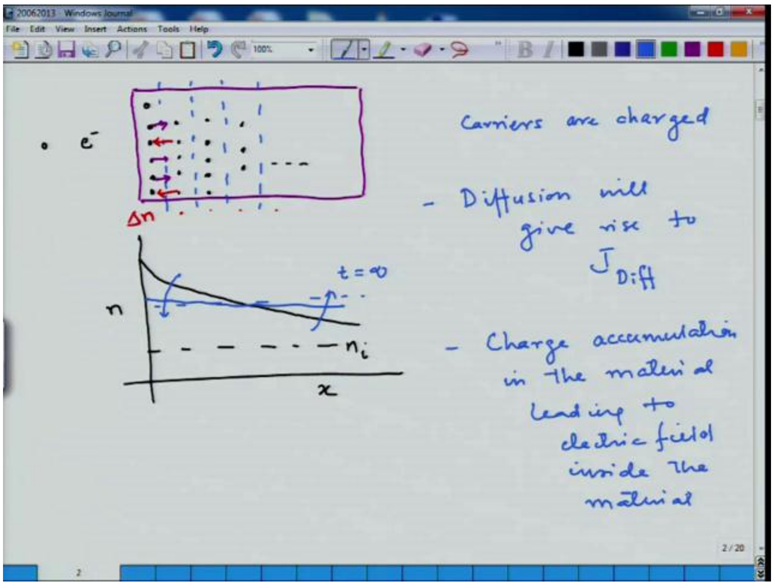

In the manner that those same sections that I have drawn earlier have now different carrier concentration. I can also plot it in terms of a graph, where I will let us take an example of a donor. So, carrier electron concentration versus x. Let us say, there are more electrons. This is being represented by electrons. There are more electrons here. As we go on, the number of electrons is getting reduced. Our doping concentration is getting reduced and so on so forth.

So, if I have to represent this on this axis; is going to be the intrinsic electron carrier concentration and some value and a change in the carrier concentration. Now, in this situation, if we look at the same random motion of carriers; you can see that the number of carriers is more here. Hence, the number coming to the right is going to be more. On the other hand, the numbers going to the left which is going to this section is going to be less.

As a result, there is going to be a change in electron concentration here vice a versa. In the same way, one can see, same thing will happen to each section as we go along because, the number of electrons leaving a particular section is not going to be always same as number of electrons coming to that section except for some special case. So, in general, we assume it is not going to be same in that situation. Eventually, with time, one would expect that this variation in carrier concentration should become less and less.

So, with time because of this diffusion process of random motion of carriers, one would expect the carrier concentration to become uniform if we have time to wait up till infinity. So, this is the reason for diffusion process. We have this in most materials. You have a situation in which the revised structures or material itself have a non-uniform carrier concentration. Now, in this particular case since the carriers are charged, diffusion also leads to a current.

So, diffusion of carriers; because they are charged, diffusion will give rise to a diffusion current. This will be of two kinds; one due to electrons and the other due to holes. By the same token whenever such a diffusion is taking place, you are going to have charge accumulation in the material. That would lead to some sort of a built in field in the material that will oppose this diffusion process. So, the two go hand in hand. Whenever you have diffusion taking place, you will have some charge accumulation in the material leading to electric field inside the material. So, diffusion in that sense is extremely important for semiconductor devices. Now, let us look at it, how do we deal with this process.

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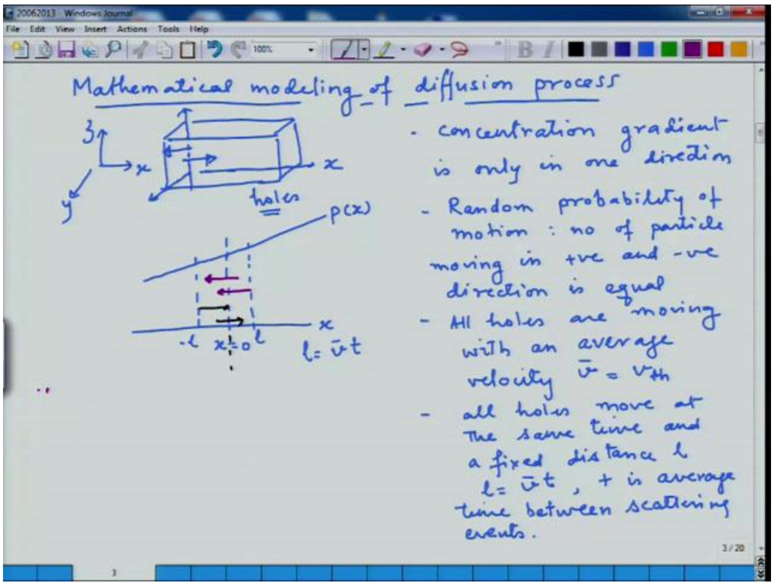

How would we account for it mathematically? So, what is the mathematical model for diffusion current? Now, in order to do this modeling, we are going to make certain assumption to simplify it and simplify the analysis here. So, in general, the material has all three dimensions and we will make sure that if you have concentration gradient. We take a example where the concentration gradient is only in one direction. So, it makes the problem one dimensional, which means if the material is having three dimensions so, semiconducting material.

Then, it is only along the x direction. We are having a concentration gradient in the y direction and in the z direction of the semiconducting material. We have uniform doping, which means that the diffusion process does not leads to any change in the concentration in y and z direction. It is only the x direction that is important for us. So, let us do the analysis for this particular case, for one dimensional diffusion. We also assume that there is a random probability of motion, which means in the x direction at any particular point.

If we take any particular point in x direction then, number of particles moving in the right direction and number of particles moving in the left direction is exactly same at any point because of this random probability of motion. So, in other words, it means that number of particles in this case. Let us make this problem more specific. Let us make this problem for holes. So, particles are holes. Here, number of particles moving in positive and negative direction is exactly equal.

We further simplify the problem. If the motion of holes in the semiconductor is completely random; then, they are all moving with the certain velocity distribution. All the holes are moving with certain velocity distribution. In order to simplify the problem, we will say that all holes are moving with the average velocity of v bar. This simplifies the problem that we take. All the particles have the same average velocity v bar, which is going to be equivalent to the thermal in the classical picture; the thermal velocity of the particles.

Finally, we in order to simplify the analysis, we also make the assumption that all particles move at the same times. So, all holes move at the same time and fixed distance l where l is given by the v bar t. t is average time between scattering events. So, we have simplified the problem quite a bit by making these assumptions. With that, we can now find a formula for finding out what would be the diffusion current in a semiconductor. So, let me take an example. In this particular case of semiconductor, let us say the hole concentration is represented by this curve.

I am looking at any particular point. For simplicity, let me say, I am looking at x is equal to 0. What we are saying here is that there is a mean free path for carriers, which is l for all holes. l is mean, this mean free path is given by the average velocity times the t the time between the scattering events. So, which means that if all carriers are starting to move at the same time carrier; a hole, which is here would have moved across this boundary in that time t, something which is here. I would have also come across this boundary in time t and in this direction. By the same token, the carriers would have moved across the boundary in the opposite direction as well. So now, let us start looking at what is happening. How the carriers are moving across this boundary at x is equal to 0. So, if we look at that then, at x is equal to 0.

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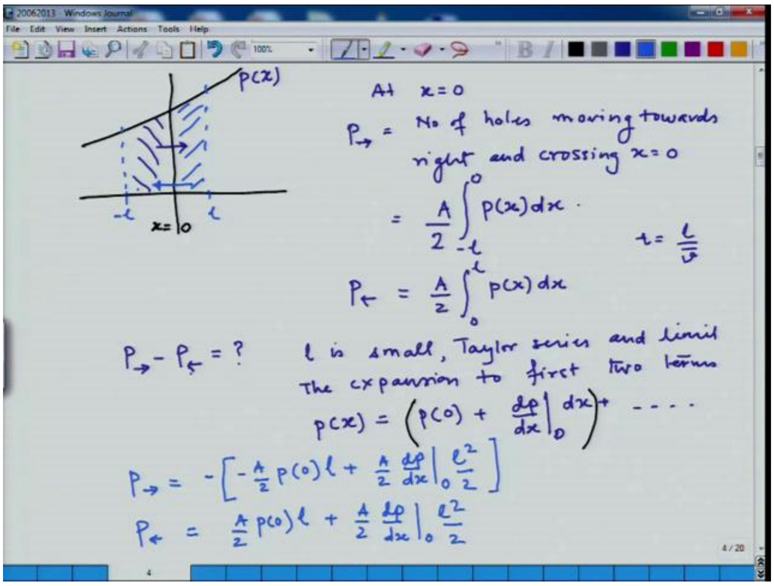

Let me just read out this quickly. You are looking at the movement of carriers across the x is equal to 0 from the length on both side equivalent to mean free path length. Because, this means that all the carriers which are in this volume would have crossed. Half of them would have crossed to the left. The carriers which are in the other volume would have also, half of them would have crossed to the right of this x is equal to 0 boundary. This is representing my hole concentration in the semiconductor.

So then, at x is equal to 0, the number of holes moving towards right is going to be this. Number of holes moving towards right and crossing x is equal to 0 will be given by the; we have to take the area of the semiconductor area multiplied by this dimension. It is the number of holes in this particular dimension, which is basically given by the hole concentration times d x this the length and the area. It has to be integrated from minus l to 0. Since, we said only half will move to right because the other half are going to move towards left.

This has to be divided by 2. So, this is a total number of holes moving from this volume. Crossing x is equal to 0 in time t, where t is being defined by length divided by the average velocity. The mean free path divided by the average velocity. Similarly, I can write the number of holes moving in the left direction. Crossing x is equal to 0 is going to be than given by A by 2 integrating over 0 to l d x. Now, we need to find out what was the total number of; what is the net exchange of carriers across x is equal to 0? So, the net change exchange of carriers across x is equal to 0 is going to be p minus p in the opposite direction.

So, this is what I need to evaluate. Now, in order to evaluate this, I know that the mean free path l is the small. The mean free path of carriers in a semiconductor which are moving around because of thermal motion is a fairly small. If you recall in the earlier lectures, we calculated that in order to prove the Drude theory. This turns out to be close to the interatomic distance in the material. So, it is a fairly small number. Hence, I can make some approximation for p of x. I can take the Taylor series and limit the expansion to the first few terms.

So then, I can write the carrier concentration of hole as carrier concentration of hole at point 0 plus the gradient of carrier concentration at 0 plus the other terms. I am only going to use these for the integration purpose. So, using this expression and then, putting it in the first two integration, I can find out what is the value of p going towards right and going towards left. So, p going in the right direction is substituting. p of x is going to be given by negative of from for negative of l integration plus for the second part.

This is going to be A by 2 value at 0 times l square divided by 2. So, this would be the value at minus l to the 0 to the value of 0. Similarly, I can write for the carriers moving in the other direction. That will be given by A by 1 p of 0, l plus A by 2 d p of d x at 0, l square by 2. Now, let us evaluate the difference of this to figure out what is the net carrier concentration across s is equal to 0.

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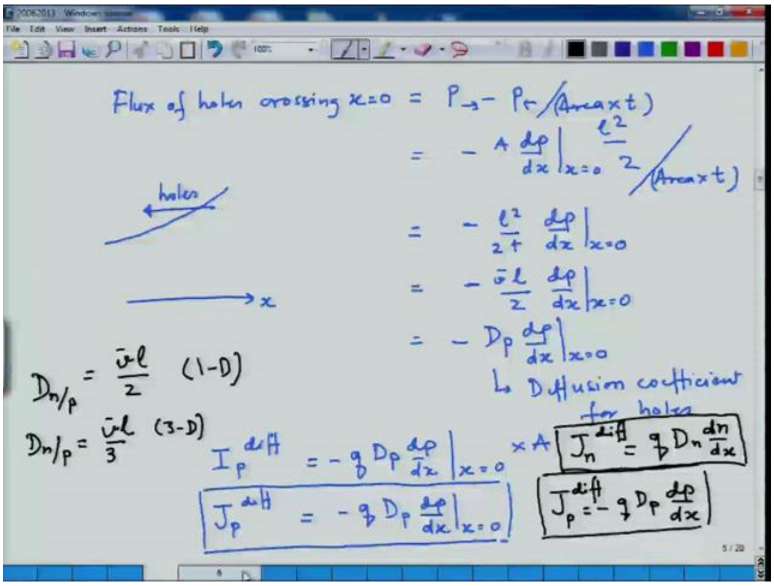

We are finally interested in the flux of holes crossing x is equal to 0. That will be given by p. This expression is coming out to be equal to at x is equal to 0, l square by two. Since, we are looking at the flux; we should divide this by the area multiplied by the time that it takes. So, if I divide this by the area and multiplied by the time then, we are looking at expression which is l square by 2 t d p d x at x is equal to 0. l by t is nothing but v bar. So, this expression is nothing but v bar l by 2 d p d x 0.

So, this is the flux of holes crossing x is equal to 0. This is the total value. Then, the sign here is negative. Why is the sign negative? Because, we have taken the positive x direction to be in this direction. This is a positive x direction. Carrier concentration is like this, which means the carriers are moving opposite to the positive x direction. That is why, this flux is negative. So, holes are moving in this direction. That is why, the negative sign comes here. If this is a flux, we define a quantity called diffusion constant for holes. It is material property. So, this is the diffusion coefficient for holes.

Now, if holes are moving in this direction, which means there is a current due to that. This current is going to be equal to due to diffusion is going to be the charge multiplied by the flux. So, this would be then, charge per centimeter square per second, which is the current multiplied by the area A. If I want to represent it in terms of current density then, the hole current density due to diffusion will be given by q sign. Negative sign missing here, q d p diffusion coefficient d x at x is equal to 0. So, this is the expression we wanted.

We wanted to figure out, due to diffusion in a semiconductor what would be the net motion of carriers which would lead to a diffusion current over here. Now, there is a little bit more generalization which is required. I took this example for looking at the motion of carriers at boundary x is equal to 0, which was a mainly for convenience. I could have taken x is equal to some value of x 1. Still, I would get the same expression. So, this choice of x is equal to 0 was mainly to keep the maths simple.

Hence, in general term, I would write this equation. As the diffusion current will be given by the diffusion constant for holes, d p d x, at any x, I evaluate. This will be giving me the diffusion current due to holes. So, this would be diffusion current due to holes. In the same manner, I one can write. One can do a similar analysis and find that diffusion current due to electrons. Here, there is going to be a change because, this is now going to be positive. Why it is going to be positive?

Because, conventionally the current is in the opposite direction to the motion of electrons; the diffusion current due to electrons will be given by this expression. Now, in this derivation, we made the assumption of having only a motion of random motion of carriers in one dimension. If one does more exact modeling and assumes that the carriers can move in all three directions. Then, the diffusion constant that we got here; the diffusion constant here has whether n or p as a value of v bar l divided by 2.

This is for a one dimensional problem. But, if I do it for a exact three dimensional problem then, this would be given by v bar l by 3 for a problem where the three motion in all three dimension is considered. Then, it gets changed by 3. So, it is not very important what exact expression this is because eventually, you will be dealing with the diffusion coefficient here. You will calculate from experimental values. So, for purpose of illustration, this one dimensional problem is much more easier to visualize. Where does the diffusion current come from? Keep in mind.

This v bar l or they have written for electron and holes will be different for electron and holes. The reason for that is because electrons are moving in the conduction band and holes are moving in the valence band. So, they will have thermal motion; is going to be dictated by the band structure of their particular band. Hence, you will have different values of v bar for electron and holes. It will not, it is not going to be the same value.

Now, having come up with an expression for diffusion current, what is important is what is this?

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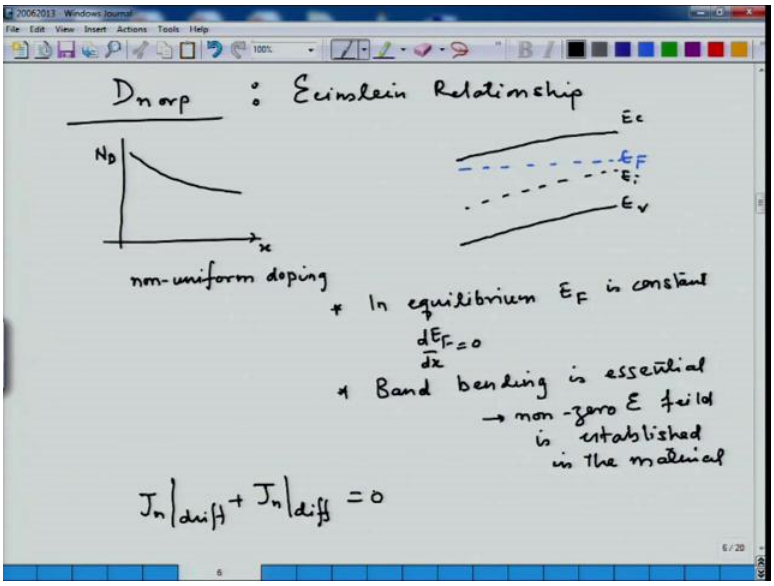

Diffusion coefficient n of p. So, when we were talking about drift, we looked at the carrier motion in response to the electric field. Then, the parameter which is important in case of drift is the mobility of carriers. Then, we looked at how what the behavior of this mobility, as a function is of may be doping concentration of semiconductor or as a function of the temperature. So, we will like to do the same thing for the diffusion constant.

But, before we do that, it becomes easier if we see the relationship between the carrier motion due to diffusion and the carrier motion due to drift. Both come from a from a similar reason. We can find this relationship and then, study what is the nature of this diffusion constant. So, in order to illustrate the relationship between diffusion coefficient and the mobility of carriers, we first develop famous relationship of Einstein relationship.

In this to derive this, let us take an example where we take a semiconductor. Let me take n-type semiconductor having a donor concentration, which is something like this. If we have a donor concentration like this so basically, this is non-uniform doping. If we have non-uniform doping, this means inequilibrium. The first condition that we must have in this material, that in equilibrium; the fermi level EF is constant or d EF d x is 0. So, in equilibrium, we have the fermi level which is constant.

Now, a fermi level is constant. I have a doping concentration which is changing in the x direction. It means I must have higher concentration of carriers here and lower concentration of carriers here. It basically means that, in this particular material, I have some amount of band bending of the semiconductor; conduction band, valence band. If I do that basically, what I am saying is, at this point, there are more electrons. At this point, there will be less number of electrons because of the non-uniformity of doping. EF will remain same. E c and E v will band in order to accommodate this doping concentration. E i will also be shown in this manner. That is the intrinsic level.

So, the first assumption here is that in equilibrium, if there is nothing else, no other applied field; the fermi level is constant in the material. The second thing is we call this fermi level is constant. You must have band bending. Band bending is essential to accommodate the non-uniformity. If you have band bending, which means you have a non-zero electrical field is established in the material. So, in this situation then, we look at what is happening in the material.

Since, the material is in equilibrium, this means that the drift current is equal to the diffusion current. What I will find in this material is the J electron for electron current due to drift plus J n due to diffusion is going to be 0. Now, what is this J n, so at any point x.

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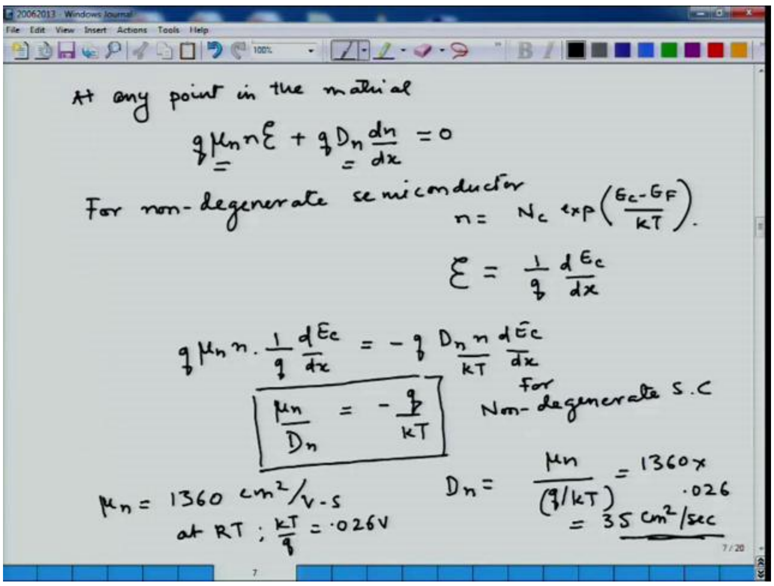

At any point in the material keeping the analysis one dimensional; I have basically the drift current, which is charged multiplied by the mobility of the electrons; concentration of electrons at that point times the electric field plus the diffusion current. It is charge multiply by the diffusion coefficient of electrons and the gradient of electrons at that point. This is going to be the two values for electrons. This should be equal to 0. Now, we lead this to the final solution; relationship between the mobility and diffusion constant in equilibrium.

So, we take help of one additional assumption, which says that let us solve this for non-degenerate semiconductors. In that case, I have an expression for n which can be written in terms of the band energy. So, I know what n is at any particular point. Then, if I know n, I can calculate d n d x. I also know from the discussion. During drift that the field inside the semiconductor can be related to the band bending due to this field by the expression 1 over q. The band bending is due to as the result of this field inside the semiconductor.

So, if I use these expressions for a non-degenerate semiconductor, I can write the electric field can be given as amount of band bending D n n d n of d x will be nothing but n time d E c d x. So, if we simplify this expression, this basically generates that mobility. This cancels out and d E c d c x cancels out. So, mobility divided by the diffusion constant is going to be, sorry, when I differentiate this, I will get expression of 1 over k T. It is going to be given by negative q over k T.

Now, this is very interesting. What it is saying is that the carrier mobility divided by the carrier diffusion coefficient ratio. This ratio is a constant. It only depends on the charge of the carrier, which is electron charge Boltzmann constant and the temperature. This then immediately says that if I know my mobility of carrier, I can calculate what is a diffusion coefficient for that carrier. Let me take an example here. So in the earlier lectures, we have taken example for let us say the mobility of electrons is 1360 centimeter square per volt second.

It would mean that at room temperature, this is going to be if I want to calculate diffusion constant; it will be mu n divided by q over k T. This k T over q is like voltage. If I am calculating at room temperature, k T over q is given by 0.026 volts. So, this gives me the diffusion coefficient will be 1360 centimeter square per volt second multiplied by 0.026

volts. This comes out to be equal to 35 centimeter square per second. So, there are two things that come out of here.

The units for diffusion constant are centimeter square per second. We can calculate if we know the mobility of the carriers. From the mobility, we can calculate what is going to be the diffusion coefficient for carriers. Similarly, we can calculate for holes, if we know the mobility. So, this then gives us a relationship between the mobility and diffusion coefficient of the semiconductor. Keep in mind. This whole derivation is for non-degenerate semiconductors. This is for non-degenerate semiconductors.

Had it been the degenerate semiconductor, we would have done the fermi direct integration in using this expression. That would be slightly different expression. Also, the other important point here is that we have derived this for a equilibrium situation. But, this Einstein relationship is equally valid for a non-equilibrium situation. We will not do that derivation here. But, this expression is equally applicable to a non-equilibrium situation. So now, we have a relationship between mu n and D n or mu p or D p. We can use that for our purpose. So, if we then look at what would be, what will happen to D?

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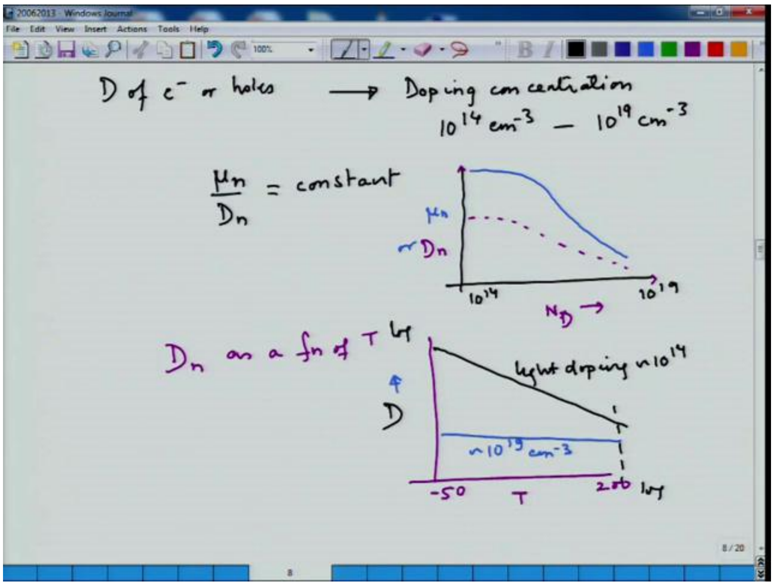

Diffusion coefficient of electron or holes; if we look at what it what will happen? If I change the doping concentration thus, the doping concentration goes from 10 to the power 14 per centimeter cube to something like 10 to the power 19 per centimeter cube. How will my diffusion coefficient change, whether it is donor or acceptor? How will it change? How would we find that expression? Here, we are going to use the Einstein relationship, which basically says that mu n.

If I am talking about electrons divided by D n for a non semiconductor, is a constant. Basically, it says then, that whatever expression we found, whatever relationship between we found for the mobility of carriers and doping concentration; the same behavior will be seen for diffusion constant. So, let me remind you what we saw in case of mobility in a schematic form. As we went from low to high concentration, the mobility drops like this.

You can also plot for mu p which basically means that D n will also follow a similar behavior. Since this is a constant, it will also drop as we go to higher concentration. Now, this is of course, physically also make sense because the diffusion coefficient is due to the thermal motion of particles. Mobility is also due to thermal motion. In addition to that, you have response to electric field. But, scattering events are there in both of them. This drop in the mobility is because as we increase the doping concentration n.

As we increase the doping concentration, you have more impurity scattering as oppose to the lattice scattering enhance. You have drop in the mobility and the same phenomenon is true for diffusion coefficient. If we try to see the same behavior for different concentration, what will happen to the diffusion constant of n as a function of temperature? Schematically, what we expect is that it will be the similar behavior. If I plot temperature range of minus 50 to 200, the mobility for low doping concentration sees on the log scale drops as a temperature increases.

As a temperature increases you have more and more of lattices scattering taking place. The mobility drops fast. This is for light doping. But, if I increase the doping concentration then, the same dependence might be more flat. This is for heavy doping approximately, 10 to the power 19; that is mean same schematically trying to plot the mobility. The reason for this more flat dependence is because at higher concentration, what we have is more of impurity scattering that is dominating over the lattice scattering.

Hence, the behavior is more flat. So, this is basically the behavior as a function of temperature for diffusion constant, which is also look similar to the mobility constant. So, this is for the diffusion constant depending on how much doping I have in the semiconductor. So, this tells me what my diffusion constant is. It tells me how it will behave if I change doping concentration. It also tells me how it will behave if I change the temperature for a light doping semiconductor or a heavily doped semiconductor.

It is going to basically following similar behavior as of the mobility of the, of the respective carrier. Now, proceeding further, let us take an example of where diffusion is going to be important before we go further.

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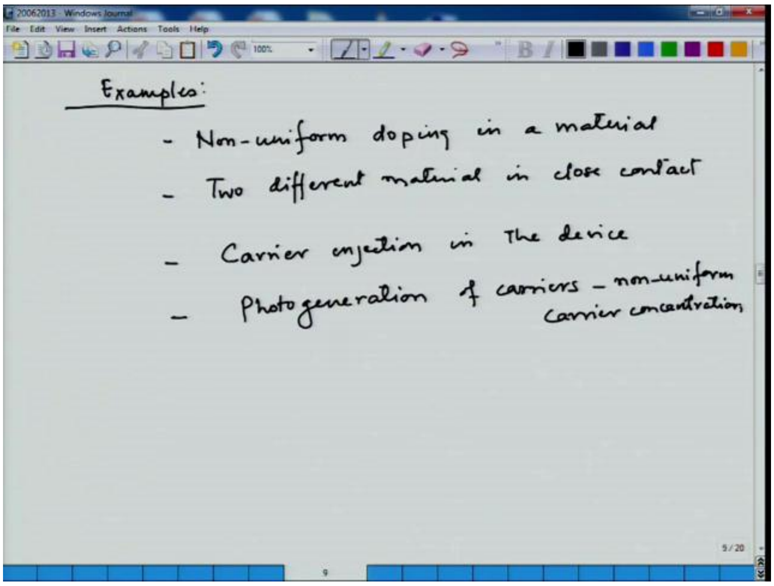

So, examples; one example, we have already seen the diffusion is going to be important when you have non-uniform doping in the material. Then, the diffusion will take place. Diffusion will be important when you have two different materials adjacent to each other material in close contact. We will see an example of that when we look at p-n junctions. One can have the same situation when we have a metal semiconductor contact. Then also, there will be a diffusion process between the two different materials.

There are other ways in which you can have concentration gradient. That is by carrier injection across the device carrier injection in the device. That will lead to non-uniform carrier concentration. Diffusion will become important. One can have a photo generation of carriers. That would also lead to non-uniform carrier concentration. So, we will see later that diffusion is a extremely important process in deciding the device behavior in many of these devices. So, to take a numerical example, let us take semiconductor.

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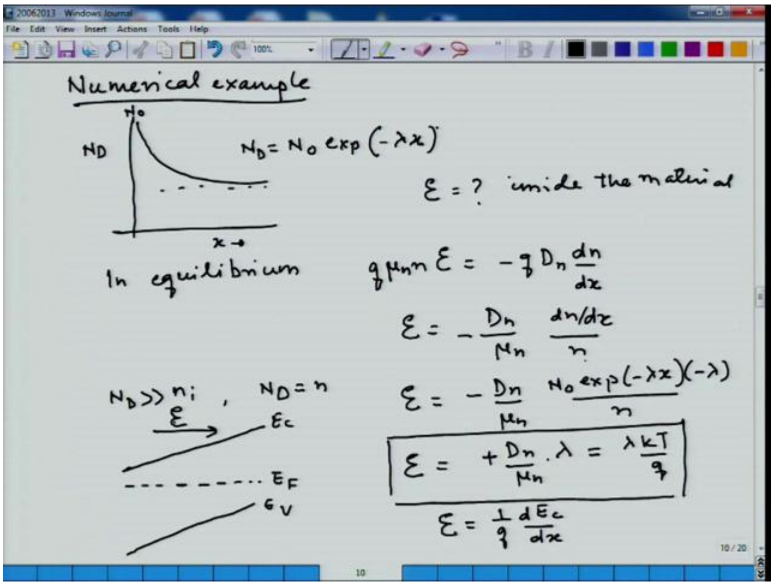

So, I am going to take us semiconductor which has donor concentration, which is being represented by a exponential equation. So, donor concentration here is being given by a concentration at the surface let us say N naught. Then, it is reducing exponentially. This is the behavior in a semiconductor. What we want to find out is what will be the electric field. What is the electric field inside the material because of this non-uniform doping of the material?

Now, from the, in the equilibrium equation, as we derived for earlier, we can situation would be were drift of the carriers is going to be equal to diffusion of the carriers. This would be the equilibrium situation. I am interested in finding out the electric field. So, electric field is going to be nothing but D n over mu n d n d x over n, the negative sign. Since I know N, I know, I do not know N, I know N of Dd. If N of D is much greater than the intrinsic carrier concentration then, I can assume that N of D is equal to n for complete ionization.

In that situation, I can write the electric field is going to be D n over mu n. The differentiation of this equation converted to the carrier rate concentration divided by n. That will lead to N naught exponential. N is nothing but this expression itself. Hence, I have the expression for electric field, which is saying electric field is going to be this coefficient multiplied by lambda. This will become positive. So, my and I know, the n D n mu divided by mu n is a constant, which is given by lambda D by mu is k T over q. so, this is the expression we get.

We get that if I have a exponential distribution of carriers in the semiconductor. I will get a constant electric field inside the semiconductor. So, if I plot the electric field inside the semiconductor, I will get in equilibrium. The band structure will be fermi level being constant. Since, electric field is given by 1 over q, the band bending, which is constant. This means that the bands are straight. This is structure E c E v. This is leading to electric field E, which is constant.

So, in this example of equilibrium, field developed in the semiconductor, we had a non-uniform concentration of dopant. That will add to a constant electric field in the semiconductor. Now, to summarize, we in addition to drift generation recombination, we have another process for transport of semiconductors, which is basically diffusion.

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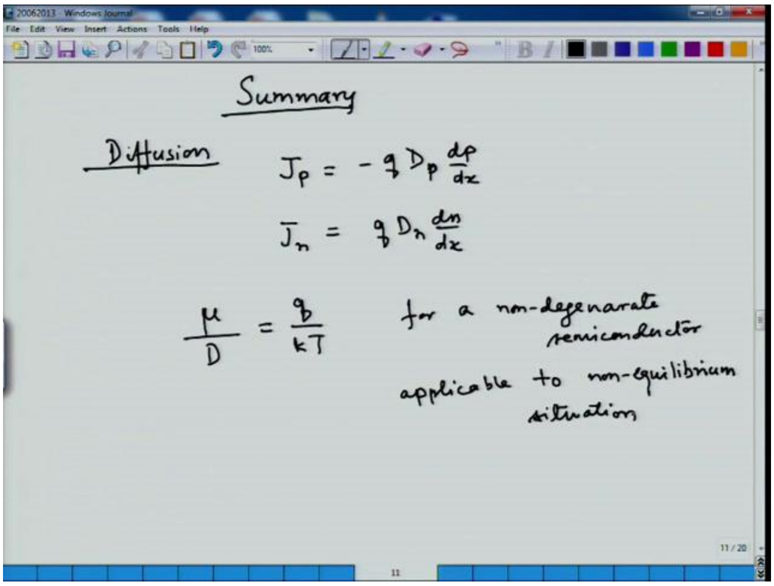

We can account for diffusion of carriers. The current generated because of diffusion can be given. The current density for holes is given by the expression q diffusion coefficient d p d x. Similarly, we derived that. We wrote the expression for the electrons that will be given by q D n d n d x. Then, we further found out that diffusion constant for any of the carriers mu n. Maybe I should write it in general form; mu over D is given by q over k T. This is for a non-degenerate semiconductor. This is the Einstein relationship.

It holds for non-equilibrium situations also. So, it is applicable for non equilibrium although we derived it for the equilibrium situation. Now, we have at the end of this lecture, we have our expression for drift; that is response of carriers to the electric field. We wrote the expression for J p and J n. For that, we have expression for current density due to diffusion. We know the rate at which the carriers will be generated or recombined. Adding all these process then, we would like to write an expression for all the responses of carriers to these fields and equation. That will help us solve the device characteristics. That we will do in the next lecture.