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JUDY HOYT: All right. We're beginning the lecture on handout number 15. This is the second lecture on dopant diffusion and profile measurement. And we're working on chapter 7 of your text. So last time, we introduced some of the basics of dopant diffusion. We talked about basic definition of sheet resistance, and the scaling requires from us that we pointed out there's a conflict between the need for smaller series resistance and the need to decrease junction depths to improve control of the channel charge.

We also talked about short channel effects and how  $d_r$  decreases as  $L$  goes down. We mentioned the use of predeposition, either in the gas phase, or by ion implantation. And then the use of subsequent driving of dopants to create a doped regions. We spoke about macroscopic diffusion from the point of view of Fick's first and second laws, and gave a few cases. There were only about three or four cases where there are simple analytic solutions to the diffusion equation.

Today, I want to just briefly review those analytic solution examples, and then talk about a brief introduction to numerical solutions to the diffusion equation. Then we'll talk about design of diffuse layers based upon certain device requirements, such as the sheet resistance. And our first deviation from Fickian diffusion, we'll discuss electric field effects on dopant diffusion. So let's go on to slide number 2 and just review from last time this pictorial view of Fick's second law.

What I'm showing here is a volume element that is shown by the blue rectangular element. And there is a flux  $f_{in}$  going in the left-hand face, and a flux  $f_{out}$  going out the right-hand face. Remember again, our basic definition of flux is, it's a number of atoms or particles per unit time per unit area. So looking at in this cube, we can calculate the net flow of atoms into this volume, into that small volume. As shown in the upper left corner is equal to the area  $a$  of one of those faces times the difference between  $f_{out}$  minus  $f_{in}$ . So that's the net flow of atoms.

And we can write that as  $a \frac{dc}{dt}$  and just looking at the geometry, it's  $\Delta x$  times the change in concentration,  $\Delta c$ , divided by  $\Delta t$ . So we can just rearrange this a little bit. The  $a$ 's go out, and what we see is that the first derivative of the flux,  $\frac{df}{dx}$ , is equal to the time change,  $\frac{dc}{dt}$ . So mathematically, if we want to write this, not in terms of  $\Delta$ 's or differences, but in terms of differentials, what we see is a time rate of change of the concentration in the box,  $\frac{\partial c}{\partial t}$  is equal to the first derivative of the flux,  $\frac{\partial f}{\partial x}$ .

And then we can substitute in the equation on the center of the page for the flux. We know from Fick's first law that  $f$  is equal to  $-D \frac{\partial c}{\partial x}$ . So that is, indeed, a way of deriving just bookkeeping and deriving Fick's second law. Now, the equation in the center of the page can be simplified somewhat if we are in the special case where the diffusivity is a constant, where it doesn't vary in space. I can pull the  $D$  out of the partial derivative with respect to  $x$ , and we just get  $\frac{\partial c}{\partial t}$ . So the time rate of change of the concentration is equal to a constant diffusivity. It's a number times the second derivative of the concentration with respect to  $x$ .

So that is-- at the bottom of the page would be then the special case of Fick's second law when the diffusivity is a constant. So let's go on to slide number 3. And these are a couple of cases we solved last time where we wrote down the solutions last time for two cases which are commonly encountered and for which analytic solutions are available. On the left-hand side, I'm reviewing the case of a predeposition. And again, by definition in this case, we are assuming that there is a supply of dopant, or atoms that are diffusing, that holds the surface concentration at a constant value  $c_s$ . That number is fixed.

And we said in this case that the shape of the profile,  $c$ , as a function of depth  $x$  and time is given by this surface concentration  $c_s$  times the complementary error function of  $x$  over  $2 \sqrt{Dt}$ . So that is the actual analytic solution to Fick's second law for a constant diffusivity. And we also know that the integral of that function integrated over our space, or throughout the silicon, has a value  $q$ . That's the dose, so the area under the curve. And that can be solved for, and it turns out to be  $2 c_s \sqrt{Dt}$ .

So this is a particular case and, in fact, showing a plot on the vertical axis is  $c$  over  $c_s$  as a function of depth. For several different times, the three curves here shown where the square root of  $dt$ -- or 2 times the square root of  $dt$  is being varied from 0.1 micron all the way up to 1 micron. And you get a feel for how the shape of the complementary error function evolves with time. In contrast, on the right-hand side, we're showing the case of a deriving that would typically be done after Pre-Dep.

And deriving takes place usually under the assumption of a constant dose  $q$ , so the constant area under the curve. And what's happening as a function of time then is the shape of the curve is changing, and it's-- we know the solution is a Gaussian, the solution to Fick's second law. And in fact, if you look at this equation as a function of time, you'll see that the concentration of the surface is dropping as a function of time according to  $1$  over the square root of  $dt$ . And the profile is broadening its width or its standard deviation is increasing according to  $dt$ . And there are a couple of different cases shown on the right.

So these solutions are valid under this particular case where the concentration of a diffusing dopant is less than  $n_{sub} i$ . And that implies in that case that the diffusivity is a constant. It doesn't vary in space. We'll talk in subsequent lectures about the case when the concentration is quite high, or higher than  $n_{sub} y$ . So let's go on to slide number 4. And this review is from last time. What we showed is an Arrhenius plot of the intrinsic diffusion coefficients of some common dopants in silicon. And what we're showing on the left axis on a log scale is a diffusivity and units of centimeters squared per second.

And the x-axis is  $1,000$  over temperature in Kelvin. The lower x-axis, the upper x-axis, actually has the temperatures actually indicated. So we are intrinsic diffusivity. So they apply when in the carrier concentration of the concentration of the dopant is less than  $n_i$  at the diffusion temperature. One thing you can notice right off the bat is that there are some fast diffusers in silicon, such as boron, phosphorus, and indium. They're the upper three curves. And the slower diffusers are arsenic and antimony and silicon.

It turns out just for practical reasons because of their high electrical solubility, that boron is often the p type opener of choice. It pretty much is. And arsenic in n type dope as you can choose arsenic or phosphorus, but arsenic is usually chosen because of its higher electrical solubility, and also sometimes its lower diffusion coefficient. It's easier to control profiles. So what-- typically, we're going to have issues with controlling diffusion in p type regions because boron is diffusing at any given temperature, almost an order of magnitude of higher diffusivity than the case of arsenic.

All right, let's go on to slide number 5. And here what we are trying to talk about is the effect of successive diffusions in, say, a [INAUDIBLE] process flow on the doping profiles. You remember from the first lecture of this course, we talked-- we kind of walked through an example of an integrated circuit fabrication process. And you know that they involve a large number of different steps at various temperatures. We don't just simply do a Pre-Dep and then a drive-in and then it's done. That could be oxidations, it could be other high temperature steps in which the dopants are going to move.

So if you have a whole series of steps, what's the question is, what is the actual final profile, and how can we approximate it? Well, it turns out in the case of Gaussian diffusion that we can write the total effective  $d^2$  product as being a measure of the thermal budget that's used in that process. And for Gaussian diffusion, we can actually sum up the products of the diffusivity in any given time step times the length of that time step,  $d$  times  $t$ . We can sum up those  $dt$  products and add them up, and end up with an effective  $dt$  for the entire process. Again, assuming that in each case, the diffusion satisfies the Gaussian assumptions.

What we'll typically find as you go through a whole process is that some of the processing steps may be negligible. And that's because the diffusion coefficients in this formula is exponentially activated, or it varies with temperature exponential. So the highest temperature steps in the process typically dominate. It's not always the case, for example, when we talk about transient enhanced diffusion. We see that's not the case.

But for normal diffusion, you expect the highest temperature steps to dominate this equation. And so you can usually zoom in on those as being the ones that primarily determine the  $dt$  product and, therefore, the shape of the profile. One thing you have to be aware of is that this Gaussian solution we've been talking about only holds if the delta function approximation for the initial profile is reasonable. We talked about this last time.

So it holds in the case where the width of the profile initially when you start is small compared to the final width, or compared to the total  $dt$ . If that assumption is not valid then, and we don't have a simple Gaussian solution, necessarily. OK, let's go on to slide number 6. And here, we're going to go through some principles and examples of the design of diffuse layers. So what we want to do is, as an engineer, a process engineer, or working with device engineers, we'll want to typically design a diffusion process, or a Pre-Dep and diffusion and a deriving process so that we end up with a certain sheet resistance that's required electrically by the device.

So that's the goal of this section. And I'm showing on the left-hand side just the example of a cube of silicon where the top region is colored in orange, and that is the little sheet through which we're going to be passing a current and measuring the voltage. And this little sheet has a particular geometry. What we're going to consider is the case where the length of this resistor is actually equal to its width. So it's a square, and it has dimension  $w$  by  $w$ .

And so we're going to define the sheet resistance of this junction. Last time we talked about it as being the resistivity, which is an intrinsic property of the material, depending on how it's doped and things, divided by  $x_j$  at the junction depth. We can see  $x_j$  marked on the left-hand side. And the units of that sheet resistance then are given it to be ohms per square.

So the sheet resistance is, indeed, the resistance  $r$  that you would get in a resistor made of 1 square of this material. And we can either write it as Roman  $r$  sub  $s$ , or  $\rho$ , Greek-- the Greek letter  $\rho$  sub  $s$ . And the  $s$  indicating it's for a sheet. The resistivity  $\rho$ , remember, is given by  $1$  over a cube with electronic charge times the carrier concentration  $n$  times mobility, which is in general, a function of  $n$ . And the resistivity has units along centimeter,  $x_j$  has units of centimeter, they cancel out. We end up with a sheet resistance in ohms per square.

That's all reasonably intuitive assuming you have a constantly doped-- a constant doped layer. For if a layer is non-uniformly doped, you need to integrate the doping profile times the mobility in order to calculate the sheet resistance. So the equation shown near the bottom of the slide says, sheet resistance can be obtained by  $1$  over the integral  $q$  times the integral from  $0$  to the junction depth of the doping-- of the carrier concentration profile, and of  $x$ , or the doping profile minus  $n_b$ . Or  $n_b$  is the background concentration that tells you where you cut off the electron concentration.

That quantity times the mobility, which is, in general, a function of  $ndx$  integrated. So that's what you would do in the case of a non-uniformly doped layer where the doping concentration is varying in thickness. Now, it turns out this equation you can solve it yourself. But this equation has already been numerically integrated by Irvin for a couple of different analytical profiles. In particular, the case of the Gaussian and the complementary error function profiles. And the solutions to those integrals are given in your text, either in Chapter 7, or there's also an appendix where the solutions are given.

So let's go on to slide number 7. And at the top of the slide we're showing an example of Irvin's curves for the particular case of  $p$  type Gaussian profiles in an  $n$  type background. And what you see in these curves on the  $y$ -axis is the surface concentration. So that would be  $c$  sub  $s$ , and atoms per cubic centimeter. The  $x$ -axis now is effective conductivity, and it has units of ohm centimeter to the minus 1.

So let's see if x-axis-- you can just go to the bottom of the slide, thinking about it, that is the effective average conductivity, so the inverse of the average resistivity. So we can write this as a signal bar and it's equal to a 1 over the product of rho sub s times xj. So it's 1 over the sheet resistance times the junction depth. So there are three key parameters we need to identify and using these curves. There's a surface concentration, which is the y-axis in the profile. There is-- again, this is for a particular type. This is for a Gaussian profile. There is the sheet resistance, which is coming into this effective conductivity. That's really part of the x-axis.

And there's the junction depth. So the x-axis has sheet resistance and junction depth built into it. And now the metallurgical junction is the place, the point in depth, where the chemical concentration in the diffuse region of the fused dopant equals the background concentration  $c_b$ . And we'll do an example shortly after this where you can see how these curves are used.

But each curve in the different color is for a different background concentration. So this, basically, tells you that you can take these three key parameters, and they have a unique relationship among themselves for the particular case where the shape of the profile is known. In this case, it's Gaussian. So in fact, let's go on to slide number 8. We're going to walk through-- the best way to understand these Irvin's curves is to go through an example.

And what we're asked to do in this example is to calculate the deriving conditions, which means the temperature, and the time to produce a CMOS p-well. So it's a p type, a region, and it's called a p-well of a certain thickness. And what we want to do, we're told that the constraint is that the sheet resistance of that p-well shouldn't be 900 ohms per square. OK. And it has to have a certain junction depth, which is shown schematically in the figure  $x_j$  to be 3 microns. And that  $x_j$ , again, is the point where the boron concentration then will reach the background concentration, which is given by  $10^{15}$  per cubic centimeter.

So again, we're informing a p-well by ion and planning bond into the region, onto the wafer. And the region on the left is blocked so we're just putting it in one region. And typically, you would implant boron at a certain dose, say,  $10^{13}$ , and energy. And then we want to drive that in. And we're interested in the driving conditions, what temperature. In time, what we need to get it to go that far and to have a particular sheet resistance.

And we're going to use Irvin's curves to do this. So let's look on slide number 9. So these are the constraints again repeated. The sheet resistance is 900 ohms per square. The junction depth has to be 3 microns, and the background concentration, either  $n_b$  or a substrate concentration, maybe  $n_{bc}$  is  $10^{15}$ . So given the requirements that we have been told, I can actually immediately find the x-axis on the Irvine curve with the average conductivity layer. It's just 1 over the sheet resistance times  $x_j$ .

So the average conductivity calculates out to be 3.7 ohms centimeter to minus 1. We can now from Irvin's curve, we can obtain, assuming this is the Gaussian, that's an assumption we need to make at this point, which we'll show is reasonable later, we can then obtain the surface concentration. So in order for me knowing the shape of the Gaussian, basically, Irvin's intervals tells us that the surface concentration has to be about 4 times  $10^{17}$  per cubic centimeter in order to achieve an average conductivity that has been specified as 3.7, assuming the junction depth 3 microns.

So that's-- and if you can-- we want to see how we actually do that, we can go on to slide number 10, and this actually shows how the curves were used. Again, this is for a p type Gaussian profile. And all we've done is on the x-axis picked out-- it's a little hard because this is a long log plot. And the x-axis picked out the average conductivity to be 3.7. And that's a little tricky to find that, but you can. And then we see-- we read off the y-axis as shown by that horizontal line surface concentration about 4 times  $10^{17}$ .

And again, we have multiple curves we can choose. I choose to use the orange curve, which is for the case of a background concentration, in this example, of  $10^{15}$ . If the background concentration, say, had been a little bit higher, say,  $10^{16}$ , or  $10^{17}$ , what you see would have happened is that the surface concentration would have actually moved down a little bit on the y-axis. So it would intersect a slightly different curve. So that's how we come up with the surface concentration.

So let's go on to slide 11. And thinking about that surface concentration,  $c_s$ , we know it's well below the solid solubility of boron and silicon. It's only  $10^{17}$ . And it's probably likely below the value of  $n_i$  at the diffusion temperature. Again, at 1,000 degrees, which is probably somewhere near or at a minimum temperature you'll be using to drive this in,  $n_i$  is about  $10^{18}$ . And so  $10^{17}$  is well below that.

So it's probably valid then to say that the profile is Gaussian. It's probably valid to say that it is a constant diffusivity  $D$ . And, therefore, we can assume this Gaussian type of solution because it's a derivation. So we can write down by inspection the equation in the center of the slide, which is the Gaussian equation. And then we know that at the point where  $x$  equals  $x_j$ , the carrier concentration, or the doping concentration,  $c$  of the boron reaches that of the background. That's the definition of  $x_j$ .

So if you look in the middle of the slide, we're saying the background doping-- background concentration  $c_b$  is equal to the surface concentration,  $c_s$ , which we just located, which is found times exponential to the minus  $x_j$  squared over  $4Dt$ . That's the definition of  $x_j$ . So we know  $x_j$  in this equation we just found,  $c_s$ . We know the background doping concentration. The only thing we don't know is  $Dt$ . So we can invert that equation and solve for  $Dt$ , plug in all the numbers and you get a  $Dt$  product.

In order to obtain this Gaussian of  $3.7 \times 10^{-9}$  centimeters squared. That's the  $Dt$  product, the so-called-- if you would like to use the term thermal budget for the deriving process. So that gives us an idea. And we don't know what  $D$  is, or what  $t$  is, but we're going to design a certain temperature in time. So we constrain to the fact that the  $Dt$  product will be this number.

So let's go on to slide number 12. And again, I'm repeating the  $Dt$  product from the top,  $3.9 \times 10^{-9}$ ,  $3.7$ . Let's just assume a temperature and see what happens, see what time is associated with that. And if it's a reasonable amount of time. So let's say we know we're diffusing pretty deep down to 3 microns. So let's just say we assume we drive in at 1100 degrees centigrade. And then you can look up from your plots, or you can calculate diffusivity of boron at 1100, it's about  $1.5 \times 10^{-13}$  centimeters squared per second.

And so then you can solve for time, the drive in time, calculate that out, you get about 6.7 hours. That's plenty long. That tells you probably from a practical point of view, you would not want to do this drive in any lower temperature because it would just take too darn long. OK. So now one thing we'd like to calculate, we have figured out the surface concentration from Irvin's curves. And we have the  $Dt$  product.

It will be interesting to calculate the initial dose, or the dose, the area under the curve, for the Gaussian profile. We have everything we need. Again, we know the dose  $Q$  is the surface concentration  $c_s$  times the square root of  $\pi Dt$ . And we have all those quantities. We can plug them in and we get  $Q$  equal to  $4.3 \times 10^{13}$ . Because the integral under the Gaussian.

It's a relatively low dose compared to our implant range. So it can be implanted. So this dose can easily be implanted into a very narrow layer close to the surface, which justifies implicitly that narrow layer might only be 1,000 angstroms deep. And that justifies our implicit assumption in using a Gaussian profile that the initial distribution would be a delta function, maybe only again, a few thousand angstroms deep. And you're going to a final junction depth that is 3 microns. And certainly, that seems justified using the Gaussian profile.

OK, let's go on to slide number 13. And now, that was the case we just talked about something we had implanted, the dose. Let's just take the case where if we used a gas phase Pre-Dep step as an example to get the boron initially into the wafer. And so that was done at 9:50. You can then use the charts in your book, or in the handouts, to look up the solid solubility of boron at 9:50, and you'll see it's pretty high, it's  $2.5 \times 10^{20}$ .

And at that temperature, we can also look up the diffusivity. It's about  $4 \times 10^{-15}$ . So you can solve for the dose in the complementary error function profile  $q$ . You have everything you need in that equation  $2 c_s \sqrt{D t}$  over the square root of  $\pi$  square root of  $D t$ . And so the time that you would require to deposit that dose into the wafer  $t$  of the Pre-Dep can be solved and you find about 5.5 seconds.

So you now see that the  $D t$  product of the Pre-Dep, which you can calculate, it's 5.5 seconds times the diffusivity at 9:50, which we see from above is  $4 \times 10^{-15}$ . So that  $D t$  Pre-Dep is about 2 times  $10^{-14}$ . And comparing that to the  $D t$  of the drive in, which we solved for earlier, which is about 1 and 1/2 times  $10^{-13}$ . So in an order of magnitude difference there. Again, this tells us that the assumption of Gaussian diffusion is justified, whether-- even if we've done a solid phase Pre-Dep.

OK, so that's the end of slide 13. That certainly gives you an idea of how these Irvin curves can be used to design a process. The alternative you could use is to read off. If you go back to just momentarily slide 10, you might-- the problem might be specified differently. You might be given some kind of surface concentration, and background concentration, and have to back out what the effect of conductivity of the layer might be. So different ways of getting those curves.

So let's go on now to slide number 14. And I want to shift gears a little bit because we have more or less covered a few cases for which the analytic solutions can be obtained. And those are important cases but, primarily, when the dopant concentration is low, or satisfying certain special conditions during Pre-Deps, it'll turn out there's most cases we cannot solve analytically. So these solutions have to be obtained by using computers using numerical methods.

And so I wanted to introduce you in the next few slides to some of the simplest types of numerical methods so you have an idea, or a feel, for how you yourself could implement these numerical techniques, if you need to do it. And there are textbooks on this topic, in particular, if you want to look at more detailed information on numerical solutions of diffusion equation. There's a book by J Crank called, *The mathematics of diffusion*, has a chapter on numerical methods for this particular equation.

The nice thing about numerical methods, they can be used to solve arbitrary initial starting profiles. So you don't have to make any detailed assumptions-- arbitrary boundary conditions, and in the case where the diffusivity varies in space. So if you have a concentration dependent diffusivity, which will be the case we'll talk about in later lectures when the dopant concentration is quite high and you can use numerical methods.

So what I'm picturing here on slide number 14 is a very schematic picture of atoms moving around between planes in a lattice. And so let's use this picture to get some physical insight into the diffusion process. So each plane here is indicated by a vertical bar. And 0, 1, 2, 3, 4. And the distance between these planes is given by the distance  $\Delta x$  as units of length. And in sub  $i$  here, so  $n_0$ ,  $n_1$ , and  $n_2$  is the planar atomic density of the  $i$ -th point. So it's the number of atoms per square centimeter in a given plane.

And  $c_i$  has a volume concentration, and it's the average volume concentration at any point. So you can calculate and you can get between the two.  $c_i$  is just  $n_i$  over  $\Delta x$ . Or  $n_i$  is just  $c_i$  times  $\Delta x$ . So let's go on to slide 15. At the top, I've just reproduced that picture. It's only a smaller version of it. And just reminding ourselves of the relationship between  $c_i$  and  $n_i$ .

Now, as we're looking at this lattice, we know that the atoms are relatively fixed in the lattice. But they do vibrate about their average position in a plane, where average position. And they're vibrating at some frequency,  $\nu_d$ , which is called the Debye frequency. And that's-- that number is typically on the order of about 10 to the 13th per second. So it's a pretty high frequency. You're vibrating about their average lattice positions at a finite temperature.

Now sometimes and during the vibration, an atom will actually be able to surmount the energy barrier that exists in going from one lattice position to the next, or one plane to the next. So it'll actually be able to hop to an adjacent plane. And there's an energy barrier, which we'll call an  $e_b$ , to get from one plane to the next. And this hopping frequency we call  $\nu_b$ , which is just a Debye frequency,  $\nu_d$ -- that's the vibration frequency-- times the Boltzmann factor exponential, the minus  $e_b$  is the energy barrier over  $kt$ .

So this  $\nu_b$ , small  $\nu_b$ , gives us an idea of the frequency of hopping from atoms from one plane to the next. And what we assume in this derivation is that there's equal probability of jumping right or left because this is a random process. So if we look at any given plane, we can say the number of atoms jumping to the right of that plane per unit time is just  $\nu_b n$  over 2 times the number of atoms in that plane  $n$ . Path 1 go right, number jumping left, per unit time is just  $\nu_b n$  over 2 times the number in the plane  $n$ . Those two are equal.

Now, if we do the bookkeeping and say, look at the number of atoms crossing a plane, the particular plane at  $i$  equals 2 in the above diagram. So the plane label 2, the number of atoms crossing that plane per unit time. Well, we can just write that as a flux. And  $f$  is an equation on the bottom. Well, that's just going to be the number of atoms, basically, per unit time jumping to the right minus those jumping to the left. So you write that as  $\nu_b n_2$  minus  $\nu_b n_1$ . Again, assuming equal probability going either way.

And then you can convert the difference between atomic density and number of atoms per cubic centimeter just by multiplying, using the definition of  $n$  is equal to  $\Delta x$  times the concentration. You have then expression for this flux crossing plane  $i$  equals 2. And then you multiply and divide by  $\Delta x$  and you end up with this equation that this flux is equal to-- looking in the right-hand side-- minus  $\nu_b$  over 2  $\Delta x$  squared times the  $\Delta c$  over  $\Delta x$ , something that's starting to look like a slope.

So immediately see some kind of thick law-- Fick's law here where a flux is related to a slope times something out in front that is a constant. So that's at the bottom of slide 15. Let's go on to slide 16. And I've just repeated that equation that we just had, but I added one more thing on the right, one more equality. And we set that flux equal to a diffusivity, a number  $D$ , times the slope  $\Delta c$  over  $\Delta x$ , where we define the diffusivity in this particular equation to be equal to the  $\nu_b$  over 2 times  $\Delta x$  squared.

So there is Fick's first law. The flux is equal to minus a diffusivity, a constant number, times  $\Delta c$  over  $\Delta x$ . And then the diffusivity has some atomic scale mechanisms of  $u$  to it. In fact, it's proportional to the jump frequency,  $\nu_d$ , and therefore, proportional be related to the energy barrier to hop between adjacent positions, or adjacent sites. So it gives you some idea of what-- at the time of scale, what goes into determining the diffusivity  $D$ .

OK. In addition to giving us an atomic scale view, we can actually use this type of formalism to go ahead and derive a numerical solution to a fix equation. So let's go on-- to do that, we'll go on to slide number 17, which is a slightly different sketch, but the exact same idea is that what we're going to be going through. And what I'm showing on the left-hand side in the bottom is a plot of concentration as a function of  $x$ , so distance. And let's say it has some shape, this dark, dark decreasing black line. And it's decreasing from left to right.

And what we'll then do is we're going to discretize this, and then look at discrete positions in space  $x$ . And we'll look at concentration  $C_0$ ,  $C_1$ , and  $C_2$ , and the spacing between those planes is going to be a constant, just like we used before,  $\Delta x$ . And so what we're going to look at is in the time interval,  $\Delta t$ , a certain time interval,  $\Delta t$ , what is the number of atoms crossing a certain plane per unit area? And we call that to the plane  $r$ , which we had labeled  $r$  above,  $q_r$ . It's just the flux,  $f_r$  times  $\Delta t$ . That's the number of atoms crossing the unit area in a given time interval. That's just basically-- this comes from the definition of what flux is.

And we then can write in for the flux. The flux is just the diffusivity  $D$  times the concentration difference across that plane, across plane  $r$ . Well, the concentration difference across plane  $r$  is  $C_1$  minus  $C_0$  divided by  $\Delta x$ . So we can approximate it that way, the flux crossing plane  $r$ . What's the flux crossing plane  $s$ ? Well, we can do the exact same thing, or the number of atoms crossing plane  $s$ . It's just the diffusivity times  $\Delta t$  times this time. We subtract  $C_2$  minus  $C_1$  over  $\Delta x$ .

So we can then do some bookkeeping and calculate the net number of atoms accumulated in that shaded region between plane  $r$  and plane  $s$ . And the time interval  $\Delta t$  is just  $q_r$  minus  $q_s$ . And we just subtract these two expressions and you see what you end up with is equal to a diffusivity  $D$  times the time interval  $\Delta t$ , times, in parentheses, the  $C_0$  minus  $2C_1$  plus  $C_2$ , that whole thing, quantity over  $\Delta x$ .

Now, if we divide that net gain in the number of atoms divided by  $\Delta x$  is shown below, that is the net gain in the concentration in that shaded region that is  $\Delta c$ . And that's just  $q_r$  minus  $q_s$ , that whole quantity divided by  $\Delta x$ . So I can substituting in  $q_r$  minus  $q_s$  and you end up with the equation near the bottom, which just says the net gain in the concentration,  $\Delta c$  in this shaded region, is just the diffusivity  $D$  times  $\Delta t$ , times this quantity in parentheses, which is related to the concentrations in those three regions, divided by  $\Delta x$  squared.

So what it says is, at a given point  $C_1$  in this curve, if I know the concentrations of the neighboring points, so I know its neighbors, I know the concentration at  $C_0$  and at  $C_2$ , if you calculate a new concentration after a certain time step,  $\Delta t$  at  $C_1$ , just by knowing its neighbors at this time step, the concentration of this neighbors. So if we go on to slide number 18, we can then use that information to come up with something called an explicit finite difference formula.

That's what the equation being shown near the top of the slide 18. What you're saying is that the concentration at any given point  $i$  in one of these slabs, at a new time,  $t$  plus  $\Delta t$ . So we're going to evolve this profile over time. So  $C_i$  plus on the left-hand side is equal to the concentration at time  $t$ . So one interval before that, whatever it was before, plus we add in this difference, this term on the right that gives the change in the concentration in the  $i$ -th slab after a time step  $\Delta t$ . Then that term is just  $D$ , the diffusivity,  $\Delta t$  divided by  $\Delta x$  squared times the quantity in parentheses.

Where again, the quantity of parentheses in order evaluated at any point  $C_i$ , all you need to know is the concentration at that point, and the concentration of its two nearest neighbors in whatever way that we've discretized. It's something we've discretized this continuous function into little intervals,  $\Delta x$ . So that is an explicit formula that you can use to evolve a concentration profile in shape over time.

And if you look at it for a few minutes, you can notice the similarity of that difference formula to the differential equation for diffusion. Which if you take the partial  $t$  on this equation shown in the center, and move it over to the right-hand side, you can see that partial  $C$  is equal to some constant  $D$  times a second derivative of concentration with respect to  $x$ . And in fact, this partial second derivative with respect to  $x$ , it can be numerically evaluated as the term in the first equation on slide 18 on the right-hand side. That is the numerical solution to that differential equation.

And I won't derive it here. If you go back to Crank's book, or any of the books on numerical methods and you find that the method is numerically stable. So it works from a numerical point of view. It gives reasonable answers for a particular condition. We have-- when we're doing the solution, we have a condition on a quantity  $r$  where this quantity  $r$  is what multiplies the concentration change in a slab at a certain time step  $\Delta t$ . That indeed,  $\Delta t$  over  $\Delta x$  squared, that multiplier has to be less than or equal to one-half.

If that multiplier gets too large, then that's-- the whole method breaks down, become unstable, and you get nonsense, absolutely, totally unmeaningful solutions. So you need to keep-- you need to adjust if you're doing this numerical, make sure you adjust your time steps  $\Delta t$  to be small enough so that this holds. And your  $\Delta x$  to be of appropriate size with respect to  $\Delta t$  so that you don't get yourself out of the physically-- out of the numerically stable solution.

It's a very powerful technique. It's very simple. That's one of the nice things about it. And it's certainly going to be required to use some method, numerical method, when the diffusivity is not a constant. If you were to sit down, you could write your own simple simulator using this very relatively easy to use finite difference 1 [INAUDIBLE]. It is not the particular type of numerical method that's been-- that is being used in Supreme 4. Supreme 4 has a more sophisticated numerical solution method for the diffusion equation.

This is much more simplified, and this particular method can be slow. It has all of its own problems. But the beauty of it is the simplicity. And just to give you an idea of how one might use numerical solutions to obtain-- numerical methods to obtain solutions of the diffusion equation. OK. Let's go on now to slide number 19. What I want to talk about at this point are from now on, and this is the rest of this lecture and the next couple of lectures, will be the so-called modifications of Fick's laws.

Fick's laws are introduced in a lot of basic courses-- material science or physics. And when we are diffusing dopants in semiconductors in practical cases, there are a few number of cases where Fick's laws need to be modified to take into account the things that are really going on in semiconductor processing. And the first thing that we'll talk about here on slide 19 is so-called electric field effect.

And this occurs in the case when the doping concentration is higher than  $n_{sub i}$ . So  $n_{sub i}$  is intrinsic carrier concentration at a diffusion temperature, again, of 1,000.  $n_{sub i}$  is close to mid 10 to the 18th or so. If the doping concentration gets higher than that, you can start to have a non-uniformity in the charge distribution in the semiconductor, and electric field effects can become important.

And this is a schematic demonstration of how electric fields can arise when dopants are diffusing and silicon. It's a plot of concentration schematically versus depth, and the red line is supposed to represent the profile at any given point in time for, say, arsenic that's diffusing. And then arsenic is a donor. It has one extra electron floating around it.

But the atom itself in the absence of this electron, this extra valence electron, the donor itself is positively charged. It's an ion. This arsenic's diffusing and there are-- the electrons associated with this heavily doped arsenic region can diffuse ahead of the dopant. And so this blue line is meant to represent the distribution or the diffusion profile of electrons, let's say.

So the electrons diffuse, and holes diffuse more rapidly than their associated donors and acceptors. Because of that more rapid diffusion, they'll diffuse-- the profile of electrons will be a little bit deeper and diffuse ahead of the dopant that they're associated with until they reach some steady state condition where the drift flux from the internal electric field is going to balance the diffusion, the diffusion flux.

And so what we look at here is there, if could just look at this schematic picture, you'll see there is indeed from your elementary electronics, or solid state physics, there is an electric field induced by the fact that there's a net positive charge on the left region. That is, if you subtract all the arsenic donors, you subtract electron concentration there, there's a net positive charge on the left. There's a little bit of net negative charge on the right that produces an electric field pointing from left to right.

So that electric field then tends to cause electrons to drift from right to left, right? Because they drift against the field. So they're going to be drifting from right to left while they're diffusing from left to right, because there's a concentration gradient. So the electric field will build up to the point where there's steady state where that drift flux just balances the diffusion flux for the electrons.

And again, the physical origin of this electric field is the fact that, well, electrons are charged in holes, and they have somewhat higher mobility. They can move around the lattice much more readily than the dopant ions themselves. OK. And again, this is only going to happen to the particular case where the concentration of the dopant is higher than  $n_{si}$ . Otherwise, the background electron concentration is set by the temperature. It's just a constant throughout space. So the electric field would not develop right at the edge of this diffusion profile.

Let's go on to slide number 20. And so what we do is, we modify Fick's first law, and we modify it in a way that's very similar and pretty much almost identical to what we do in our electronics, or solid state physics classes. We say that the total impurity atom flux in the presence of both a concentration gradient and an electric field can be written down as a sum of two fluxes. One is  $f$ , which is the normal Fickian diffusion flux, which is given by  $-D \frac{\partial c}{\partial x}$ , plus  $f'$ , where  $f'$  is now the drift flux due to the electric field.

And for the drift flux, I wrote down  $z$ , which is going to get the charge. The charge number  $z$  would be 1 for electron, depends on the number of electronic charges associated with whatever is drifting, times the mobility  $\mu$ , times the concentration  $c$ , times the electric field. That is the flux due to drift. Again, it's not a diffusion processes, that's the drift process, a different physical process. You can add these two together and write down as the total flux. So we have a non-Fickian term on the right.

But because of the Einstein relation, we can actually, when we're talking about the diffusion of carriers, like electrons and holes, we know that their mobility is directly proportional to the diffusivity and the proportionality constant is  $q$  over  $kt$ . So  $\mu$  is equal to  $d$  times  $q$  over  $kt$ . So we can substitute in for the mobility in the upper right-hand equation with a substitute in  $q$  over  $t$  times  $d$ .

We can also substitute in the fact that electric field  $e$  is the gradient of the potential where the potential  $\psi$  can be related to the carrier concentration in as  $-\frac{kt}{q} \ln \frac{n}{n_i}$ . So basically by substituting in the expression proportional diffusivity for  $\mu$ , and substituting in for the electric field, how it relates to the potential and, therefore, to  $n$  over  $n_i$ , we get the equation near the bottom for the flux  $f$ , which is the usual Fickian minus the times  $z$ ,  $\frac{\partial}{\partial x}$ , times  $-D$ , times the concentration  $c$ , times now we've come up with this  $\psi$  term,  $\frac{\partial \psi}{\partial x}$  of  $\frac{q}{kt} \ln \frac{n}{n_i}$ .

So now this is the new flux equation, and we can-- now we use for the carrier concentration. And you have to be careful. It's not just equal to  $n_d$  because  $n_i$  can be of order  $n_d$  in this. So we need to make sure we use the full expression for the carrier concentration. And it's one-half-- the bottom equation here is one-half times the quantity, square root of  $n_d^2$  plus  $r$  and  $i$  square plus  $n_d$ . That comes from charge neutrality.

Given that, we-- therefore, there's a relationship between  $n_d$ , the carrier concentration, and the concentration of the dopant  $c$ . Because again, the concentration  $c$  is just  $n_d$  minus  $n_a$ . So it's the net concentration. So we have a relationship between  $n$  and  $c$ . We're going to use that to make this flux equation  $f$  to be written only in terms of the concentration  $c$ .

So we go on to the next page, slide 21. What we find is that we can do this compression in this equation, and we find that the total flux now  $f$  is written as something called minus  $h$  times the diffusivity of a dopant  $D_a$ , partial  $c$ , partial  $x$ . So we've been able to actually write down an equation that looks just like Fick's first law, but there's an  $h$  factor multiplying it. And this  $h$  factor, it turns out to be equal to  $1 + c$  divided by the quantity square root of  $c^2 + 4n_i^2$ .

So basically, it looks-- in the presence of an electric field, it looks just like we have an enhancement in the diffusivity of the dopant by a factor called  $h$ . And you can-- we just worked that out. So interestingly, we see that it-- electric field effect on a dopant that is creating the field on that dopant itself, it enhances the diffusivity, and it turns out  $h$  has an upper bound of 2. So  $h$  is not going to be any larger than 2, and that means that the electric field enhancement term can enhance the diffusivity of the dopant that causes the field by as much as, or a maximum of a factor of 2.

And this happens when the doping concentration term, or  $c$  is much, much greater than  $n_i$ . And you can see that by substituting in and calculating out what  $h$  is in certain conditions. In the special case where  $c$  is  $n_i$ , then  $h$  goes back to being 1. So how do we get to this equation where the simplified  $h$  factor? Well, if you go on to slide number 22-- actually, I'm not going to go through all the algebra. But basically, what we did was, we used a particular fact, which is that-- along the top of slide 22-- partial partial  $x$  on the logarithm of  $x$  is equal to  $1/x$ .

And what we needed to find in that earlier diffusion and that earlier drift term, there was a term that went partial partial  $x$  of  $\ln n$  over  $n_i$ . And so just by going through the algebra shown on-- we can substitute-- on slide 22, we can substitute for the carrier concentration  $n$ , and we can find an expression for partial partial  $x$  of  $\ln n$  over  $n_i$ . And you see that in the middle of the slide.

And then we substitute in that the dopant concentration  $n_d$  is equal to  $c$ . And we're able to see then that the flux, the total flux is the usual thickening term  $D_a$  minus  $D_a$  times partial  $c$  partial  $x$ , minus this other term, which ends up being able to be written just like partial  $c$ , partial  $x$  in terms of partial  $c$ , partial  $x$ , times the  $h$  factor where  $h$  is equal to, as I show on the bottom,  $1 + c$  over the square root of  $c^2 + 4n_i^2$ . So that's just justifies the derivation of the  $h$  factor on slide 22.

OK, so just go back to slide 21 for one second and just want to remind ourselves that the total flux  $f$  now in the presence of a high carrier concentration can be written just like the Fickian diffusion, but the  $h$ , there's a multiplier  $h$  from the diffusivity of the dopant atom  $a$ . Let's skip on to slide 23 now. However, so that's what we're talking about the amount of enhancement you might get in the high concentration species.

But you may have two different species diffusing. And in the case where the species are at different concentrations, the electric field term can actually cause an even larger change in the diffusivity of the low concentration [INAUDIBLE]. So let's look at a particular example shown on slide 23. And what we're showing here is concentration as a function of depth, and the red curve in high concentration, let's say the high concentration arsenic profile.

The initial arsenic profile looks-- it was on a planet or something it looks like this as shown in the solid red curve. The background doping is initially all constant, it's p-type. So this boron is shown by the solid blue line. Now, we're going to simulate including electric field effects at 1,000 degrees, the diffusion of the arsenic and the boron. Well, it turns out the arsenic does indeed diffuse, as shown by the dashed line. But that the electric field that it produces right near its-- the slope right near the edge of its profile, actually, that electric field can cause a flux of boron ions, which can cause the bond to itself to move.

So the final boron profile now is shown by the blue dashed line, has this little hump in it and then a dip. And that little dip occurs right near where the junction is, right where the boron-- the arsenic in the boron cross. And there's no way by Fickian diffusion you would ever predict that a constant profile of boron would end up being-- looking the way it does in this particular plot. Again, that's because of the second term, the electric field term, non-Fickian term.

So when you want to think about that, how that occurred, look at the electric field arrow drawn from left to right. Again, drawing from positive, net positive to net negative charge, that direction of  $E$  pulls the bond-- and again, remember, the boron ions, as they diffuse, they're  $b^-$ , these acceptors and that negative charge. So they're going to be pulled in, they're going to move to the left by the electric field. They'll be pulled into the  $n^+$  region and deplete some of the boron in the region past the junction.

And so you end up with this sort of clump and dip, which is a non-Fickian type of motion, but induced by the electric field created by the higher concentration arsenic species. So this can have quite a bit of an effect on the diffusion profiles near a junction. And we see this all the time in our devices. In fact, you go on to slide number 23, showing a simulation example of an MOSFET. These are two Supreme simulations, both around 1,000 degrees.

For MOSFETs, you'll recognize the polysilicon gate here in magenta. And the source and drain regions are arsenic, and they are shown in black. And if you look first at the left in the case of an electric field, you see these different contours, the green, yellow, sort of light orange, and then a dark orange, or red.

We see the boron uniformly doped, and its contours are shown by the different colors. And now what happens on the right in the presence of an electric field, instead of these uniform lateral doping controls for the boron, you see there's an electric field that acts on the boron and it changes the doping distribution in its shape. In fact, they dominate-- it dominates the shape of the bond distribution, particularly, near the source drain junctions of the MOSFET device.

The boron basically gets pulled in to underneath the source and drains, and there's quite a bit of loss of boron from the channel region into the source drains that do electric field effect that's not predicted on the left-hand side. So even though  $D$ , the  $D$  factor has been in the arsenic, diffusivity is limited to, at most, a factor of 2. So there's not too much effect on the junction of the arsenic, if it's in the black junctions. The regions don't change that significantly. But it dominates the diffusion of the boron underneath, or at a lower concentration.

So let's go on to slide number 25. I just want to summarize this second lecture on diffusion. We reviewed a few cases of simple constant diffusivity. These generally apply well to the case of low doping concentrations in a seamless process flow that usually means the diffusion of the seamless wells, which are fairly lightly doped, say, below mid 10 of the 17th, or below 10 to the 18th. They're usually diffuse in at very high temperatures so  $n_i$  is large. And they satisfy the fact that the dopant concentration was less than  $n_i$ . So you have constant diffusivities.

But beyond that case, turns out most diffusion problems in devices need to be solved numerically. And we introduced a very simple but powerful method for numerical solution of the diffusion equation. And it actually was a finite difference formula. It's not that sophisticated, and it's not actually the formulation that is used in Supreme 4, but it gives you an idea if you needed to write your own simple method.

We talked about the first type of modification we need to make to Fick's first law, and that was for electric field effects, which can enhance the diffusivity of a high concentration species up to a factor of 2, but can dramatically impact the motion of species at lower concentrations. And what we're going to talk about next time are further corrections to the simple Fickian diffusion that we've been talking about, and more realistic dopant profiles, such as the case when we have concentration dependent diffusivity.

OK, that's all I have for today, and thanks very much.