VLSI Technology
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Lecture - 16
Diffusion II- Infinite source and constant impurity diffusion

In our discussion regarding diffusion, we have seen that if the diffusion co-efficient D is assumed to be a constant, then the doping profile can be expressed simply as del N del t is equal to D del 2 N del x 2.

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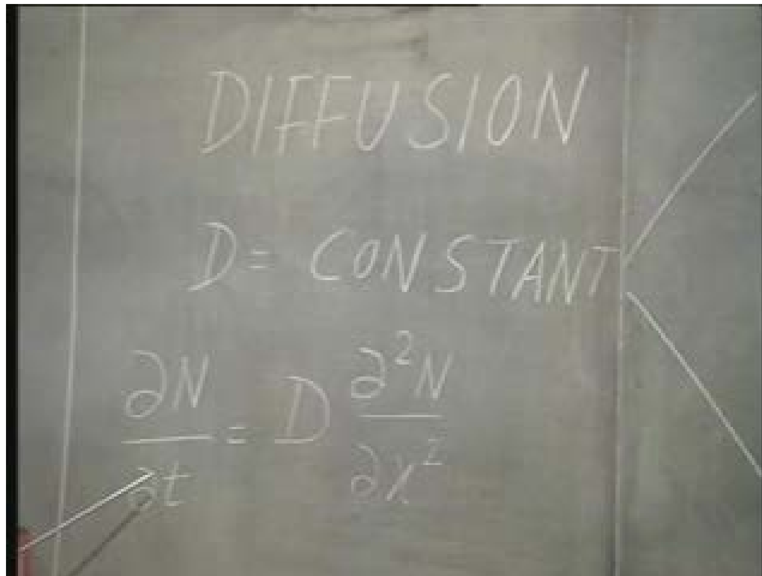

Now, all that remains is to solve this differential equations subject to various boundary and initial conditions and we have seen that for this D equal to constant case, there are two possibilities. One possibility is when we have an infinite source. When we have an infinite source that means the surface concentration is dictated only by the solid solubility limit. So, we also call the infinite source diffusion as the constant surface concentration case.

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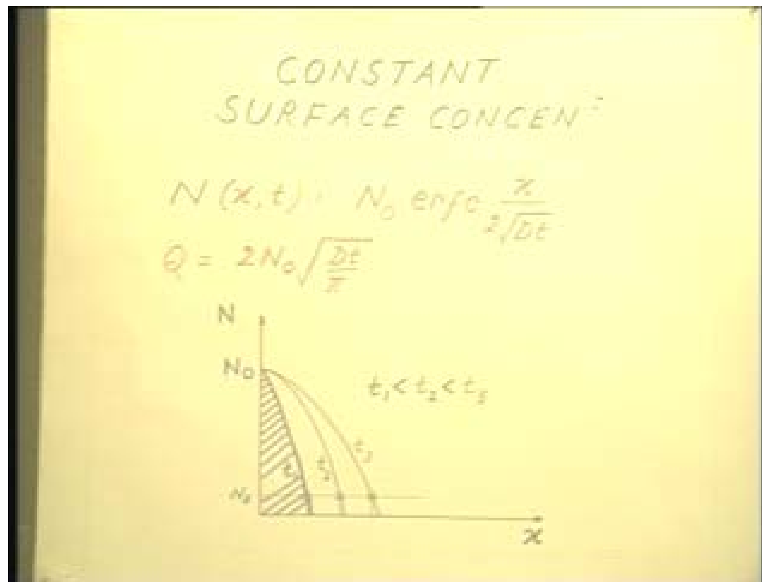

That is in this case, the surface concentration is fixed at the solid solubility limit and under that condition we have already derived the expression for the doping profile that is N as a function of x and t, space and time, is given as N 0 complementary error function x by 2 root over D t and this N 0 is actually the solid solubility limit. In a doping profile, the important parameters are the surface concentration, which in this case is fixed at N 0, the total impurity that is the area under the doping concentration profile curve which is obtained by integrating this expression for N (x, t) from zero to infinity and you obtain the total impurity as 2 N 0 root over D t by pi. So, this is one possibility where we have constant surface concentration or the infinite source diffusion.

In the language of diffusion in VLSI technology, this is very often referred to as the pre deposition. That is this deposition is carried out, this diffusion is carried out with the source on. The silicon samples are put inside the furnace in an ambient of the dopant, whatever be the dopant, phosphorus or boron, the ambient surrounding the semiconductor sample contains this impurity and with the source on the diffusion is carried out at a given temperature for a specified amount of time, so that the doping profile that we obtain is given by this error function profile. So this is the pre deposition.

Let us now focus on to the case two that is when we have constant total impurity.

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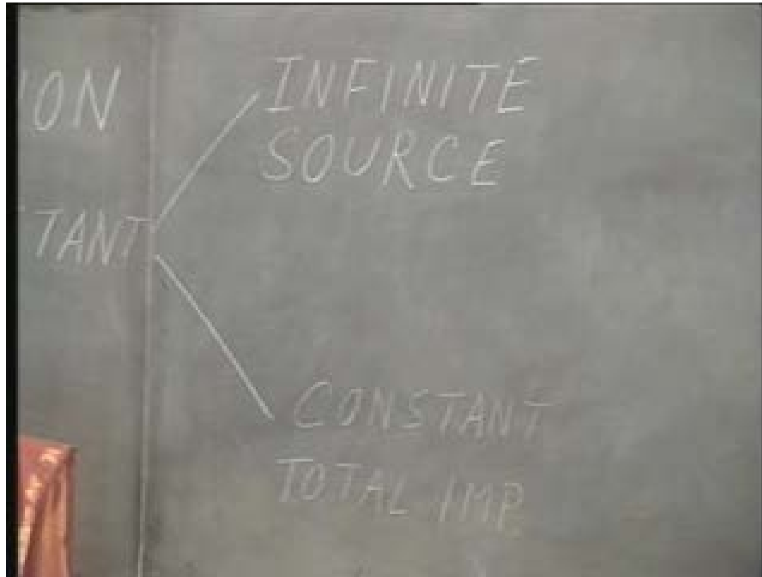

In a practical system what is done is this. We carry out the pre deposition at a given temperature for a specified amount of time, so that some amount of dopant is incorporated in silicon. It follows the complementary error function doping profile which is very abrupt. That is junction depth is very small. It is a, this total amount of impurity lies in a thin sheet of charge very close to the surface of the semiconductor. In the next step, the source is shut off and the sample with this thin sheet of dopant material already incorporated very close to the surface is subjected further to high temperature processing.

As the source is shut off there is no possibility of any new impurity coming into the semiconductor. That is why we call it the constant total impurity case. That is the total amount of impurity is fixed by the time of pre deposition, by the time and temperature of pre deposition. Whatever amount of total impurity has gone into the surface remains there and gets further driven inside the semiconductor material. So, this step is also referred to as the drive-in step. The infinite source diffusion is called the pre deposition step and the constant total impurity diffusion is called the drive-in step.

Now, let us see what is going to happen at the time of drive-in. We will have to solve, fix simple equation subject to the various initial and boundary conditions just as in the previous case. Only thing is the boundary conditions will change. So, what are the boundary conditions now?

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As we are saying that it is the constant total impurity case that means integral zero to infinity N dx is a constant that is Q. That is one boundary condition. The other boundary condition is of course that at a very large distance from the surface, the doping concentration falls to zero; N at x equal to infinity that is very much deep inside the surface is zero. These are the two boundary conditions and of course the initial condition is that, sorry, the initial condition is at the beginning of diffusion, the doping concentration is also zero.

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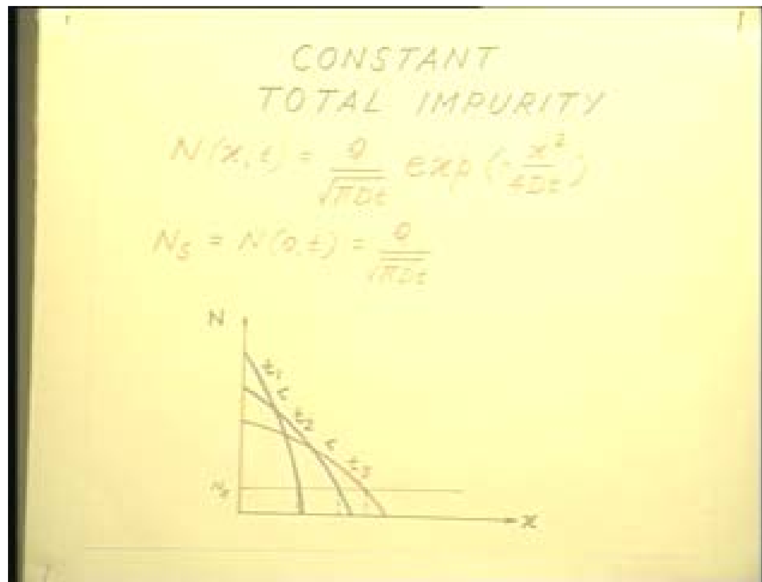

When we solve the differential equation subject to these boundary and initial conditions, the doping profile we obtain is given by N as a function of x and t is given by Q by root over pi D t exponential minus x square by 4 D t and this is a Gaussian profile. In the previous case, for the infinite source diffusion we obtained a complementary error function profile, in this case we obtain a Gaussian profile. Q is of course the total impurity which is constant in this particular case.

Now, as before let us try to analyze the important factors, important parameters associated with this doping profile and what are these? Now that we have obtained the equation for the doping profile, the first important thing is of course the surface concentration. Notice that in this case the surface concentration is no longer fixed by the solid solubility limit as in the previous case. In the previous case for infinite source diffusion, we said that the surface concentration is fixed at the solid solubility limit. But now as drive-in progresses, the surface concentration is going to come down. So, what is the surface concentration? Well, by definition the surface concentration is nothing but N at x equal to zero. x equal to zero is the surface. So, we have to solve this equation for x equal to zero.

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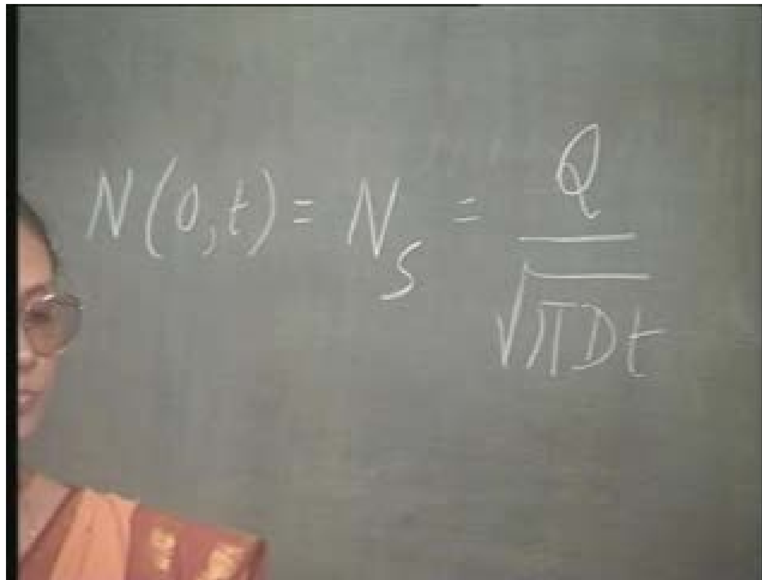

Now, at x equal to zero that is the surface concentration is given simply by .... Putting x equal to zero in this equation, this term becomes 1 and therefore we get N S. That is the surface concentration is nothing but the doping concentration at x equal to zero and given as Q by root pi D t. So, you note one very interesting point. That is as the time progresses, t, small t, as time progresses the surface concentration keeps falling and that is depicted here in this curve.

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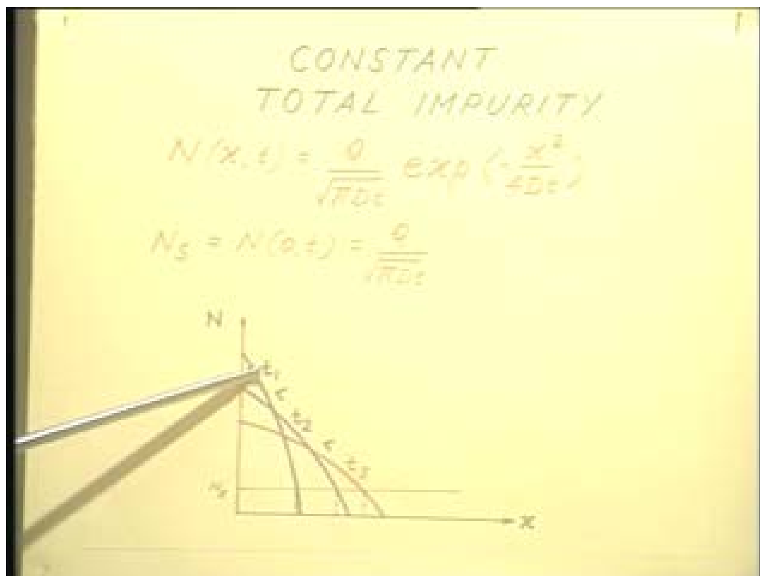

Let us say we carried out the drive-in for a time t 1 and the surface concentration was at some value here. As the drive-in progresses, if we carry out the drive-in for a longer time, t 2 being greater than t 1, then look at this violet curve. The surface concentration has come down. Carry out drive-in for even longer time, t 3 greater than t 2 and the surface concentration falls even below. So, as the drive-in progresses, as the duration of drive-in is increased the surface concentration decreases and obviously the dopants move further and further inside the semiconductor.

So, that brings us to the next important parameter which is the junction depth.

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In order to find the junction depth x j, how is the junction defined? The junction is defined as that point inside the semiconductor at which the impurity concentration equals the substrate background doping concentration. In other words that is the point where N becomes equal to the background doping concentration. So, x j corresponds to N equal N B, N B being the background doping concentration. So, if I put N equal to N B at the left hand side of this equation, then what do we get? We get N B is given as Q by root pi D t which is N S exponential minus x square by 4 D t and this x is actually x j. So, at x equal

to x j, N should corresponds to N B and therefore you obtain this equation that is N B equal to N S exponential minus x j square by 4 D t.

In other words, x j is a function of D t as well as the ratio of N B and N S. These are the two factors which determine the junction depth. So you see, this D t is a very important factor as far as diffusion is concerned, D multiplied by t, diffusion co-efficient which has a unit of centimeter square per second and time is usually given in seconds. D t actually has the dimensions of centimeter square or square root of D t, it has the dimensions of length. So, square root of D t is actually, I could say that it represents how much the dopant has moved inside the semiconductor material. It affects the junction depth, because it is going to dictate how much the dopants have moved inside the semiconductor. So, this is the constant total impurity case.

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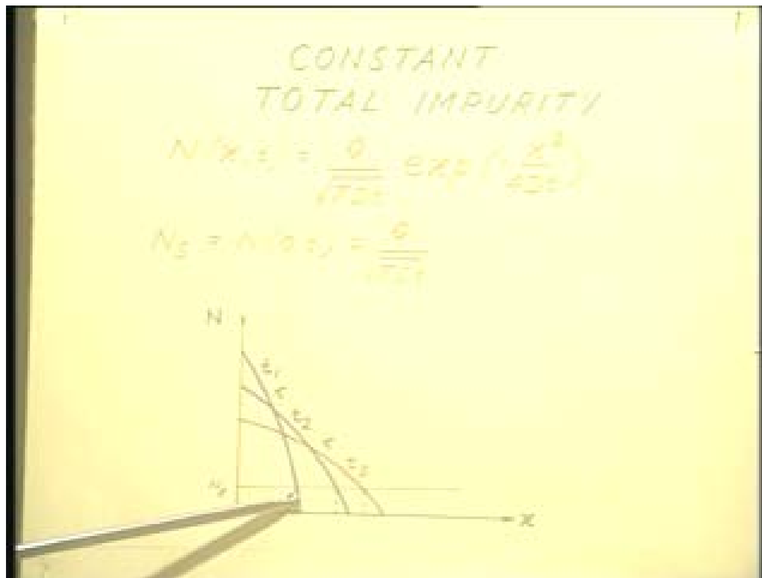

Again let me draw your attention to this curve. In this particular case you see, as the time progresses the junction depth increases. This is the junction depth for t equal to t 1 case, this is the junction depth for t equal to t 2 case, t 2 being greater than t 1 and this is the junction depth for t 3, t 3 being greater than both t 2 and t 1 and obviously because this is the factor which is x j is going to be directly proportional to square root of D t. So, as

time increases, the junction depth is going to be larger. That is the dopants are going to move deeper and deeper into the semiconductor material.

So, so far we have discussed the cases where the diffusion coefficient is assumed to be a constant. Only in that case we can use, fix simple diffusion equation and solve the differential equation, subject to the conditions of infinite source or the condition of constant total impurity. But now suppose, if the diffusion coefficient D is not a constant, but instead it is a function of doping concentration, then what happens?

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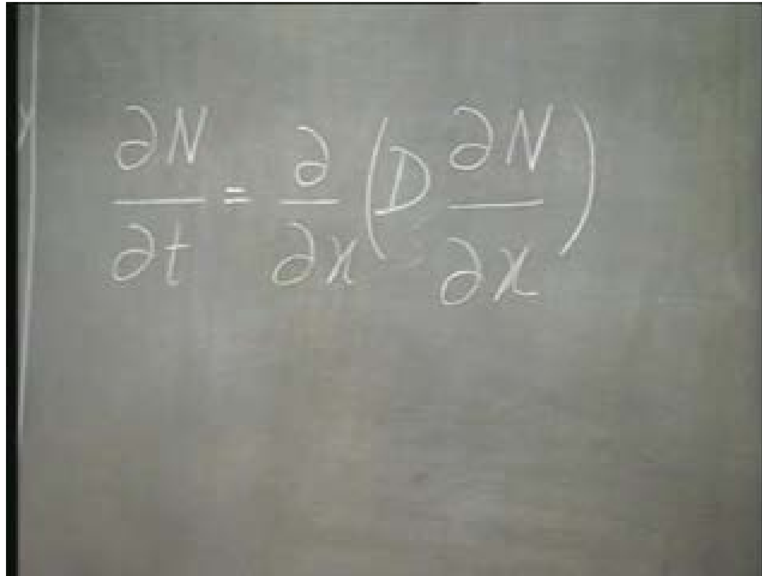

Well, in that case obviously, we cannot use the simple diffusion equation, we have to go back to the original equation that is del N del t is equal to del del x of D del N del x. Since D is no longer a constant, we cannot take it out and make it the simple diffusion equation. The analytical solution of this equation is more difficult, but it can be done and people have tried to do computer simulation of the cases for D being a function of concentration. Now of course, the question remains as to what really is the case. Is D a constant or is D really a function of the concentration?

We will see later that in a practical situation, depending on the circumstances D can either be a constant or D can be a function of concentration. But, first of all let us see what happens if D is a function of the doping concentration N.

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Under such conditions, I could say that D is, let us say, D is proportional to N. Let us assume the case where D is proportional to N, so that I could write that D is equal to some constant K into N, so that at the surface where the surface concentration is N S, I could say that it is associated with a diffusion coefficient D S. This is the surface diffusion coefficient which is given by K times N S. Therefore in general, I could write D is equal to ....., given in the normalized fashion D is given by the surface diffusion coefficient D S multiplied by N by N S.

Similarly, if D is proportional to N square, I could say D will be given by N square by N S square D S. If D is proportional to N cube, then D will be given by N cube by N S cube into DS. That is to say I can define three possible cases.

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$$D \propto N \rightarrow \frac{N}{N_S} D_S$$
$$\propto N^2 \rightarrow \left(\frac{N}{N_S}\right)^2 D_S$$
$$\propto N^3 \rightarrow \left(\frac{N}{N_S}\right)^3 D_S$$

D proportional to N in which case D is given by ...... We have defined these three cases: D proportional to N, D proportional to N square and D proportional to N cube. Computer simulation of these cases that is where D is proportional either to the doping concentration or to the square of the doping concentration or to the cube of the doping concentration, computer simulation taking these things into account and assuming an infinite source diffusion will have the profile like this.

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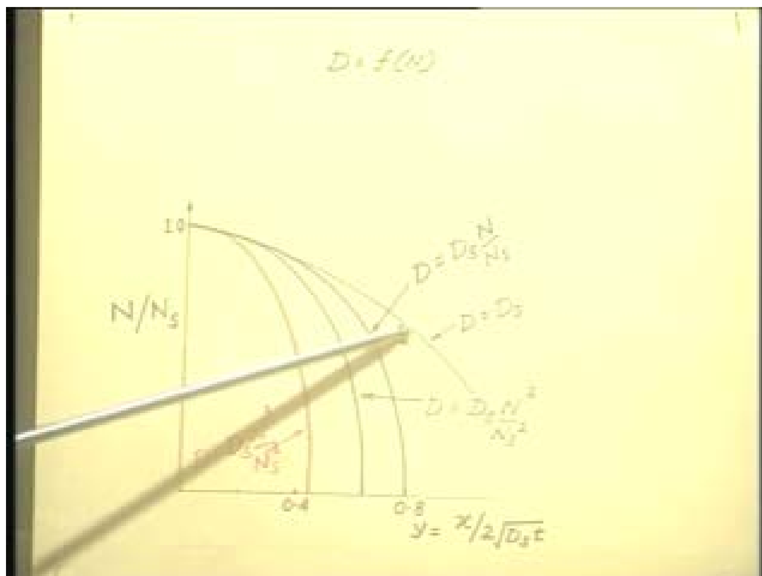

See, here this curve is for the constant diffusion coefficient that is the complementary error function case, infinite source, D is the constant. Therefore, this is for the complementary error function case. The next one is for D being proportional to N. D is given as D S N by N S and the green one is for D is proportional to N square, the red is D being proportional to N cube. So, one thing is very clear from this figure. That is compared to the complementary error function profile, all the other three are much steeper, they are more abrupt. What do we mean by that? That is you see, the surface concentration in all these cases is given by N S, it is normalized; N by N S is 1.

Now you see, the junction depth is here for the rate curve, at around the value of 0.4. In this particular case, this is at around the value of 0.8 So, one thing is the junction becomes shallower, as D becomes a more power; this shows a more power dependence on the doping concentration. The junction becomes shallower and over larger part of this junction, the doping concentration remains close to the surface concentration. In the complementary error function profile, you see the junction is much deeper compared to the other three cases and the doping concentration is falling; right from the surface it is falling gradually, whereas compare it with D equal to D S N cube by N S cube the junction is much shallower and it remains at the surface concentration level for a much larger part of this junction and then falls more steeply. This fall is much steeper compared to this, this fall.

So, when D is a function of the concentration we obtain a more abrupt, more box like profile. It is called a box like profile. That is it can be approximated as a rectangular box. This fall is almost vertical. That is why this can be approximated as almost a box and for these three particular cases, the junction depth can be given as this.

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x j is given by 1.616 root over D S t for D proportional to N, it is equal 1.019 square root of D S t for the case D proportional to N square and it is equal to 0.87 square root of D S t for the case where D is proportional to N cube. That means if we have the same surface concentration and the same time, then for D proportional to N case, the junction depth will be given by 1.616 times square root of D S t and in this case, it will be about half of that 0.87 times square root of D S t. That means as D shows a higher power dependence on the doping concentration, the junction becomes shallower and of course the profile also become steeper as can be seen from the chart. The profiles have progressively become steeper as D becomes a, shows a higher power dependence on the doping concentration.

Now of course, the question is what really happens? In a real life situation, should D be considered as a constant or should it be considered as a function of the doping concentration? What is usually taken, accepted is that you see diffusion is carried out at high temperature and you know that the intrinsic concentration of semiconductors that is also a function of temperature. As the temperature increases, the intrinsic carrier concentration of semiconductor is also going to increase. Now, at the diffusion temperature if the intrinsic carrier concentration is much higher than the impurity

concentration, then the diffusion coefficient D can be modeled as independent of concentration that is the D equal to constant case.

On the other hand, if the impurity concentration is very high, much higher than the intrinsic carrier concentration of the semiconductor even at the diffusion temperature, then the diffusion coefficient is assumed to be a function of the doping concentration. That is D is equal to f (N). This is because, actually what is going to happen at the time of diffusion? Let us consider the substitutional impurities, because they are electronically active and therefore the most important as far as VLSI technology is concerned. You know that for substitutional diffusion, the dopant atoms are going to replace silicon in the lattice site. In order to do so, there must be vacancies, there must be point defects; vacancies are point defects.

These vacancies must be available in the lattice, so the diffusion is primarily a process where the dopant impurity is going to interact with these points defects and these point defects can be in various charge states. They can be neutral, they can be positively charged, they can be negatively charged. So, the reaction of the dopant atoms with these vacancies, depending on their charge states, will depend on the concentration, on the electron and hole concentration and therefore the diffusion coefficient will become a function of concentration.

On the other hand, if at the diffusion temperature the intrinsic carrier concentration of the semiconductor is going to dominate, then the diffusion coefficient can be taken to be independent of the doping concentration and in that case, the doping profile can be modeled for the infinite source case as the complementary error function profile and the constant total impurity case as the Gaussian profile and usually as I have already told you in a practical diffusion system, it is a combination of both. First of all pre deposition is carried out which is an infinite source diffusion and at the end of that pre deposition, some amount of total impurity is put at a layer very close to the semiconductor surface.

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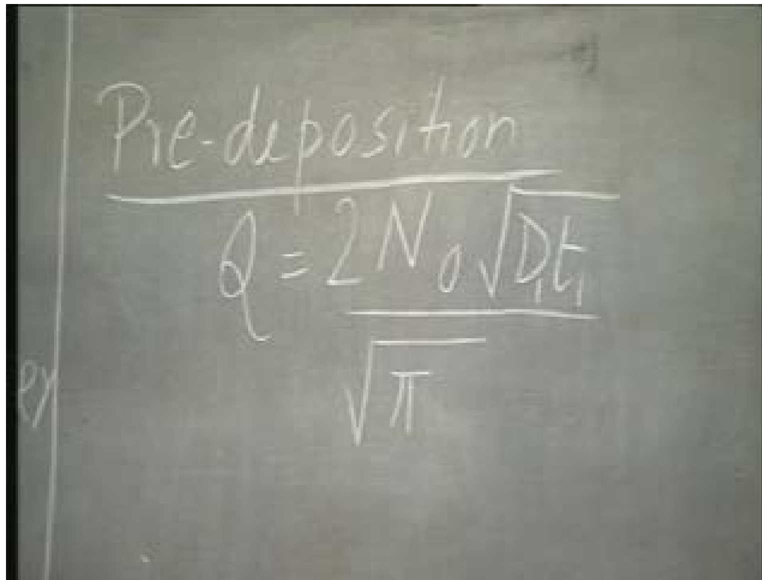

So you know, that this infinite source diffusion followed the complementary error function profile and the total amount of impurity that is put after carrying out the diffusion will be given by ...... So, in a practical diffusion system, the first step is pre deposition which is an infinite source diffusion and at the end of this infinite source diffusion, the total amount of impurity that is put inside the semiconductor is given by 2 N 0 square root of D t by pi. Now, let me use the suffix 1, D 1 and t 1 in order to characterize the pre deposition process, because this is the first step in the diffusion. So, Q is given as 2 N 0 square root of D 1 t 1 divided by root pi.

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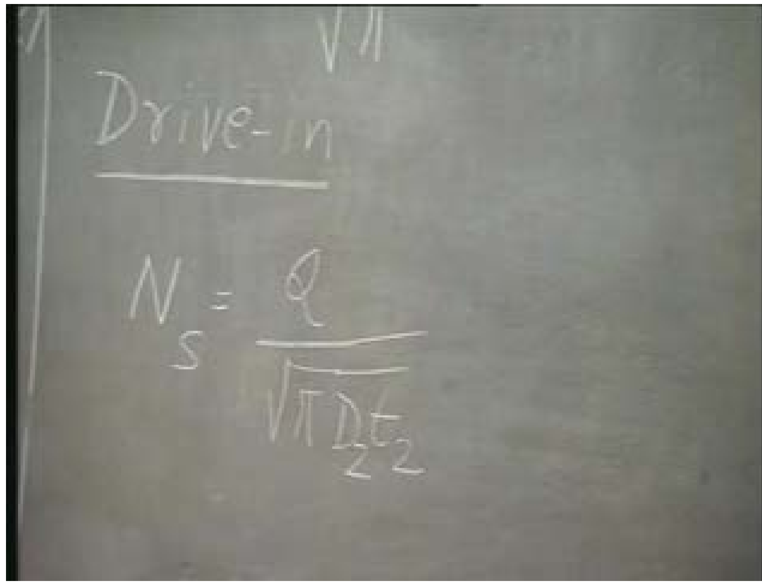

Now in the second step, the samples are going to be subjected to drive-in. Drive-in is nothing but the constant total impurity case. That is now the source has been shut and this amount of impurity is going to be there that is the total amount of impurity. We are not going to put any additional amount of impurity, this is the only amount of impurity which is going to be there. So you know, that for this case, the surface concentration is given as, let me use suffix 2 for this, because this is the second step, drive-in is the second step and these two processes are not necessarily carried out at the same temperature. That is why the diffusion coefficients are different, D 1 and D 2 depending on the temperature. Of course, the pre deposition time and the Drive-in time are also different, t 1 and t 2. Now I know what Q is, because Q was put during the pre deposition case.

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So, substituting for the value of Q, I can write that the surface concentration N S is given as 2 N 0 square root of D 1 t 1 divided by pi square root D 2 t 2 or simply.... This is a very interesting relationship. As I have already told you that pre deposition is carried out at a temperature corresponding to which the diffusion coefficient is D 1 for the time t 1 and drive-in is carried out at a temperature corresponding to which the diffusion coefficient is D 2 and the time is t 2.

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So you see, in a practical situation, D 1 t 1 will be much, much less than D 2 t 2. That is pre deposition will be carried out at a much lower temperature, so that D 1 will be much smaller than D 2 and for a much lesser amount of time, so that t 1 will also be much lesser than t 2. Therefore, the product D 1 t 1 is going to be much, much lesser than D 2 t 2. If that is so, then you can see that the surface concentration is going to be very much less than the solid solubility limit, N 0. N 0 was the surface concentration at the end of the pre deposition case and after the drive-in, the surface concentration is going to fall considerably by the factor square root of D 1 t 1 by D 2 t 2 and this 2 by pi is also less than 1, so that after drive-in the surface concentration is going to be much, much less than the solid solubility limit.

Another point what I want to mention in this case is very often, one diffused layer will be subjected to further high temperature process. For example, let us consider the case of base diffusion in bipolar junction transistor. You know, in a bipolar junction transistor, we first have to diffuse the base and then we have to diffuse the emitter. So during base diffusion, pre deposition and drive-in, we have obtained some junction depth, some surface concentration for the base region. Now, during emitter diffusion, the base is also being subjected to further drive-in. We are carrying out the emitter diffusion also at high temperature. So, even though we are not putting any new base dopant, the already present base dopants are being subjected to a further drive-in process and therefore, both the junction depth as well as the surface concentration of the base region is going to change. So, this has to be taken into account when one is designing the process steps for fabrication of a bipolar junction transistor, because you know the base width is going to be a very important factor.

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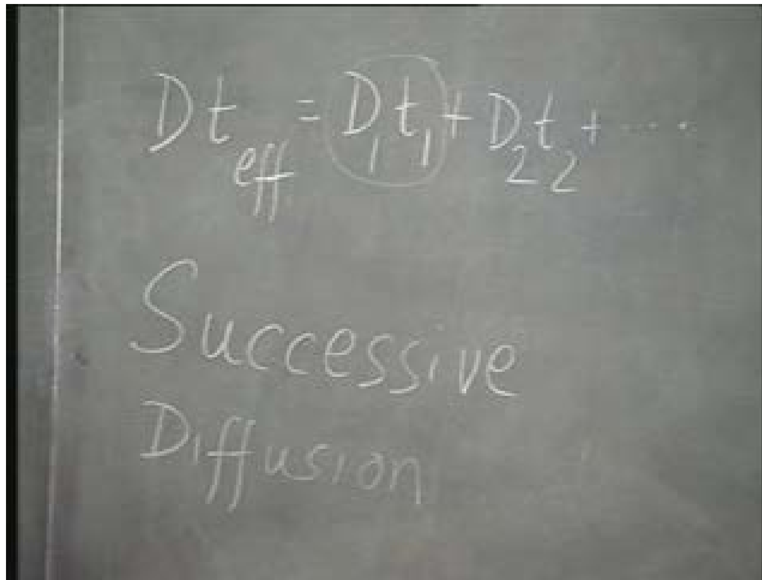

So, when you design for transistor with a particular base width, you must take into account not merely the base junction depth during the actual base diffusion, but also the additional effects during the emitter diffusion and in such cases the effective D t, because you know D t is the very important parameter, D t in fact represents how deep the dopants have gone inside. In such cases, D t is given as ...... That is each D 1 t 1 D 2 t 2 they are all corresponding to the particular processing step.

Let us say this processing step is for the actual base drive-in. Drive-in was carried out for a time of t 1 at a particular temperature, so that the diffusion coefficient was D 1 and then in the next instance, the emitter diffusion was carried out; emitter drive-in was done for a time of t 2 and at a temperature corresponding to which the diffusion coefficient of boron was D 2. So, in that case the effective D t will be given as D 1 t 1 plus D 2 t 2 plus if there are any further processing steps. So, this is called successive diffusion. So, this is quite an important aspect of diffusion. That is any high temperature processing will modify the diffusion profile. Any high temperature processing is going to modify the diffusion profile and that is one reason why in VLSI technology one goes more and more for low temperature processing, so as not to affect the already obtained diffusion profile.

The more you subject it to high temperature, the more you are going to affect the diffusion profile. So, this is the successive diffusion.

The other thing is of course if we carry out a two step diffusion like I said a predeposition followed by drive-in, then what is going to be the final shape of the doping profile? Well, in most cases since the drive-in time and temperature is much larger than the infinite source predeposition time and temperature, the final doping profile will be approximately Gaussian that is when D 2 t 2 is going to dominate the case as is true for most practical situation. So long as D 2 t 2 is much larger than D 1 t 1, the doping concentration profile will be given by approximately a Gaussian profile. Mathematically speaking this is, these are the laws by which the diffusion is governed and this is how the doping profile is obtained.

In a practical situation, however we will see that the diffusion coefficients cannot be expressed so simply. That is we cannot blindly give a blanket ruling, either they are going to be independent of concentration or it is going to be proportional to the concentration or proportional to the square of concentration. In a practical situation, the diffusion coefficient may have various component, one independent of doping concentration, one proportional to doping concentration and like that and which term of the diffusion coefficient is going to dominate will depend on the particular situation. For example, closer to the surface where the doping concentration is very high, it may be dominated by the constant dependent case. On the other hand as we move inside and the doping concentration falls, may be it falls below the intrinsic carrier concentration and then the diffusion coefficient becomes independent of concentration.

So, in a practical situation, the diffusion coefficient will have a number of terms and therefore the profile will be somewhere in between, like it will not be a straight forward case as we have shown here.

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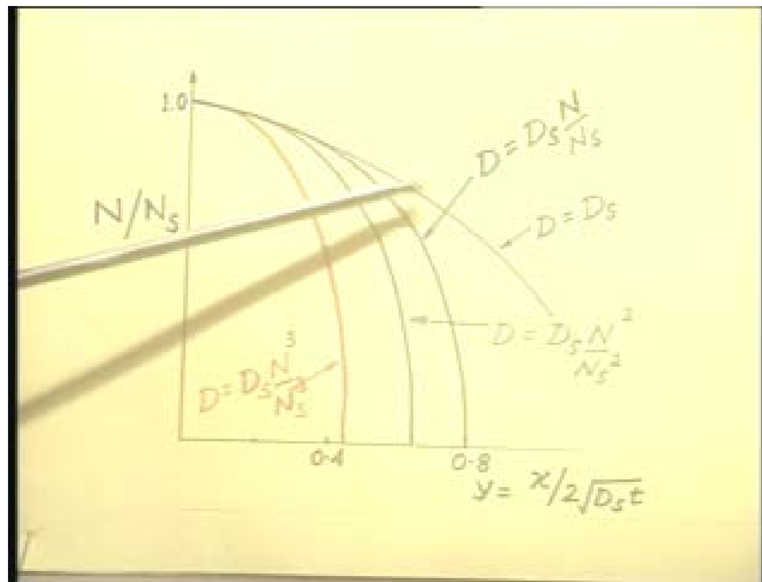

That is this is for the complementary error function profile when D is constant and for D proportional to N or N square or N cube, it follows a much steeper path, it may be somewhere in between.

These are the things we shall investigate in the next class. We will see what are the factors which cause the diffusion coefficient to depend on the concentration and where these particular terms are going to dominate and then, we will investigate for the actual situation that is boron or phosphorus or arsenic, the real dopants in silicon. In that case which terms are going to dominate and how the diffusion profile is going to be modeled.