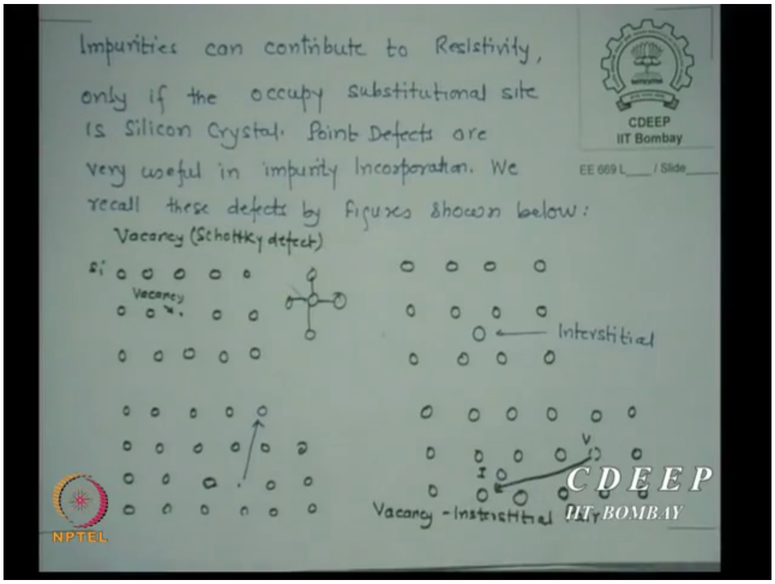
Fabrication of Silicon VLSI Circuits using the MOS technology

Professor. A N Chandorkar
Department of Electrical Engineering
Indian Institute of Technology Bombay

Lecture 07
Diffusion

(Refer Slide Time: 0:17)

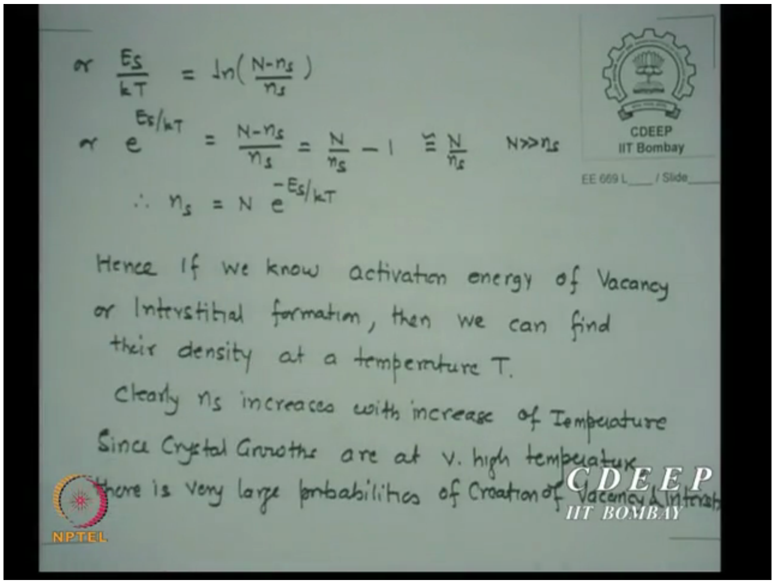


Impurities can contribute to Resistivity, only if the occupy substitutional site is Silicon Crystal. Point Defects are very useful in impurity Incorporation. We recall these defects by figures shown below:

Vacancy (Schottky defect)

Okay. So let us go we were looking of impurity contribute to resistivity of the seen last time. This is what we were doing it.

(Refer Slide Time: 0:38)



$$\text{or } \frac{E_s}{kT} = \ln\left(\frac{N-n_s}{n_s}\right)$$

$$\text{or } e^{E_s/kT} = \frac{N-n_s}{n_s} = \frac{N}{n_s} - 1 \cong \frac{N}{n_s} \qquad N >> n_s$$

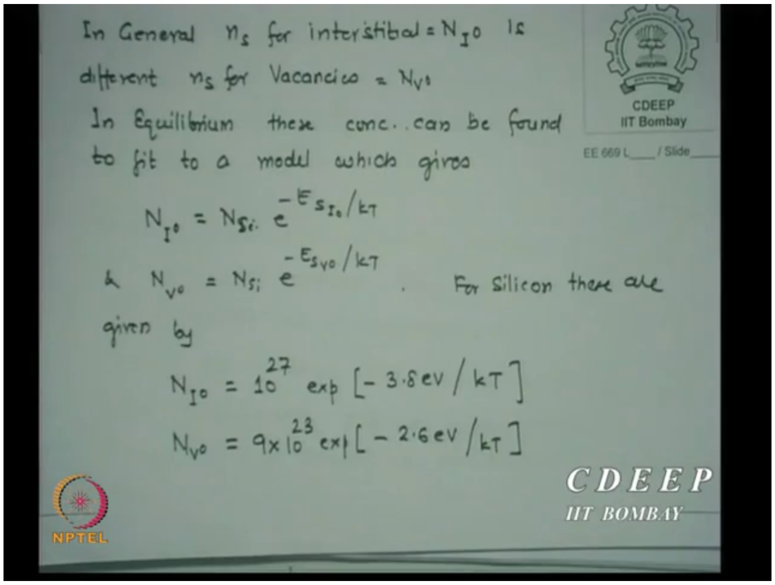
$$\therefore n_s = N e^{-E_s/kT}$$

Hence if we know activation energy of Vacancy or Interstitial formation, then we can find their density at a temperature T.

Clearly n_s increases with increase of Temperature Since Crystal Growths are at v. high temperature there is very large probabilities of Creation of Vacancy & Interst

We also calculated, I just want to quickly go through what we did last time. We calculated the available substitutional impurities or interstitial impurities by putting this thermodynamics. And we then said that these are available to the N e to the power minus Es by kT where N is number of atoms available in the lattice per cc.

(Refer Slide Time: 0:52)



In General n_s for interstitial $= N_{I0}$ is different n_s for Vacancies $= N_{V0}$

In Equilibrium these conc. can be found to fit to a model which gives

$$N_{I0} = N_{Si}\, e^{-E_{sI_0}/kT}$$

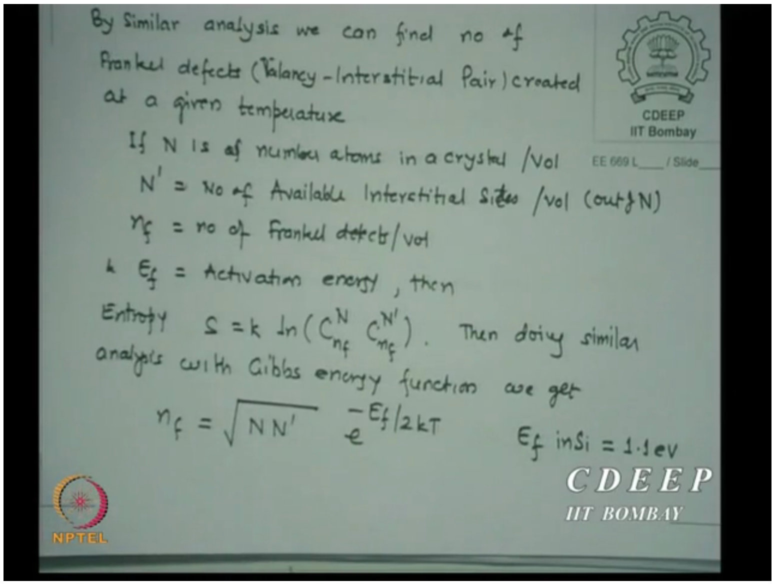
& $N_{v0} = N_{Si}\, e^{-E_{sv0}/kT}$. For Silicon these are given by

$$N_{I0} = 10^{27} \exp\left[-3.8\,\text{ev}/kT\right]$$

$$N_{v0} = 9\times 10^{23} \exp\left[-2.6\,\text{ev}/kT\right]$$

And then we also said if it is interstitial, we declared it NI0. If it is vacancies, it is Nv0 and we derived an expression which NI0 is 27, 10 to power 27 times this. Nv0, this is all that we did last time.

(Refer Slide Time: 1:10)



By Similar analysis we can find no of Frankel defects (Valancy - Interstitial Pair) created at a given temperature

If N is af number atoms in a crystal /Vol

N' = No of Available Interstitial Sites /vol (out of N)

n_f = no of Frankel defects/vol

& E_f = Activation energy, then

Entropy $S = k \ln(C^{N}_{n_f} C^{N'}_{n_f})$. Then doing similar analysis with Gibbs energy function we get

$$n_f = \sqrt{NN'}\, e^{-E_f/2kT}$$

E_f in Si = 1.1 eV

Today we start with quickly something more about it. There is also possibility as I said last time, Frenkel defects are also available and they can also be created at given temperature. If N is the number of atoms in crystal per cc or per volume. N dash is number of available interstitial sides, sorry it is sites per volume and nf is number of Frenkel defects per volume. And Ef is the activation energy. Then by similar arguments we have entropy is equal to k times Boltzmann's constant time ln of Cnf.

Please remember I am now looking for vacancy interstitial, so both these are we have taken into care. And by same argument I can show you that by similar d, we can write S by into kT and T delta G. Delta G, by same method we can calculate. The available Frenkel pair will be N into N dash e to the power Ef by 2kT where silicon, Ef and silicon is 1.1 electron volt. Please remember this energy is smaller, so Frenkel pair creations are not smaller.

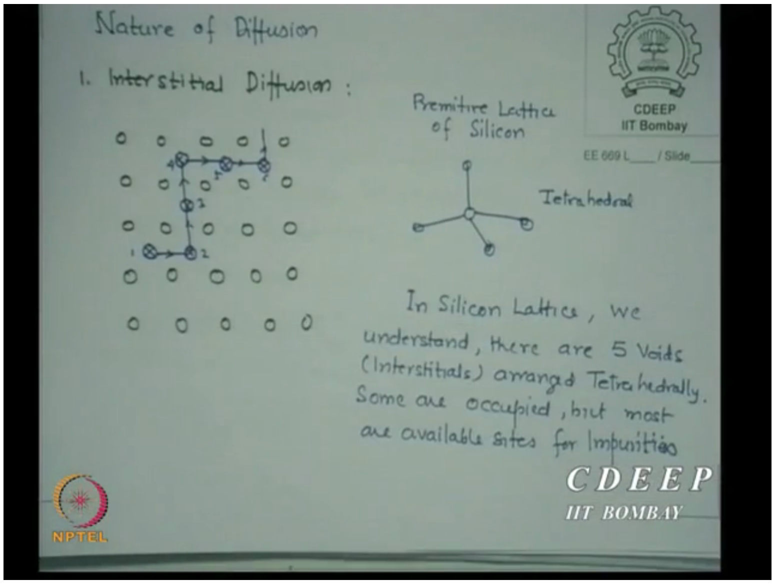
Frenkel pair creations are not smaller simply because on interstitial side vacancy can pair very easily and move together. One jumps there, then the vacancy is created on the backside. A slight electron volt transport. So this of course is not so important. So maths you can do again, I have not done it. I just wrote down the final answer. The method is same as I we did for interstitial and vacancies.

Okay, once we say the, we know the defects at a given temperature, we like to know how these impurities move inside a crystal and we are not looking impurities concentration in amorphous semiconductors and in polycrystalline semiconductor. Though we are interested at least in the case of solar cell, doping of amorphous materials and we are interested in the case of CMOS, poly gates or silicon gate devices, poly diffusions.

However as we say we will first look into crystalline structure in which impurities are entering. Now these impurities if they sit only on the substitutional sides as I say other day, then only they can contribute to resistivities. Otherwise they will sit into interstitial side and do nothing except creating strain. If you have written down, I may move further. Please remember this is available on Google sites. If you wish to read sometimes, find time if not very much busy with other more important activity like TV, mobile and or Internet. Look for this, maybe interesting.

This is a diffusion process has nothing to do with electrical engineering or something, it is a diffusion in anything. So basically it can be available on chemical engineering sites, chemistry sites, material science sites. Many places you can get same expressions because it is a thermodynamics related situation. Is that okay? So let us start how impurities move.

(Refer Slide Time: 4:39)



Nature of Diffusion

1. Interstitial Diffusion :

Premitive Lattice of Silicon

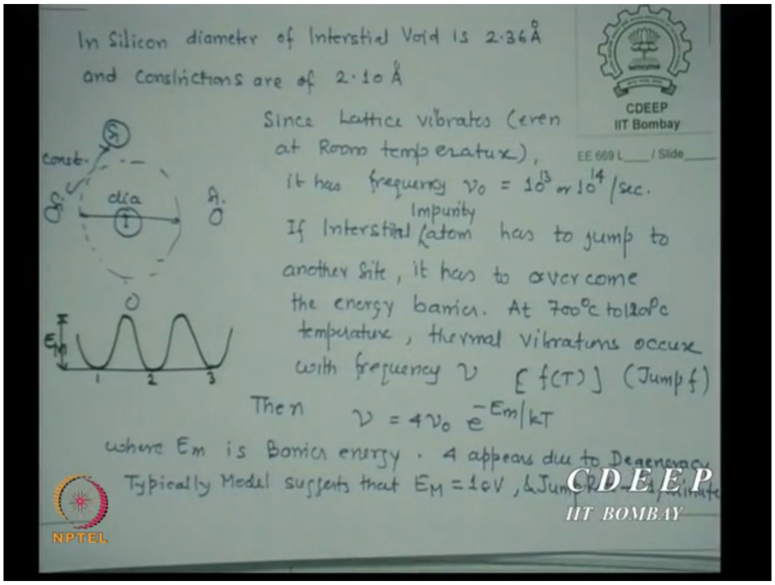
In Silicon Lattice, we understand, there are 5 Voids (Interstitials) arranged Tetrahedrally. Some are occupied, but most are available sites for Impurities

Please remember silicon has a primitive cell which is shown here which is one silicon atom is bonded to nearest neighbor by four atoms. And this is called primitive cell. If you have seen our unit cell, there was a primitive cell colored shown by. The corner one, the one which is just interposed from 1 by 4, 1 by 4 site and three other this. So these are essentially is called primitive cell. The minimum amount of bonding which makes silicon atoms go is, silicon lattice go is this cell, primitive cell.

Now there are if you see, primitive cell, there are five voids, they are arranged in tetrahedrally, 1, 2, 3, 4 and back one side, so 5 sides. Here are some are occupied but most are available sites for impurities not all voids are substitutional by something. But they are voids available. So one of the possible mechanism is how interstitial diffuses through interstitial. So let us say an impurity sits a position 1, it can hop through to 2, to another interstitial site, it can hop to 3, another (interst). Of course this is random, this is only shown one method, one place but can have any random placements. 3 can go to 4, 4, 5, 6 and maybe further ahead.

So this is called interstitial diffusion. Impurities hop from one void to the other, this is called (substitu) interstitial diffusion. Even now though it is doing, this process may not contribute to resistivity but it has more importance because as it releases, the void strain releases and there is a possibility of silicon moves from here. It can occupy another void and release a vacancy down. So the whole purpose is how vacancies also can be moving with interstitial motion. Now in case of silicon, this is of course few lines, so you can always see.

(Refer Slide Time: 6:43)



In Silicon diameter of Interstitial Void is 2.36 Å
and Constrictions are of 2.10 Å

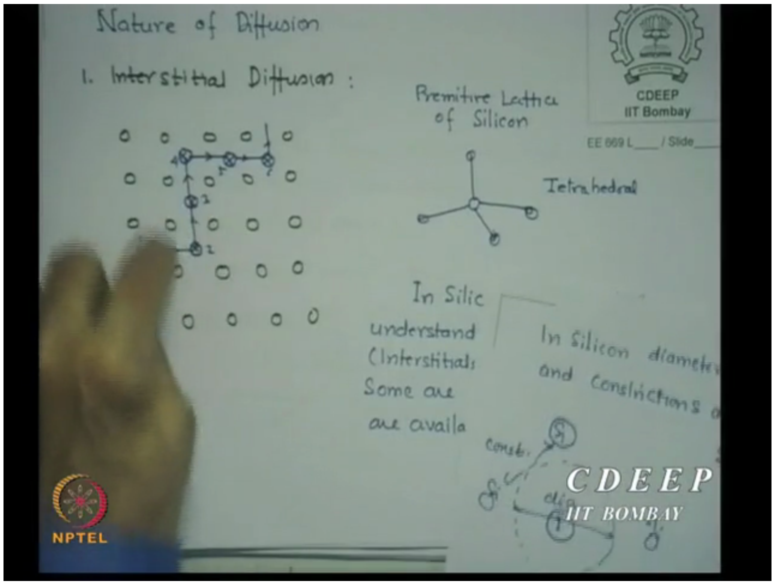
Since Lattice vibrates (even at Room temperature), it has frequency $\nu_0 = 10^{13}$ or 10^{14}/sec.
If Interstitial (Impurity) atom has to jump to another Site, it has to overcome the energy barrier. At 700°C to 1200°C temperature, thermal vibrations occur with frequency ν [f(T)] (Jump f)

Then $\nu = 4\nu_0 e^{-E_m/kT}$

where E_m is Barrier energy. 4 appears due to Degeneracy.
Typically Model suggests that $E_M = 1eV$, & Jump [illegible] /minute

Silicon diameter of interstitial void is 2.36 Armstrongs. What is the void essentially I am saying?

(Refer Slide Time: 6:53)



Nature of Diffusion

1. Interstitial Diffusion :

Premitive Lattice of Silicon

Tetrahedral

In Silic

understand

(Interstitials

Some are

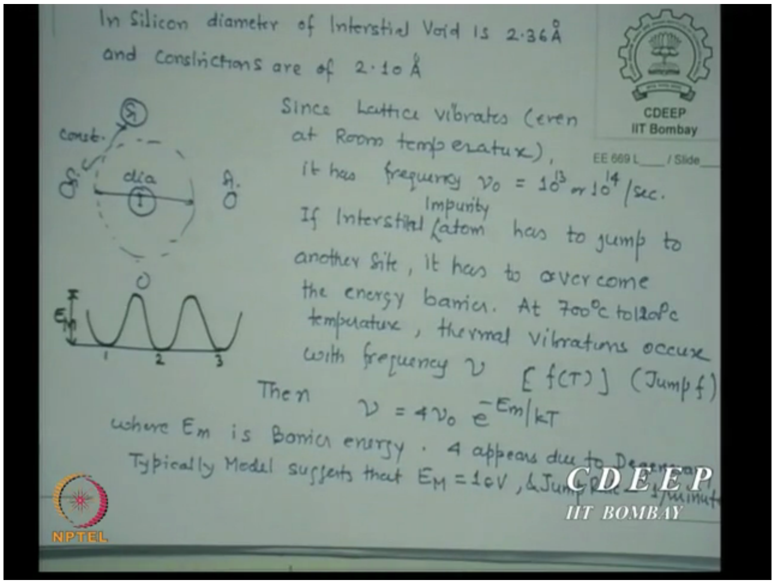
are availa

In Silicon diamete

and Constrictions a

Between this the circle which touches all four or rather backside one as well, is called sphere there.

(Refer Slide Time: 7:01)



In Silicon diameter of Interstial Void is 2.36 Å
and Constrictions are of 2.10 Å

Since Lattice vibrates (even at Room temperature), it has frequency $\nu_0 = 10^{13}$ or 10^{14}/sec.

If Interstitial Impurity atom has to jump to another Site, it has to overcome the energy barrier. At 700°c to 1200°c temperature, thermal vibrations occur with frequency ν [f(T)] (Jump f)

Then $\nu = 4\nu_0 e^{-E_m/kT}$

where E_m is Barrier energy. 4 appears due to Degene

Typically Model suggests that E_M = 1eV, & Jump rate 1/minute

And that is circle which is shown here, has a dia of 2.36 Armstrongs which means radius is 1.18 Armstrong. This is called tetrahedral radius, 1.18 Armstrong is called tetrahedral radius. And of course between the two constriction, between the two atoms on the constriction side, the gap is 2.10 Armstrong. Since lattice vibrates at any temperature, there is a lattice vibrations, the lattice keeps on rocking as well as stretching. More physics, some day.

And it has some frequency which is called jump frequency or frequency of oscillations or vibration. And typically it is 10 to power 13 to 10 to power 14 per second in different lattices. This is typical monitored number derived from and measured from atomic spectroscopies. If interstitial impurity has to jump from one side to the other, it has to overcome energy barrier. It cannot just go, it has to cross some barrier. Now this barrier which is 700 to 1200, thermal vibrations occur with frequency new which is given by 4 mu 0 e to the power Em.

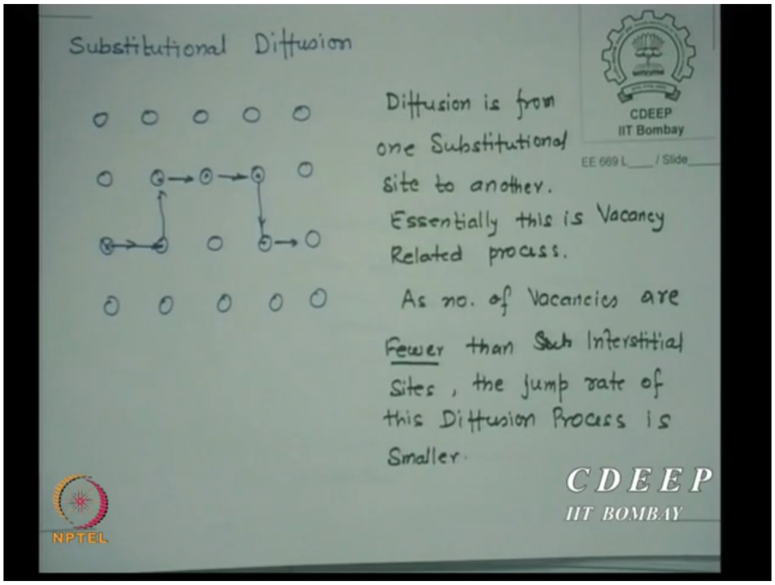
Em is the barrier energy, it has to cross this much energy to come out. It should get excited enough, pass through barrier and jump to the next side. This 4 of course is called degeneracy, from where it comes? It is a random, it can go this side, it can go this side, it can go this side, it can go this side, so it has four possibility of motion. So it is called degeneracy factor. So typically the jump frequency is 4 mu 0 e to the power minus Em by kT.

Typically Em for this substitutional sides, the barrier is something shown here. So if atom has to go from this side to this side, it must cross this much energy. This is equivalent model of energy. I hope in second year or maybe earlier you might have done chronic pain model, this is replication of that to some extent. So you have one atom here and it has to occupy this. It must cross the barrier of energy, Em to reach to the next side.

This essentially is what this expression shows. Typical jump rate or frequency is 1 per minute at around between 700 to 1200 date, varies little bit but it is around 1 jump per minute is what the rate with which substitutional this, sorry interstitial actually jump. This is important because how many atoms are where at a given instant is relative to, at a given temperature is some way relevant to know how many impurities are available where.

I introduce some impurity in silicon where they will lie. So I like to know where they can at best go and how will they go. So this is physics telling that there is a possibility. Now these jumps, impurities can come and occupy that void, so they are entering in. Now this jump frequency, why I have got it? There is something this equation has to do with diffusion coefficient but maybe we will see this later. This relationship which I am drawing, I need to have for creation of constants, diffusion constants or diffusion coefficients. Is that okay? Everyone? Okay. So this is something called interstitial.

(Refer Slide Time: 10:50)



Substitutional Diffusion

Diffusion is from one Substitutional site to another.

Essentially this is Vacancy Related process.

As no. of Vacancies are ~~Fewer~~ than Such Interstitial Sites, the jump rate of this Diffusion Process is Smaller.

The most important transfer of impurities inside a material is through substitutional sides. Substitutional means wherever silicon atom is there and if there is a vacancy, an impurity atom can occupy that vacancy and sit there. But it can actually jump from say let position 1, if it finds a vacancy here, so it actually may jump here. If it finds a vacancy here, it may jump here and keep jumping wherever it finds another vacancy. So impurity can move from one vacancy side to the other vacancy side by process called substitutional diffusion.

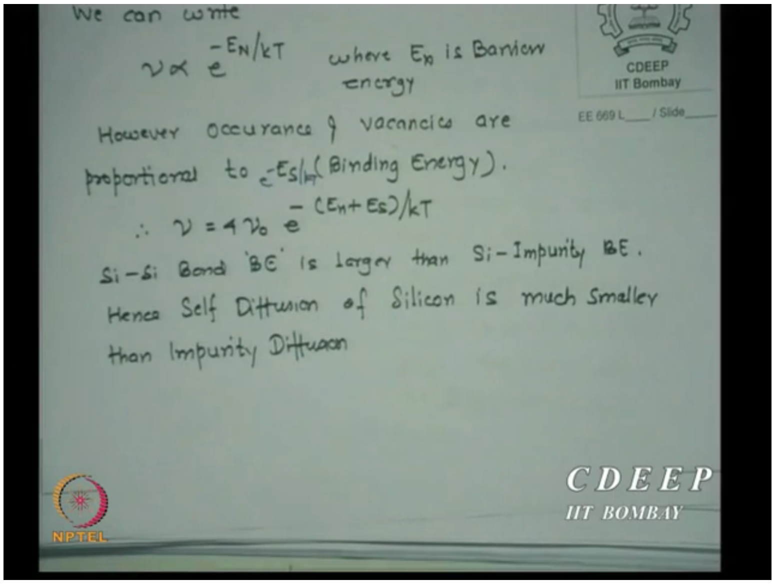
This is most important diffusion, how impurities actually travel inside silicon. That is what our aim. Why are we doing all this? Maybe it should be very clear to you that my interest in doing all this is not just because I want to understand physics alone or maybe I am interested x of you, I am maybe interested. But the interest part is how much resistance it finally offers because of the profile it gives. Because current is related to that, there are some wear, I am very keen to know how much is the current I can get if I apply x voltage.

My interest in electrical engineering is only IV and CV. If anyone hurts me on IV or CV, I am going to look into you. Why cannot I do better? So I look into physics, I look into material, I look everything because at the end of the day circuit must function the way I thought I have designed. And to do this, I must understand everything around that which helps me to improve. So please do not think this technology course is only of this side. This is essentially covering those areas which normally we do not cover anywhere. Normally, I do not say…..

Please remember generally vacancies are fair compared to voids. So essentially you can say the jump rate of diffusion process will be smaller because available sites are smaller compared to interstitials. Interstitial side almost everywhere. Vacancies are need to be created by some energy, e to the power Es by kT. So you have now two energy, one Es you have to first create a vacancy and then allow it move. So that will be now new energies will be, will have actually energy creation for vacancy plus energy (creati) energy for barrier to cross.

So actually it will be two energy sum now which will be required for vacancy motion. Is that point clear? Voids are not to be if they are there. But in case of, first vacancy have to be created. Once vacancy, it can jump only if it crosses a barrier.

(Refer Slide Time: 13:36)



We can write

$\nu \propto e^{-E_N/kT}$ where E_N is Barrier energy

However occurance of vacancies are proportional to $e^{-E_S/kT}$ (Binding Energy).

$\therefore \nu = 4\nu_0 e^{-(E_n+E_S)/kT}$

Si-Si Bond 'BE' is larger than Si-Impurity BE. Hence Self Diffusion of Silicon is much Smaller than Impurity Diffusion

So based on the same, similar analysis, one can write mu is now 4 mu 0, e to the power En plus Es where Es is, the En, Es are binding. Es is binding energy and En is the vacancy creation energy. Is that okay? I just now said. To create a vacancy, I need En energy. To move it I need barrier to cross which is Es. Now silicon-silicon bond, binding energy is larger than silicon impurity bond. Is that word clear? Two silicon atoms, okay maybe first you write down.

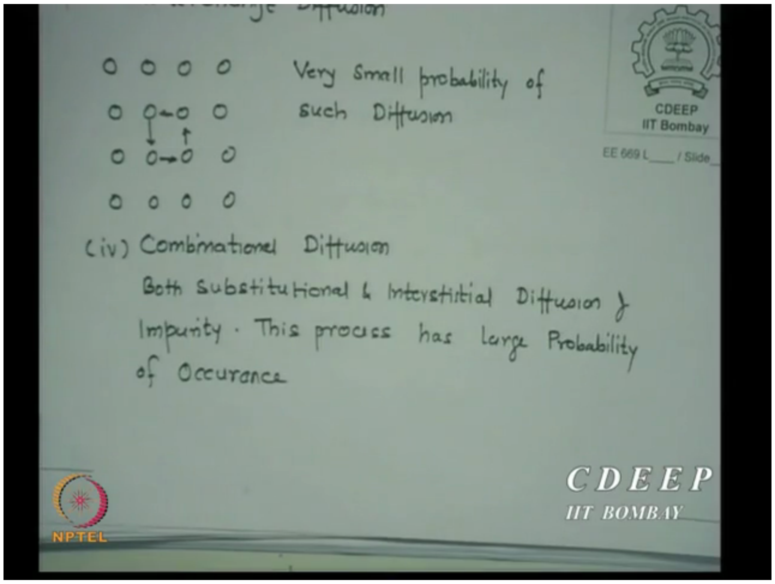
This part is most important to show that substitutional impurity diffusions has much lesser chance compared to void ones because there are enough voids, so many many of them can actually enter which is very contrasting. People believe that impurities must be sitting on first vacancy. No, first they may likely to sit to the voids itself, interstitial sides and then maybe move for seeing a vacancy around.

This very interesting part, silicon is also, atoms are also moving because of thermal energy. Some bonds are broken anyway but silicon-silicon bond is very strong, very very strong in case of bond strength. That is (())(14:50) law if you apply. The bond and force is very high. Compared to silicon impurity atoms, the binding energy for silicon-silicon is much higher. So it is unlikely that silicon bonds maybe keep breaking every now and then unless you heat it very heavily.

Give lot of thermal energy, otherwise silicon does not break, bonds does not, do not break very easily. Therefore silicon self-diffusion going from one side to the other is lesser event, not that it will not happen but lesser chance of moving one silicon atom to the other silicon side is very smaller probability event compared to impurities getting inside the crystal. Because after all you are giving temperature, enough thermal energy is provided.

Every possible mechanism can happen. So we want to eliminated saying that okay, silicon-silicon self-diffusion is smallest among all of them, does not mean 0, finite, small compared to the interstitial and substitutional.

(Refer Slide Time: 15:59)



Very Small probability of such Diffusion

(iv) Combinational Diffusion

Both substitutional & Interstitial Diffusion of Impurity. This process has large Probability of Occurance

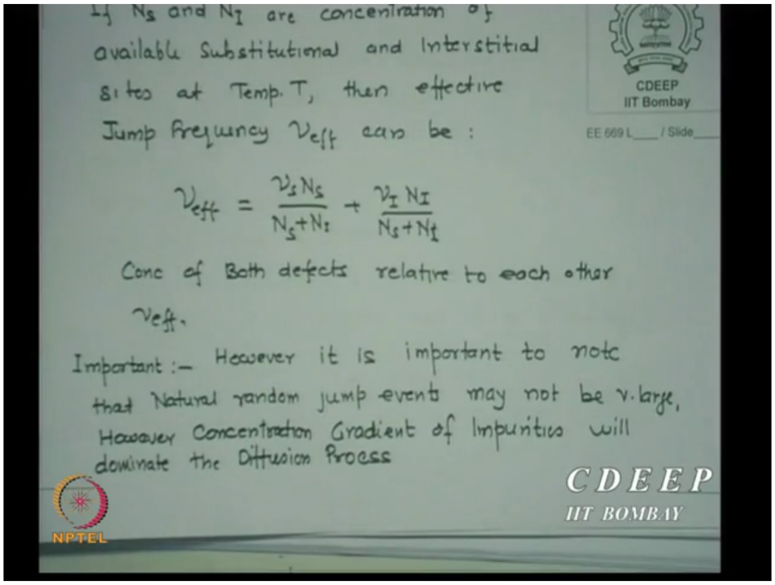
There is one more (possi), maybe two more possibility that there which also are very low, maybe this one. There is a possibility that atoms may move either vacancies are at silicon atoms and they can actually keep moving around nearer sides. This is very interesting which is very very small probability that this atom of impurity or silicon jumps to the next side, next side, next side and come apart.

This has a very very small, this is called interchange diffusion, very very unlikely event but can occur. One in billion or even lower probable but can occur. But at given temperatures higher than it may occur as well to some extent. However which is the best possible diffusion therefore? Substitutional and interstitial together is very possible. Atom first come to interstitial side, jumps to vacancy, allows another impurity come to interstitial side, jump to vacancy.

This vacancy atom may move to another vacancy, it may create another void there from where interstitial move, another vacancy is brought in and this is called cooperative diffusion. This is the most likely diffusion in which interstitials and vacancies go together to push atoms inside. Is that okay? They both can help each other to actually get more and more impurities getting diffused inside the crystal. This is most likely event and has the largest probability.

I can do some quick calculation for this as well. Is that okay? Two possibly, so there are four possible mechanism in which impurities can get inside. Most likely is the last one but the first two actually tell you that together they will help in the fourth case. Is that okay? Everyone?

(Refer Slide Time: 18:00)



If N_S and N_I are concentration of available Substitutional and Interstitial sites at Temp. T, then effective Jump Frequency ν_{eff} can be :

$$\nu_{eff} = \frac{\nu_S N_S}{N_S + N_I} + \frac{\nu_I N_I}{N_S + N_I}$$

Conc of Both defects relative to each other ν_{eff}.

Important :- However it is important to note that Natural random jump events may not be v. large, However Concentration Gradient of Impurities will dominate the Diffusion Process

If Ns and NI are concentration of available substitutional and interstitial sites at temperature T, then the effective jump frequency can be given by available substitutional site into total sites into jump frequency for substitutional plus available interstitial site to the total sites into jump frequency for interstitial. This is very standard average method. Available ones to the total with a jump rate, available one with ratio to the total into that jump rate. This is the net possibility. If it is only substitutional, what will happen?

NI will be much smaller than Ns. Then you say this term will be negligible. Only substitutional impurities may move. If NIs are much larger than Ns, we say only interstitial diffusion. But in a given this, both are together and Ns, Ni also concentration keep changing as numbers start getting more and more inside. So relative to, for considering both defects relative each other is effective new. Please remember this is most important thing which you should understand.

This expression is only trying to say both together can happen. And this expression I have derived from the average method, one among so much into this, second among so much into this. However it is important to note that natural random jump events may not be very large. These are called natural random jumps. Most of the impurities actually travel because of concentration gradient. Larger comparative is here, smaller impurity is here and they try to diffuse through to make equalization.

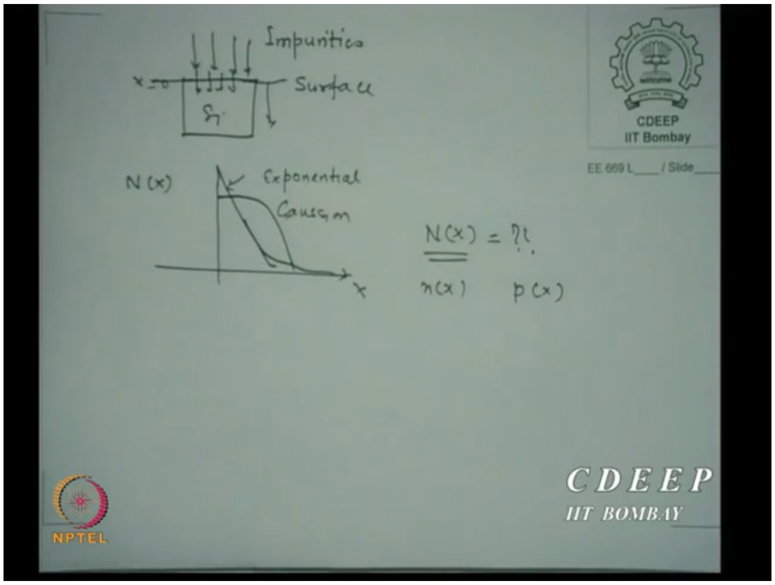
So question arises and why do we argue this if we know it is only gradient dependent? No, some of the effects what I should call them, anomalous effect. I see some profile, none of the standard expression fit to that. Then I come and see is this material at this time has some other diffusivity going on. So I look into which is the other mechanism which might have added or reduced it so that the profile should have gone up but it is moving down.

So to understand the actual profile which I will get in real diffusion, I will have to model it. And to model it, I should know from where these possibilities can occur. So it is not that these are very strong forces there but in case the profiles do not match as in the case boron it does not match, phosphorus it does not, mostly it matches with arsenic in normal this. But all other impurities show what is called as anomalous effects.

Anomalous means from standard diffusion theory it does not match my profile. So I say why. This is more important if you are actually looking into very very highly doped crystals areas or very very low dope area. In between the diffusion coefficient, diffusivity is essentially governed by gradients. Most devices are in that range but source drain, 10 to power 20. Some kind of PI diodes, 10 to power 13. So on those areas, these diffusion techniques are very very important, other ones.

We have two hours, so now we will start with this how the diffusion starts and I want to find at the end of the day, maybe I will show you one figure what is my ultimate aim of doing all this. Why I am so much worried?

(Refer Slide Time: 21:59)



By some way this is my crystal. Maybe silicon right now and this is my surface I call it. And I introduce impurities. This is what I will do. Technique of doing it, we will discuss in techniques, how impurities are introduced actually. Now if they are getting, since there is a large concentration of impurities at the surface compared to what silicon it has, it can be p-type, n-type, smaller doping, higher doping but difference.

So there is a gradient. These impurities tend to enter the lattice and keep moving downwards because of the gradient it created. If I, let us say this is x is equal to 0, then if I plot concentration of impurities Nx versus x, impurities getting down, this is x down. Then I may say there are number of profiles. One possible profile is this. Other possible profile is, sorry exponential. This is Gaussian, this is exponential and one more we shall, that is what we will start with.

So this Nx is what I am interested to know, what is the profile? That means from the surface the concentration will be normally very high but as you go down the concentration starts reducing. Now this profile decides some kind of resistance available to you because carrier available will be proportional to x now. Normally we say dopants are equal to the electrons or holes depending on the what dopant.

If it is n-type, all the doping impurities actually are equal to available electrons, not everyone of it but mostly. We say n is equal to Nd plus ionized one, p is equal to Na plus ionized ones. They are almost equal. So resistivity decided by n and p, so that that means Nd and Nes. But if Nd, Ne they are not constant, that means there is a profile. So n and p are also functions of x which means if I calculate the resistivity or resistance, I will find it is a function of x.

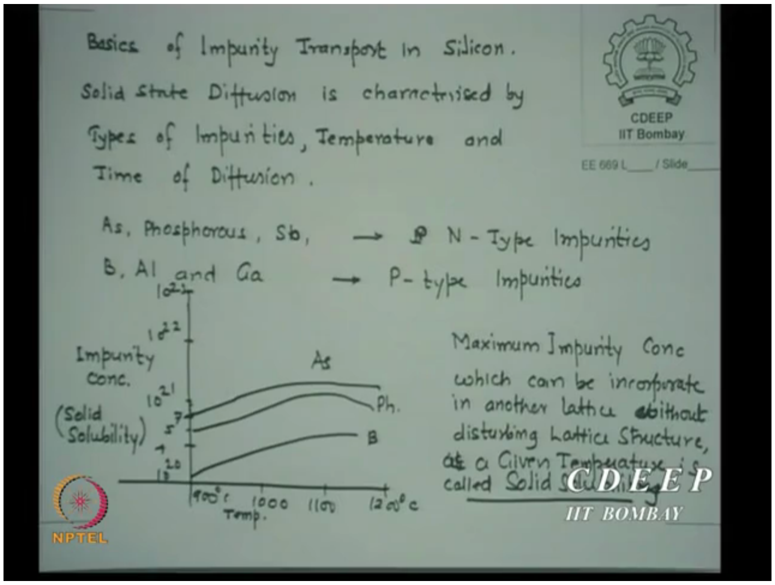
In many cases the way I do it, I take average of that value, integral over that range and say okay average resistivity is this. But in real life resistivity will higher have up, sorry, resistivity will be smaller up or conductivity higher up and will go down. Now this matters lot in smaller devices now because your channel length is of the order of 14, 10 nanometers. Your diffusions or substrate are 10 to power 19 kind of things, very thin layer of channel is going to be created.

Of course there are other physics effect called quantum effects but some other day. Now there how many real items are available to us? How much really Nx I have? Do I have a profile say uniform? All those issues will finally decide IV of the MOS transistor or BJT transistor. So this number is very crucial for me. How many actually? And this how many makes me actually go through all of it. Since I am interested to know Nx, Px for my electrical properties, I am now looking into how are impurities going to contribute to this Nx and Px profiles.

Is that clear? So that is the purpose of doing all this. I am not just doing this physics because I like. Maybe I like it, as I keep saying I really like it. Over the years you will also like it. When there is no stress of exam, you also start liking, I mean this is natural. So there are two laws in which impurities, diffusion can be modeled. First is called Fick’s first law and second is Fick’s second law. I think what I will do is I will leave it Fick’s first and second law for a while.

I will first finish the impurities because someone say lab you want some numbers. So I will show you actually how diffusion is done there. So what we are essentially doing here is the impurity which are coming inside the silicon, how they get inside and what is the profile it creates, is what is our major interest of doing all of it. So I start with something which is related to that and as I say time permitting I will come back to that.

(Refer Slide Time: 26:52)



Basics of Impurity Transport in Silicon.

Solid State Diffusion is charactrised by Types of Impurities, Temperature and Time of Diffusion.

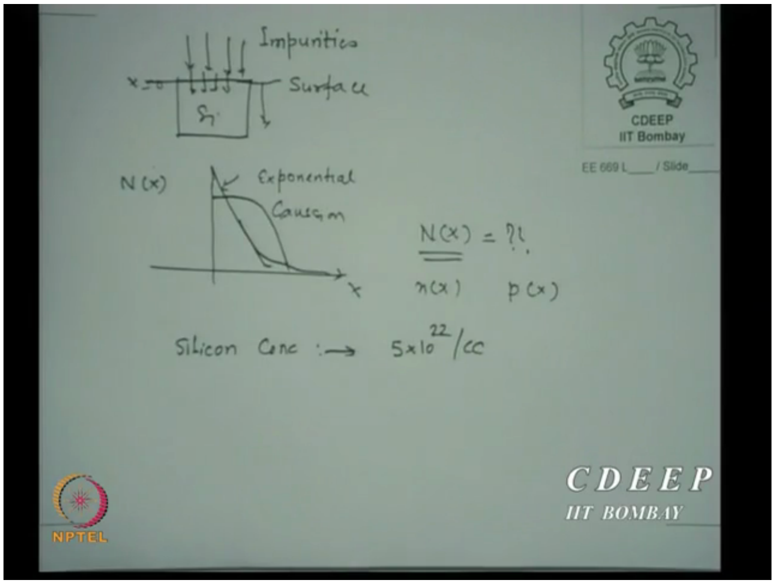
As, Phosphorous, Sb, → ~~P~~ N-Type Impurities

B, Al and Ga → P-type Impurities

Maximum Impurity Conc which can be incorporate in another lattice without disturbing Lattice Structure, at a Given Temperature is called Solid Solubility

This is very interesting. Since our diffusion is solid impurities are getting into solid material, if it is liquid-liquid system which we have solid bits getting into liquid, both forming liquid crystal growth. There we can as if stir it and uniformly dope it but that is not so in the case of diffusion in normal sense. So we are interested in, if I start these impurities diffusion from the top let us say of the wafer, what is the maximum concentration I can get at the surface. For your kind information maybe, just a minute I will just say numbers and come back to this.

(Refer Slide Time: 27:37)



N(x) = ?!

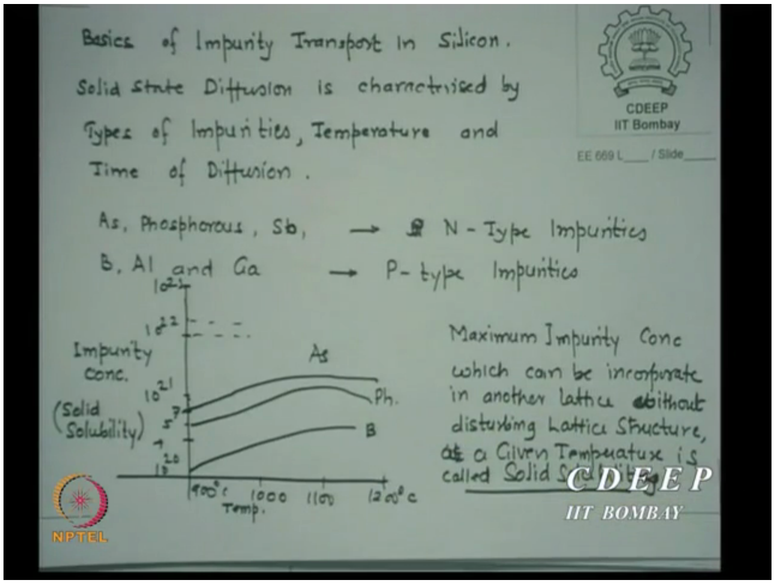
n(x) p(x)

Silicon Conc :→ 5×10^{22}/cc

The maximum silicon concentration at a normal temperature is 5 into 10 power to 22 atoms per cc. This is the maximum carrier concentration or maximum doping, maximum atoms per cc available to you. Based on this our density recalculations we perform or rather from the major densities this number has been found. Okay, for the lattice of 8 atoms in per cell. So this is the maximum atoms, so how much doping we can do? Certainly not 5 into 10 to power 22.

Because if it replaces all the atoms, then there is nothing silicon. So obviously it has to be less than 5 into 10 power 22. So this is a natural limit up to which silicon can get into, impurities can get into silicon. That at a given temperature is different and this term is called solid solubility. Solubility is essentially between liquid and solid but here is the case we are talking, terming it as solid solubility. Is that clear? Atoms, how many atoms per cc are inside at the surface, we will like to know how maximum can reach there at the surface. That is called solid solubility.

(Refer Slide Time: 29:06)



Basics of Impurity Transport in Silicon.

Solid State Diffusion is charactrised by Types of Impurities, Temperature and Time of Diffusion.

As, Phosphorous, Sb, → N-Type Impurities

B, Al and Ga → P-type Impurities

Maximum Impurity Conc which can be incorporate in another lattice without disturbing Lattice Structure, at a Given Temperature is called Solid Solubility

Here is some type of impurities you know which contribute to electrons and holes. There are some story about if there is why do not you buy, put impurities from the second group or even the first group. Then it can create two electrons or two holes, three electrons or three holes. Why only one kind of thing, three or five we take. There is answer later when I calculate diffusion coefficients. What will happen if there is a double such system appears?

However as of now arsenic, phosphorus, antimony are standard n-type impurities and boron, aluminum, gallium are mostly p-type impurities. 99 percent now we use arsenic as n-type dopant and boron even now is the only good dopant for p-type. Yeah, there are some devices in which boron plus aluminum has been tried but it is not great success. There is some new methods are being tried there, some other day about this.

P-type impurity concentrations, difficult to get into the much numbers. We will see this number soon. So here is some graph shown here. This is temperature versus solubility. I can say this is my 10 to power 22 or maybe 5 into 10 to power 22 is the limit of silicon. So nothing much can go below. Also the graph shown here, arsenic, phosphorus, phosphorus deep at higher temperature. We will explain, this is anomalous. At high temperature phosphorus, why it comes out?

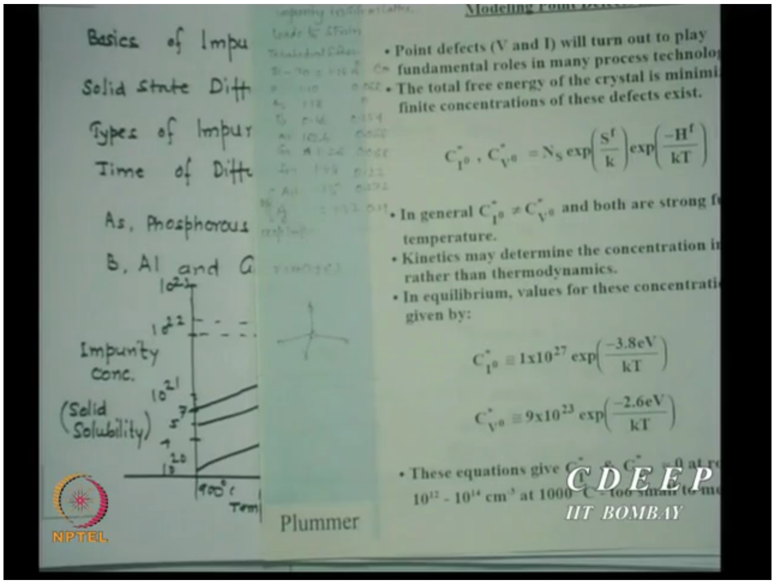
So it actually reduces the concentration. Boron of course at 1200 does not do much. Now one can see from here the numbers were, roughly it is 4 into 20 for arsenic, boron but arsenic can go up to 10 to power 21, 4 into 10 to power 21. What does that means? Arsenic is much easier to get in compared to boron. So what is the problem? Why solid solubility of arsenic is highest compared to boron? So here is some numbers which, a sheet which last time I forgot, so maybe taken from Plummer yesterday and hand-written on something.

If you have taken down the graph, these graphs are also available in Plummer, so nothing great about. Of course they, if you see their book, I do not know, yesterday I wanted but there will be also two such graphs. One is this and the other is dotted lines for both arsenic, phosphorus. Can you think what could be they? This will be slightly lower than all of them. Say arsenic, 4 into 21, maybe this is let us say 5 into 21 but actually dotted curve will be slightly below, 3 into 21 or 4 into 21. Why these dots come lower then, is that clear to you? Something?

Not all atoms actually get ionized, they may come in only at the substitutional sides. If they sit, they ionize which essentially means this is the actual number which have come in. But the actual ionized atoms will be slightly lower than the available. So actually our interest is in that number not even this. But for theory let us look into solubility at given temperature. So please look at the books, they will show you three graphs for solid solubility, three graphs solid solubility with activated impurity. Activated means ionized, they are actually sitting at substitutional side.

In this everything which is getting into lattice without straining it, is possible. Is that okay? So this fact has to be understood why that number is slightly smaller and in other calculation when I will give you graph, I will give both, I mean the full graph. We will have to always choose the dotted pairs which are activated numbers for the concentration. Is that point clear? You must use dotted curves instead of the hard ones because dotted are activated impurities. Activated means these are the ones only contributing to resistivity and we are only interested in currents and voltages, no more. So we will say okay, they are dotted. So we will see that graph later.

(Refer Slide Time: 33:36)



Basics of Impu

Solid State Diff

Types of Impur

Time of Diff

As, Phosphorous

B, Al and G

Modeling Point Defe

- Point defects (V and I) will turn out to play fundamental roles in many process technolo
- The total free energy of the crystal is minimi finite concentrations of these defects exist.

$$C^*_{I^0},\ C^*_{V^0} = N_S \exp\left(\frac{S^f}{k}\right)\exp\left(\frac{-H^f}{kT}\right)$$

- In general $C^*_{I^0} \neq C^*_{V^0}$ and both are strong f temperature.
- Kinetics may determine the concentration i rather than thermodynamics.
- In equilibrium, values for these concentrati given by:

$$C^*_{I^0} \cong 1\text{x}10^{27} \exp\left(\frac{-3.8\text{eV}}{kT}\right)$$

$$C^*_{V^0} \cong 9\text{x}10^{23} \exp\left(\frac{-2.6\text{eV}}{kT}\right)$$

- These equations give $C^*_{I^0}$ & $C^*_{V^0}$ ≈ 0 at r 10^{12} - 10^{14} cm^{-3} at 1000°C - too small to m

Whenever impurities try to get into a lattice, it try to, even if we say strain-free, it does strain the lattice. For example, when the, even if interstitial side between the two atoms, when there is a constriction there, so it has to pump in, it has to push in. Now that means some of the earlier atoms may not retrace back to its original position, maybe slightly moved. So there is this partial strain which always exists even if we do room temperature. The problem is we recover it by some other technique that is another issue.

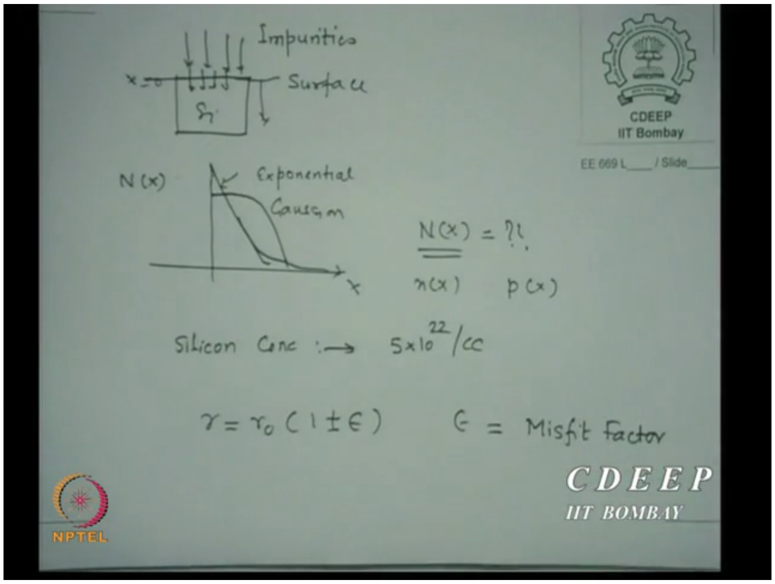
For a silicon we have actually discussed other day or just now that there is a tetrahedral radius which is 2.36 Armstrong was dia, so 1.18 Armstrong was the radius. For each such atom size of phosphorus, arsenic, antimony, I think there are given boron, aluminum, gallium, indium, gold, silver, all impurities we have actually found out the tetrahedral radius for their lattices. Now one of the these impurities may come into silicon. This is, is that clear? They are impurity atoms, they also have a crystalline structure, many of them, not necessary all of them.

So if their tetrahedral radius is known and I know silicon tetrahedral radius. Now we say if the tetrahedral radius of silicon matches with tetrahedral radius of that impurity, then the maximum will come because they will not strain anything. Same size, if the size is bigger, the smaller atoms and one is bigger sitting there, so it will strain the lattice anyway. If it is smaller, it will be inverse stress. So if the size tetrahedral radius of an impurity is not identical to silicon or tetrahedral radius, then it strains the lattice, marginally but it does. This is essentially called replaced by, this is explained by term called misfit factor. It is called misfit factor, so maybe I write down in that sheet. I come back and this number maybe read out for you so that you know.

For silicon R0 is the tetrahedral radius, 1.18 Armstrong. Phosphorus, it is 1.10, okay. Arsenic, it is 1.18. Boron, it is 0.88. Please note, when I say please note down. Silicon, 1.18; phosphorus, 1.10; boron, arsenic, 1.18; boron, 0.88; aluminum, 1.026; gallium, 1.26; aluminum, 1.026, in gallium, 1.26; indium, 1.44 largest atom around. But gold and this is even higher. Gold is 1.5 Armstrong, silver is 1.52 Armstrongs. Is that okay?

And the difference between R0 to this tetrahedral radius are that it is called misfit factor epsilon. Is that clear to you? The difference between silicon tetrahedral radius and impurity tetrahedral radius is called misfit factor. It can be plus or minus. If the impurity atom is larger tetrahedral radius, it will be minus. If it is smaller, it is positive. So what I define, you have noted these numbers, you noted down what I wrote.

(Refer Slide Time: 37:26)



$\underline{\underline{N(x)}} = ??$

$n(x)$ $p(x)$

Silicon Conc :→ $5 \times 10^{22}/cc$

$r = r_0 (1 \pm \epsilon)$ ϵ = Misfit factor

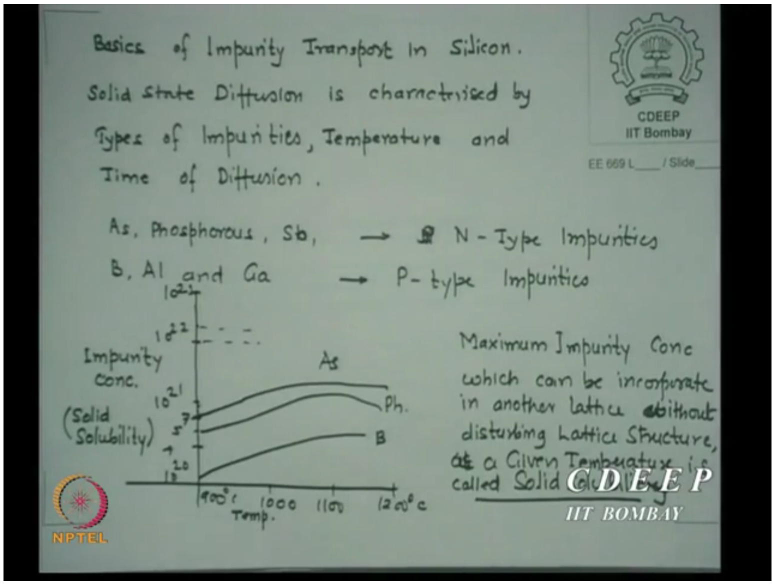
What I am now saying you that I have a formulation which says r is equal to r0, 1 plus minus epsilon where epsilon is called misfit factor. You subtract 1.18 from each impurity atoms, each impurity atom tetrahedral radius and find out what is epsilon for each. r0 is for silicon, r is the tetrahedral radius for impurities. If epsilon is 0, when this can occur? When r is r0. If r is r0, epsilon is 0. Which impurities according to you has? Arsenic.

Since arsenic has the least misfit factor, the possibility of number of atoms of arsenic getting in silicon is the highest at solid solubility. Is that point clear? Because they do not strain the lattice compared to others. Next will be which? Depending on of course, 0.68 is for phosphorus. So next best may be phosphorus. Boron has 0.254 as epsilon difference, so it will have a smaller number. So do you get the point that graph which I showed you is someway related to misfit factor. Is that point clear? Why those graph, arsenic shows highest concentration followed by phosphorus, followed by boron.

And if you plot for all the impurities, correspondingly you get solid solubility curves for all impurities. But since we are only interested into silicon IC process, I am restricting only these three. But please remember in case I needed, I get those values for my other impurities as well. So this fact that misfit factor decide solid solubility should be understood that why people actually say that arsenic is the best n-type dopant or best dopant in silicon.

But if the gallium arsenide lattice, it may have different kinds of misfit factors for different impurities there. Of course there is no, by the way which is the easiest doping this in the case of gallium arsenide? Silicon. Okay, some other time. Of course, I am not teaching gallium arsenide but my own PhD work for some gallium arsenide, 35 years, 40 years ago. So I still enjoy that.

(Refer Slide Time: 39:55)



Basics of Impurity Transport in Silicon.

Solid State Diffusion is charactrised by Types of Impurities, Temperature and Time of Diffusion.

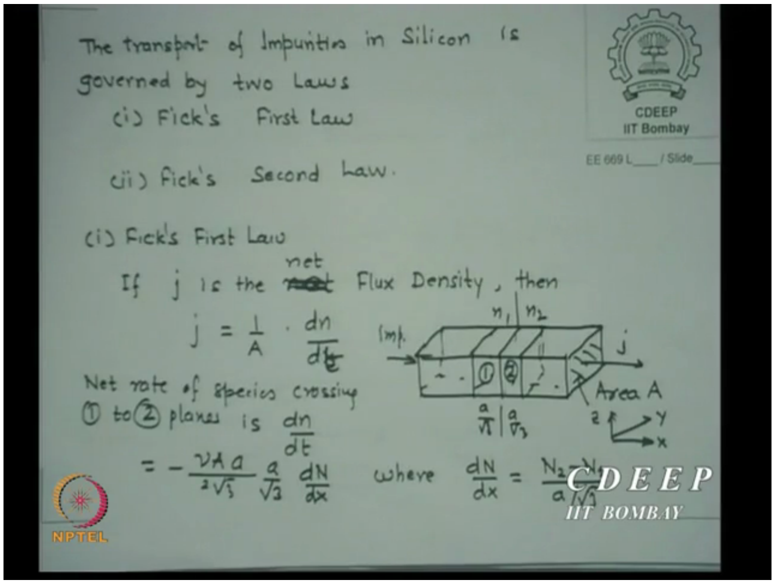
As, Phosphorous, Sb, → N-Type Impurities

B, Al and Ga → P-type Impurities

Maximum Impurity Conc which can be incorporate in another lattice without disturbing Lattice Structure, at a Given Temperature is called Solid Solubility

And as I said those days when I shifted to silicon, my guide was saying that oh, this is the area of future, why are you shifting? Then I told him ki sir, woh future never comes. So I would prefer to be in present, so I shift to silicon. So my choice was not bad as far as technology goes but if I would have continued, I would have published many more poor papers. For silicon there were 20 lakh people working, gallium arsenide 100. So I should have been there but did not realize that I will become teacher. Maybe I should have become the otherwise. Though I did try work in industry as well as R&D labs, before I became teacher.

(Refer Slide Time: 40:36)



The transport of Impurities in Silicon is governed by two Laws

(i) Fick's First Law

(ii) Fick's Second Law.

(i) Fick's First Law

If j is the ~~net~~ net Flux Density, then

$$j = \frac{1}{A} \cdot \frac{dn}{dt}$$

Net rate of species crossing ① to ② planes is $\frac{dn}{dt}$

$$= -\frac{\nu A a}{2\sqrt{3}} \frac{a}{\sqrt{3}} \frac{dN}{dx} \quad \text{where} \quad \frac{dN}{dx} = \frac{N_2 - N_1}{a/\sqrt{3}}$$

That is why we say technology was my first jobs where I did for 15 years. So I understand more of technology compared to many not because they are smarter, they are, they know more knowledgeable maybe. Many of them I have been taught by me, so maybe more better than me but simply because I enjoy. And after great fight with my head, you are the sufferers for that but I forced them to give me this course for the last time because I said I want to record it once.

Many of my old student who learnt technology from me, 20 years, 15 years, they kept on saying sir, aapka yeh course web par nahi hai. Mein bola okay, last time I will record it. Now this was the old time case that students ka thinking has changed, student attitudes has changed. Maybe I have also changed. So things may not be as good or as bad, as they were earlier. But I am known as technology scene earlier phase of my career and suddenly I became designer for no good reason.

These days I am working on meta materials and antennas and something else. There are two laws of diffusion. One is Fick’s first law, and the other Fick’s second law. As I said we will derive them or I will leave it to the posting. What is Fick’s first law says? Let us say there is a semiconductor bar, it has two planes I have made, A by root 3, A by root 3 are the two planes. This Fick's law statement, I am just showing a figure.

This is called cross-sectional area. Impurities are coming inside this area and getting inside. This is my x direction. This is my y direction and this is my z direction in a crystal. Now it can be found by not going too detail on this, this we derive again. I just wrote down there, maybe I said, j is called flux density. This plus, please us this word j which is current density but here I am using a flux density because over the years I have been using it. Some other books may give something else.

What is flux density? Number as, someone asked you what is the definition of flux density, number of atoms or number of particles moving per unit area per second is essentially called flux density. So when someone asked us many years ago that why IIT Bombay and many other IITs only have electrical engineering department and not electronic as communication instrument, I have some mixture of n of them. So I said, my statement was simple.

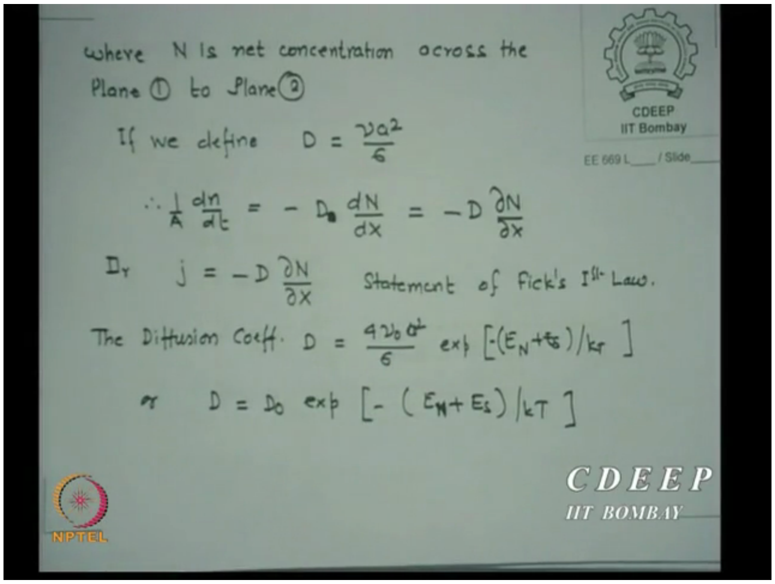
After all in all electrical engineering we are interested in the electron transport and nothing else. Maybe hole is additional feature and it is only the flux density matters. If it is very high flux density, we say it is a power area, very large flux, large amount of currents amps, tens of amp, fifties of or hundreds of amps. Flux density is very high actually. If it is very very small, we say nano. In between if the signal you need moderately, flux density requires for electrons motion.

So all areas are covered essentially by number per cc per second. So electrical engineering is only electron transport and nothing more. So we keep working only on electron transport. So this flux density is per unit area, so it is dn by dt. This is the statement. We will derive this later, 1 upon A, dn by dt where n is the number which essentially we are saying per unit volume actually. Impurities are coming and going from this plane in one or one into two and there is a diffusion process remains.

Some numbers can go from 2 to 1 but there will be net numbers going from 1 to 2 if there is a gradient set. Now this gradient is let us say if N2 is the number here and N1 is the number here per cc. So dn by dx is N2 minus N1 upon, if this plane distance is a root 3, so N2 minus N1 by a root 3, what is this a root 3? The distance between the plane, which distance I am talking? Is the Miller distance, we will see next time.

You have the planes, so Miller planes, so we will see what is the minimum distance they have along 100, 111, other planes. So if I do this which I have done there again, please just note down, do not note down because I am going to post this. I just wanted to rewrite because to show you.

(Refer Slide Time: 45:45)



where N is net concentration across the Plane ① to Plane ②

If we define $D = \frac{\nu a^2}{6}$

$$\therefore \frac{1}{A}\frac{dn}{dt} = -D\frac{dN}{dx} = -D\frac{\partial N}{\partial x}$$

Or $j = -D\frac{\partial N}{\partial x}$ Statement of Fick's Ist Law.

The Diffusion Coeff. $D = \frac{4\nu_0 a^2}{6}\exp\left[-(E_N+E_s)/kT\right]$

or $D = D_0 \exp\left[-(E_N+E_s)/kT\right]$

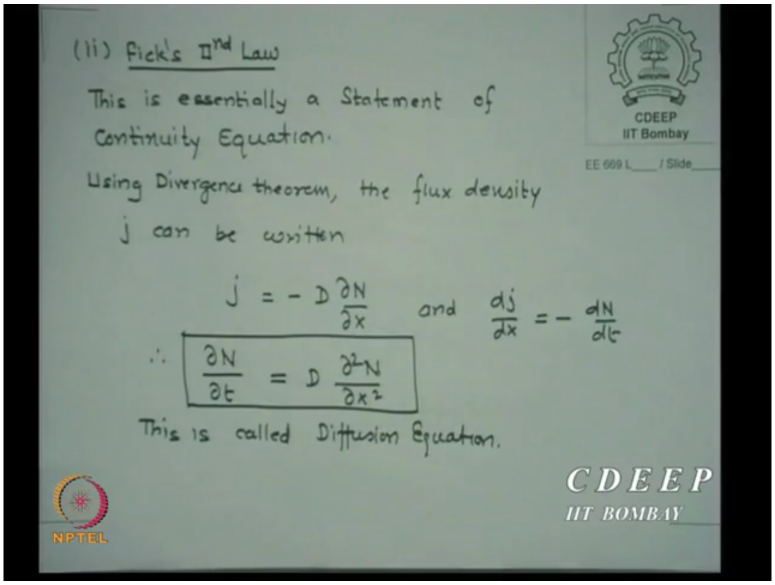
And then we define this mu a square by 6, whatever term is coming here as diffusion coefficient or diffusion constant D. Then I write 1 upon A dn by dt is minus D dn by dx or j which is this minus dn by dx. This is Fick's first law, that the flux density is related to gradient, proportional to gradient. I repeat the flux density is proportional to gradient, this is the Fick's first. Why this minus sign? Gradient down, okay, minus sign.

D is the diffusion coefficient or diffusion constant and we know diffusion coefficient can be rewritten as 4 mu a square by 6, exponential En plus Es by kT for vacancy transport. So D is equal to D0, this term is called D0 exponential minus En plus Es by kT. So first Fick's law says j is equal to minus dn by dx, gradient, that is our first thing. So if the impurity concentration is higher here and lower here, impurities will move towards the lower side, it is like a potential difference.

Unless there is a potential difference, energy does not move. The only difference there is one can say it is not a random motion. In this case the way it is as I say probability wise, 50 percent chance going ahead, 50 percent, but keep going plus minus, plus minus, at some number if there is a gradient, you will be further away from the starting point. So this is essentially statement of Fick's first law. That the amount of impurities per unit area, per unit time at the surface of silicon or rather when they enter silicon, it will be proportional to the gradient it has set in.

Now that is the term we want to calculate. So we must first get j value somewhere and must get dn by dx relationship with that later. If I can calculate Nx, that is what all that my interest is. Is that okay? So for you this of course, you need not have written but I have written there again. But just to repeat in case I do not, then I feel I will show where from Fick's first law is coming.

(Refer Slide Time: 48:23)



(ii) Fick's II^{nd} Law

This is essentially a Statement of Continuity Equation.

Using Divergence theorem, the flux density j can be written

$$j = -D\frac{\partial N}{\partial x} \quad \text{and} \quad \frac{dj}{dx} = -\frac{dN}{dt}$$

$$\therefore \boxed{\frac{\partial N}{\partial t} = D\frac{\partial^2 N}{\partial x^2}}$$

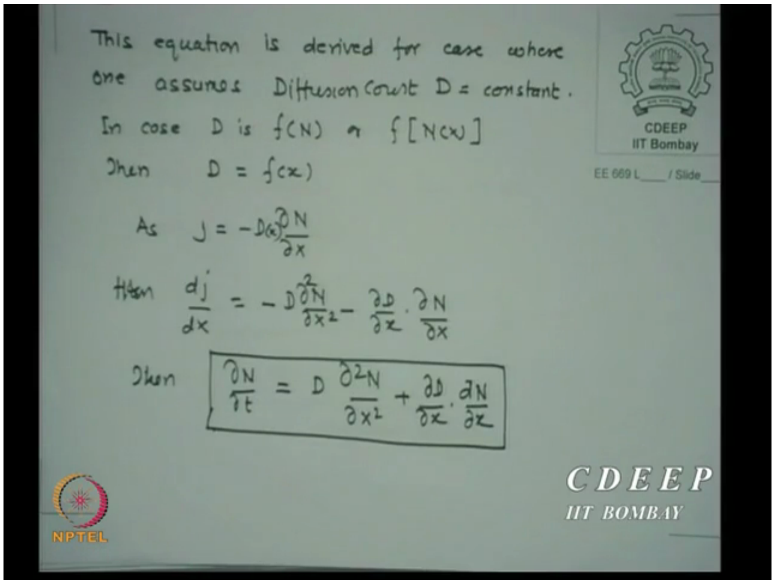
This is called Diffusion Equation.

The Fick's second law is essentially a statement, I do not know how many of you have done your devices well but hopefully. So but any other's devices we bound where we talk lot of it but continuity equation has nothing to device. Continuity of transport of any fluid, solid, gas, anything is continuity. And according to the divergence theorem, the dn by dt, dj by dx that is the flux density gradient is equal to minus dn by dt. This we will discuss, this is called continuity equations. So time dependent term is related to space dependent term. This is called continuity equation, we will derive this next time or as I say may post it.

And if I use dj by dx is minus dn by dt, use this j here, differentiate j here, so I get this equation. dn by dt is D d2n by dx square. This is called diffusion equation. This is what we want to solve. At the end this is what we want to solve, why? For a given time impurities are coming in and also moving in, is that point clear why this equation is relevant? Impurities are coming inside, going with time but also moving in space. So I am not interested in only Nx but I am also interested in Nxt. But if t is known, I know I will only get Nx profile at the end of t. Is that clear?

That is what I want to do. This equation is my precursor of finding Nx functions. This equation is what we are going to solve now. And once we solve this, only thing catch word in this maybe I have said it, okay. Here I assume D is a function of nothing, that is constant. D is independent of everything. But in real life that is not so. D is a function of concentration itself. You can understand some way. If there are larger atom, the other impurities will require more effort to get in. So it is a gradient dependent term. So if Nx are present, that means D will be get affected by N itself. N is larger, D will be smaller you take from me. Because they will be stopped by some other people. It is a crowd business.

(Refer Slide Time: 50:47)



This equation is derived for case where one assumes Diffusion Const D = constant.

In case D is $f(N)$ or $f[N(x)]$

Then $D = f(x)$

As $J = -D(x)\frac{\partial N}{\partial x}$

then $\frac{dJ}{dx} = -D\frac{\partial^2 N}{\partial x^2} - \frac{\partial D}{\partial x}\cdot\frac{\partial N}{\partial x}$

Then $$\boxed{\frac{\partial N}{\partial t} = D\frac{\partial^2 N}{\partial x^2} + \frac{\partial D}{\partial x}\cdot\frac{\partial N}{\partial x}}$$

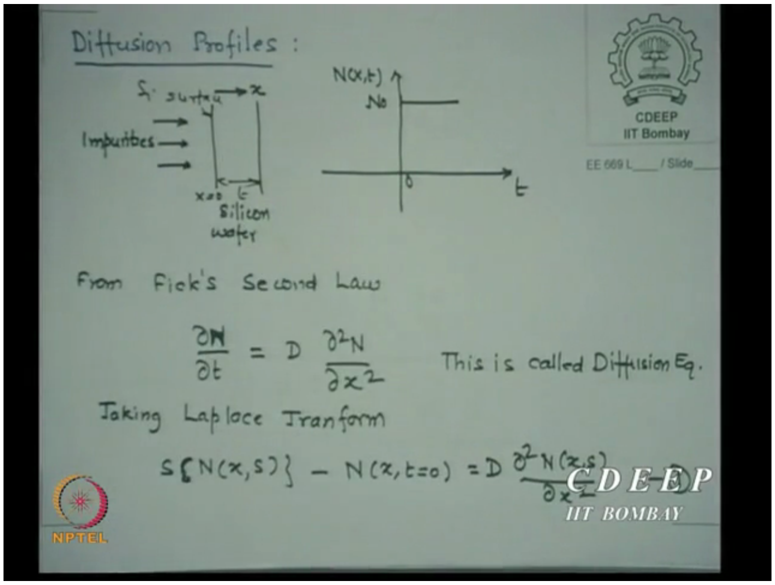
Since D is a function of Nx, D is a function of x, so if I differentiate J, D dn by dx, then I must write this as a function of x. And if I then differentiate, I will get two terms. One related to Dd by dx, the other related to d2n by dx square. Now this term many cases, this equation is not linear equation, it is a non-linear equation. And therefore analytically cannot be solved easily. Some people can do by linearization. If you are expert in maths, there are certain condition in which you can linearize it.

If you cannot, what is the easiest way? Own a system and solve numerically this equation. Any non-linear second order differential equation can be solved by N methods. Whichever method you prefer, you can solve. Linearize it also, by then come to Gauss- Seidel, Gauss–Euler, whichever method, you can choose (())(51:44) methods. N methods are solving second order non-linear differential equations. I will assume right now linearity for analytical purpose. But in real life the models which I will substitute in software for process simulation, I will use D as a function of N itself.

And let it take, because there is a grid, it will find what N and find D there. Why should I care for it? But why I care many times? Even if in a software when I write, what is the criteria I normally put for writing good software? Time taken to solve is the major criterion writing a good software. You may have very interesting software written but if it takes ages to solve, then there is no point in using that.

So as much as simplicity you can create, so put some small model inside which may not be accurate but enough for that and partly linearize it. So there are tricks in all modeling people, they keep using some tricks and then say oh, so fast it works. It works fast because you have assumed some few things. If you do not, it takes hours or ages. So please remember you will do only linear system because that is easy to solve analytically. Real life, since this is not very strong term, D by dx, Dd by dx, so for first order this term can be neglected and you can use only first ones.

(Refer Slide Time: 53:22)



Diffusion Profiles :

From Fick's Second Law

$$\frac{\partial N}{\partial t} = D \frac{\partial^2 N}{\partial x^2}$$ This is called Diffusion Eq.

Taking Laplace Tranform

$$s\{N(x,s)\} - N(x,t=0) = D \frac{\partial^2 N(x,s)}{\partial x^2}$$

The first thing we start is now looking into profiles, that is our ultimate, that is what we are going to do, work at. So we start with profiles. First, let me say and then draw. This is silicon surface and as I say this is the depth in silicon surface, shown x, this is the silicon surface. This is silicon surface, this is silicon wafer of thickness t and t is very large compared to anything. t is, for a boundary condition what will say? t equal to infinite, means our thickness is infinite.

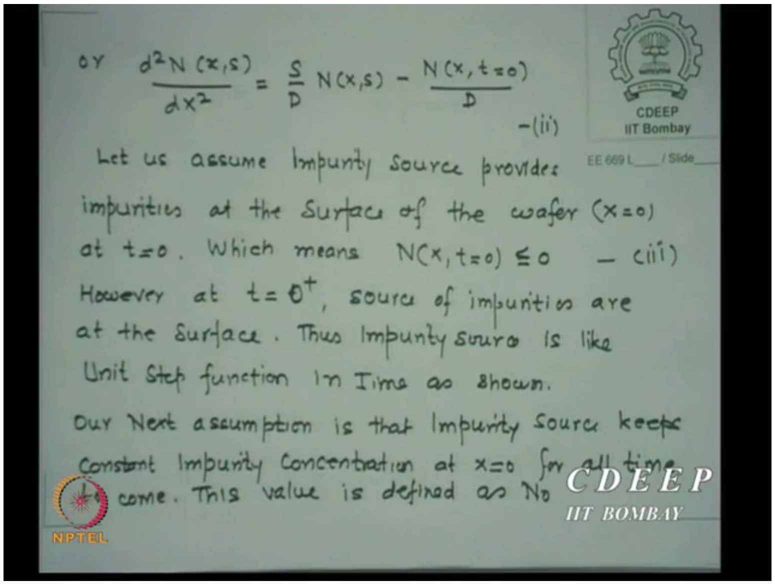
So I have impurities introduced from surface side. Essentially wafers sit in a rack like this and source of impurities are impinging on it in any technique. I assume and that is very important, in time frame, okay maybe we will come back to this later. Is that model clear what I am saying?

Impurities are impinging at x is equal to 0 at which is silicon surface and they will get inside silicon along the x axis. The assumption is it is isotropic diffusion, means y and z do not play. It is not true, actually I should do Nxyz or delta as a term we should solve for.

But most cases this is good enough. dn by dt is D d2n and this is our diffusion equation. Just now we wrote, Fick's second law. We take, of course this we will come back. This is the condition I am putting because I need to solve, so initial condition I create. I take a Laplace transform, I hope 99.9999 people know Laplace transforms. If not, what you did? At least communication people if they do not know Laplace transform, 4-year transform, they will not be within communication, next day bahar khada kar denge.

Microwave terms mein chal jata hai. loag match kartehi nahi udhar, so udhar chal jate hai. Of course, this is a trivial maths, any network person must know it. S NxS is equal to the Laplace transform or this is S Nx S, minus the initial condition, Nxt equal to 0, equal to D times d2Nx S upon dx square. This is the Laplace transform or diffusion equation. I can rearrange these diffusion equations slightly, is it okay? Nahi, kisiko doubt hai toh bol dena, there is nothing wrong with this. Laplace transform sikh lijiye baba, nahi hota toh aisa nahi chalega. Life is very tough without transforms. Is it okay?

(Refer Slide Time: 56:34)



or $$\frac{d^2N(x,s)}{dx^2} = \frac{s}{D}N(x,s) - \frac{N(x,t=0)}{D} \quad \text{-(ii)}$$

Let us assume Impurity source provides impurities at the surface of the wafer (x = 0) at t = 0. Which means $N(x, t=0) \leq 0$ — (iii)

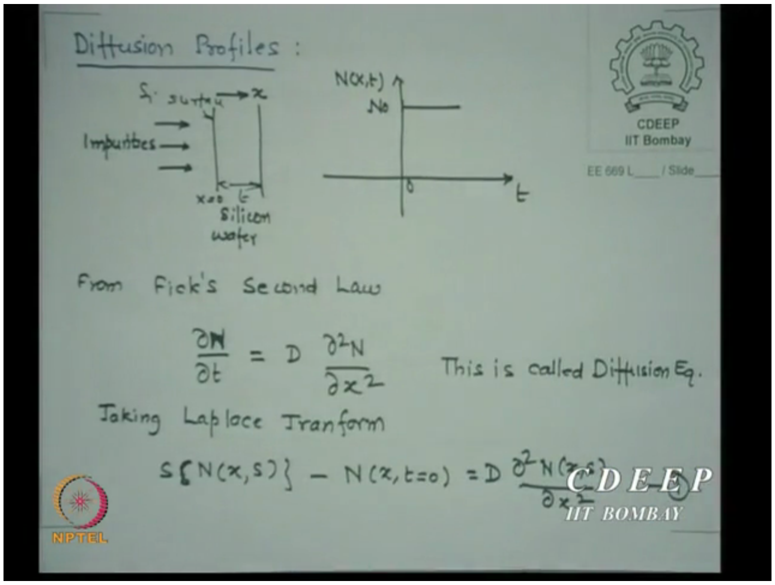
However at $t = 0^+$, source of impurities are at the surface. Thus Impurity source is like Unit Step function in Time as shown.

Our Next assumption is that Impurity source keeps constant Impurity concentration at x = 0 for all time come. This value is defined as N_0

I rearrange this, that equation again. I write d2Nx S by dx square is S by D, please remember Laplace transform is only for time, x does not change. So d2Nx S upon dx square is S by D Nx S minus Nxt0 by D which is why initial condition term. Now here is my to solve this equation, this is very easy to solve if I know this. This equation I can solve, if I know this, that means I must know my initial condition. So I have conditions which I impose myself and say this is my initial condition.

So let us assume, if you have written down the formula which is trivial, let us assume impurity source provides impurities at the surface which is x is equal to 0 at t is equal to 0. So that means, what does that mean? Prior to t equal to 0, there are no impurities. At t is equal to 0, source starts. Is that clear? Prior to t equal to 0, there is but once it starts, it never ends. Certain number of atoms per cc are constantly available to me infinite times.

(Refer Slide Time: 57:58)



Diffusion Profiles :

From Fick's Second Law

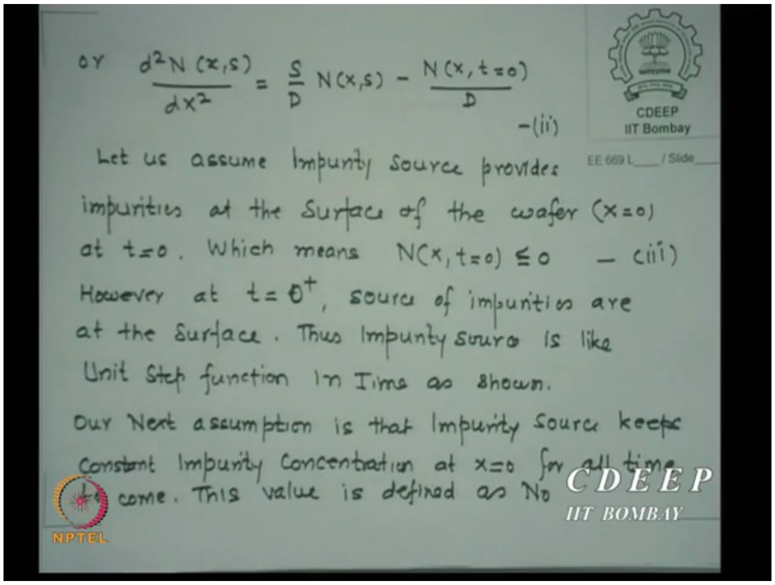
$$\frac{\partial N}{\partial t} = D \frac{\partial^2 N}{\partial x^2}$$ This is called Diffusion Eq.

Taking Laplace Tranform

$$s\{N(x,s)\} - N(x,t=0) = D \frac{\partial^2 N(x,s)}{\partial x^2}$$

Just a minute before I show this. At t is equal to, less than equal to 0, no impurities are impinging. At t is equal to 0, the available concentration is in N0 which remains constant for all times to come. This is my initial condition which I start with and this is real life condition, that is why I did it. Is that okay?

(Refer Slide Time: 58:14)



$$\text{or}\quad \frac{d^2N(x,s)}{dx^2} = \frac{s}{D}N(x,s) - \frac{N(x,t=0)}{D} \qquad -(ii)$$

Let us assume Impurity Source provides impurities at the Surface of the wafer $(x=0)$ at $t=0$. Which means $N(x,t=0) \leq 0$ — (iii)

However at $t=0^+$, source of impurities are at the Surface. Thus Impurity source is like Unit Step function in Time as shown.

Our Next assumption is that Impurity Source keeps Constant Impurity Concentration at $x=0$ for all time to come. This value is defined as N_0

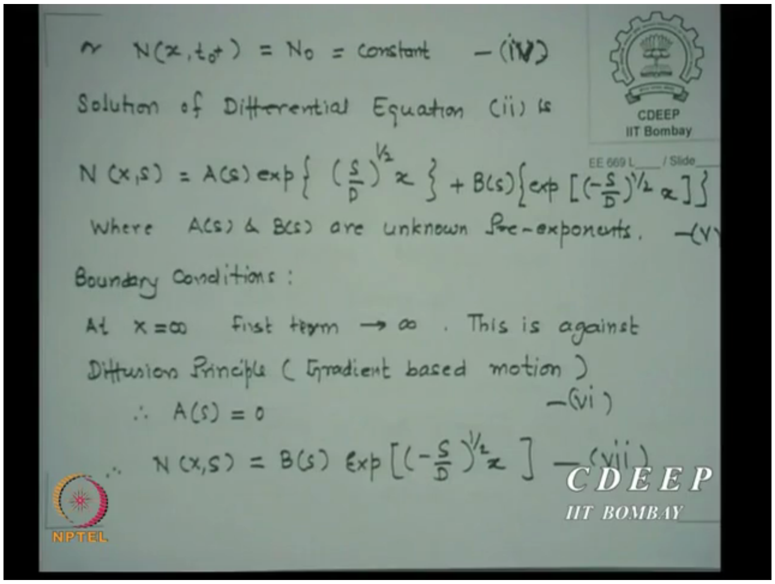
At t is equal to 0, no impurities, we start the source at t is equal to 0 and some fixed number appears for all time to come. Which means Nxt0 is less than equal to 0. However t equal to 0, plus what I said, I have written again. Source of impurities at the surface, thus impurity source is unit step function in time as shown. Our next assumption, yeh to ekk condition lag gai, what is the other assumption I need or other conditions I need?

x ki condition chahiye naa, t ka toh dikha diya, ab x ka bhi chhahiye. How many conditions you need, boundary conditions? Second order equation need two BCs, so let us see which are the two boundary conditions we have. Our next, first assumption is it is unit source. t is equal to 0, then it starts, I have constant source available or also called infinite source, why? It keeps coming, there is no stopping on that. So either it is called infinite source diffusion or called constant source diffusion. All the time in infinite or constantly available for all times.

The second BC or secondly we want to see BCs, so we say our next assumption is that impurity source keeps constant impurity concentration at x is equal to 0. At the surface we always get N0 whatever number all the time. At x is equal to 0, this number is fixed, how much? N0. And how much will be N0 roughly? Solid solubility because at that temperature the maximum available to enter there is so much. So N0 will be actually you pick from solid solubility graph, is that correct? N0 will be picked up from solid solubility graph. Because we know at that temperature how much N0 can reach at the just below surface of the silicon.

Okay, This value is defined as N0 because that is the number which we were constantly pushing. So we said x is equal to 0, this number is fixed. So the first boundary condition therefore say, Nxt0 plus onwards is N0 which is constant.

(Refer Slide Time: 60:42)



$\sim \quad N(x, t_0^+) = N_0 = \text{constant} \quad -(iv)$

Solution of Differential Equation (ii) is

$N(x,s) = A(s) \exp\left\{ \left(\frac{s}{D}\right)^{1/2} x \right\} + B(s)\left\{ \exp\left[\left(-\frac{s}{D}\right)^{1/2} x \right] \right\}$

Where A(s) & B(s) are unknown Pre-exponents. $-(v$

Boundary Conditions :

At $x = \infty$ first term $\rightarrow \infty$. This is against Diffusion Principle (Gradient based motion)

$\therefore A(s) = 0 \quad -(vi)$

$\therefore N(x,s) = B(s) \exp\left[\left(-\frac{s}{D}\right)^{1/2} x \right] \quad -(vii)$

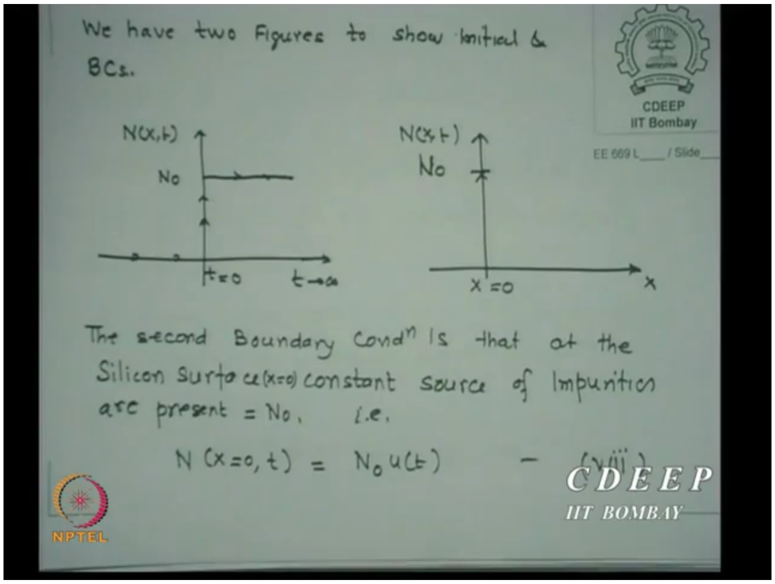
Now once I know my initial conditions, I know the equations which are wrote, has equation analytical equation given by, solution is AS exponential under root of S by D into x plus BS, exponential minus S by D to the power half x. This is the solution of second order differential equation which I have used. This is very simple, second order differential equation ka simplest solution ye hai. Now the first boundary condition you have said here, the second boundary condition, boundary is what? First is x is equal to 0, where is the second boundary? Far away.

x is equal to infinite. If the impurities are coming in with the constant this, why should it become 0? All impurities will go there naa. Why should it go 0? So there is an issue, means this is what you are saying. If infinite source is there, the infinite N it will reach because there is no stopping it, it just goes there. Now the problem is if I put first x is equal to infinity in this term, what does that mean? This is positive, S by D is constant, x is positive, x is infinite, what does that mean?

This Nx will become infinite but I already told you diffusion is always gradient based. So obviously impurity concentration cannot reach from N0 to infinite, that is not possible. So what should be happening? AS must be unequivocally 0, the first constant pre-exponent must be unequivocally 0. Is that point clear? If x is equal to infinity, the first term will go to infinite, that means concentration will reach infinite which is never possible because impurity will diffuse down with the gradient which essentially means the first term must vanish, which means AS must be guaranteedly 0.

If that is so, the second term has removed the first term itself, second boundary condition. Then I get NxS is BS, exponential minus S by D to the power half into x. So this is the solution but what is still not known to me? BS, first AS, because of the second boundary I just removed that. But now I must know BS, so I look into the real life situation. Let us see what it happens. Is that okay? Please note down. This is the solution. If x goes to infinity, this term blows and since this term blows, it is again the principle of diffusion and therefore AS must be 0. So the actual solution in this specific case is BS times exponential minus S by D to the power half, is that okay everyone?

(Refer Slide Time: 64:01)



We have two Figures to show Initial & BCs.

The second Boundary Cond^n is that at the Silicon surface(x=0) constant source of Impurities are present = No. i.e.

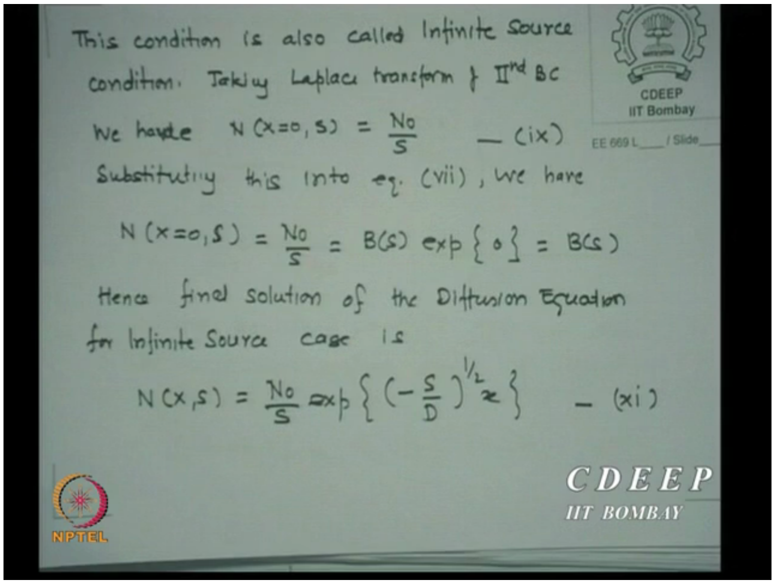
$$N(x=0, t) = N_0 u(t) \quad - (viii)$$

The first of course initial condition I already showed, a step function of source I have introduced. The second is I say at the surface the concentration is fixed, that is what I said, is N0, solid solubility limit. That is the number which is available at x is equal to 0. If you are not very satisfied, say x is 0 plus because at the surface we do not know outside, but just below surface you can say or at the surface we say the concentration is N0.

If I know this boundary condition, x is Nx, so we can see. From below that, we do not know, in the silicon there is no concentration. x minus, there is no concentration. But just at x is equal to

0, it becomes N0. Now this essentially means Nx0 at all times, your impurity source are coming anyway, all times is N0 ut. Is that correct? It is a step function. So if this is my second boundary or rather first boundary condition, that at x is equal to 0, concentration is N0 ut. Why this ut has to be done? Because step, so I have to because in Laplace transform it will give something. What will it give? What is Laplace transform, N0 ut? N0 by S. So we have to take care of that ut term, constant by S. ut is only giving me that constancy.

(Refer Slide Time: 65:44)



This condition is also called Infinite Source condition. Taking Laplace transform of IInd BC

We have $N(x=0, s) = \frac{No}{s}$ — (ix)

Substituting this into eq. (vii), we have

$$N(x=0, s) = \frac{No}{s} = B(s)\exp\{0\} = B(s)$$

Hence final solution of the Diffusion Equation for Infinite Source case is

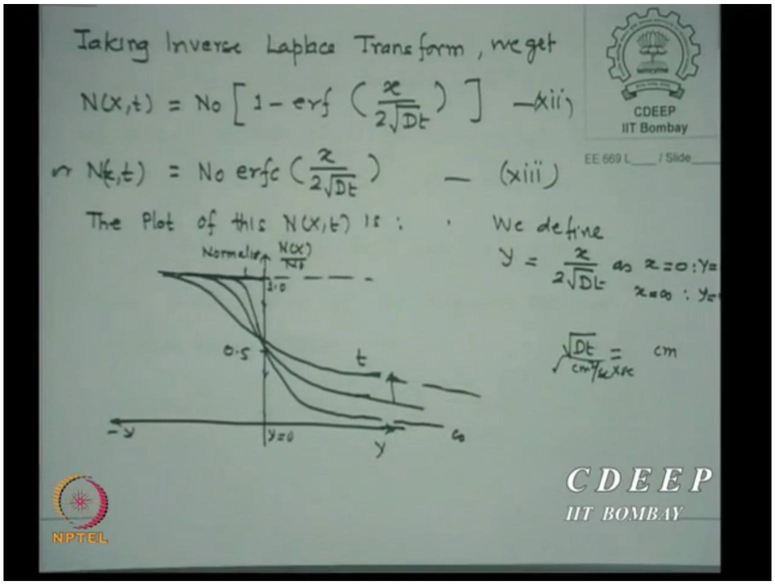
$$N(x, s) = \frac{No}{s}\exp\left\{\left(-\frac{s}{D}\right)^{1/2} x\right\} \quad \text{— (xi)}$$

This condition is also, the kind of boundary condition initially when I used is also called infinite source condition or constant source condition. If you have a constant source, so we have Nx0 S is N0 by S taking Laplace transform the second boundary condition, rather first boundary condition. So we write Nx0 S is N0 by S equal to BS exponential 0. x is equal to 0, so exponential 0, so we get BS is equal to N0 by S. Is that correct? Second boundary condition, first boundary condition removed AS.

The first boundary condition give me the BS is equal to N0 by S. This is just substitution of x is equal to 0 in the equation. And therefore the infinite source or a constant source case, the solution of diffusion equation is NxS is N0 by S, exponential under root of minus S by D times x. This is the solution of diffusion inside silicon when starts with constant source at x0, constantly N0. This is the equation you get for it. Is that okay, solution? So now I have the diffusion equations solving done for profile, this is my profile which, this is in what this, this is explained and I want to come back to time frame.

So what should I do? Take inverse Laplace transform of this, kay hoga? Anyway it is not so easy for you and you have not seen that function, so do not try unless you have done a course somewhere or done something.

(Refer Slide Time: 67:42)



Taking Inverse Laplace Transform, we get

$$N(x,t) = N_0 \left[1 - \text{erf}\left(\frac{x}{2\sqrt{Dt}}\right) \right] \quad \text{—(xii)}$$

or $$N(x,t) = N_0 \, \text{erfc}\left(\frac{x}{2\sqrt{Dt}}\right) \quad \text{— (xiii)}$$

The Plot of this N(x,t) is :

We define

$$y = \frac{x}{2\sqrt{Dt}} \quad \text{as } x = 0 : y = \quad x = \infty : y =$$

$$\underset{\text{cm}^2/\text{sec} \times \text{sec}}{\sqrt{Dt}} = \text{cm}$$

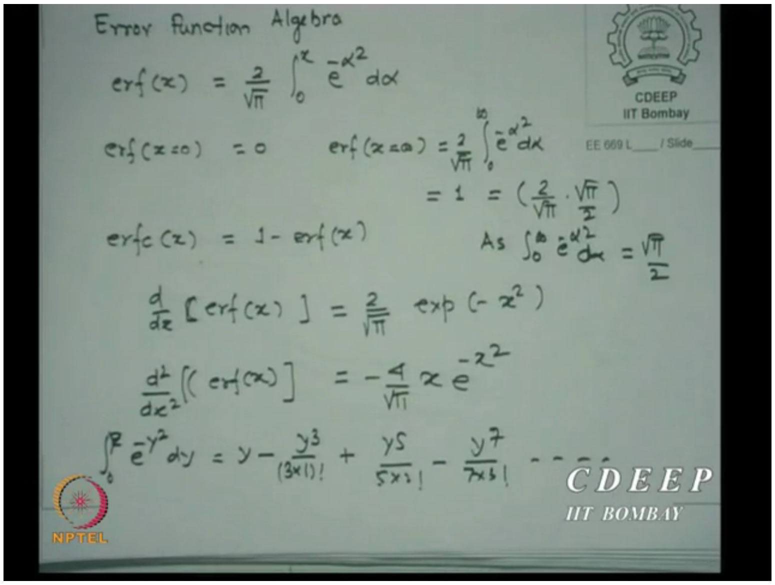
Taking inverse Laplace transform, Nxt is N01 minus error function of x upon 2 root Dt. That is very important. I will explain the error function soon quickly before we leave. Can anyone tell me what is the unit of this? D is always defined as centimeter square per second. Is that correct? Into time, under root of that means it is centimeter if everything is, so Dt is, root Dt is essentially distance, is that correct? Root Dt is essentially a distance, we will see D is a function of temperature T, some temperature dependence.

So what does that mean? If Dt term which is temperature dependent and time dependent, so for a given temperature for a given time, I have fixed root Dt, 2 root Dt. Is that clear? So now I know where the impurities are going for this time and temperature at every x. Is that point clear? D is fixed for a given temperature, T I have fixed, okay I will do 1 hour diffusion, so I know the time. Please remember everywhere we do seconds, so 1 hour yaani 3600 seconds. Is that okay to you?

So please 3600, do not mischief 1 there. So if I plot this function, normally Nx0 by N0 versus y, y I define x by 2 root Dt, I define y to plot, nothing this. So if I say between plus y and minus y, this is symmetric function. It is initial value is this, and as time proceeds, and at where it will all go finally? Infinite. It will go to 0 and infinite. Some way this has reached to 1, actually it is isotropic, it should reach to 1 isotropically. Now this function is called error function. Now for those last slide for the day, this is please note down this.

Some data about error functions. And since I am going to use this constant source diffusion very often, I first want to give little expression for error function because those will be used directly by me in my solving the actual profile evaluations. Is that okay? Everyone, noted down? Those who wish to, everyone does not but those who wish to.

(Refer Slide Time: 70:31)



Error function Algebra

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-\alpha^2} d\alpha$$

$$\mathrm{erf}(x=0) = 0 \qquad \mathrm{erf}(x=\infty) = \frac{2}{\sqrt{\pi}} \int_0^\infty e^{-\alpha^2} d\alpha$$

$$= 1 = \left(\frac{2}{\sqrt{\pi}} \cdot \frac{\sqrt{\pi}}{2}\right)$$

$$\mathrm{erfc}(x) = 1 - \mathrm{erf}(x) \qquad \text{As } \int_0^\infty e^{-\alpha^2} d\alpha = \frac{\sqrt{\pi}}{2}$$

$$\frac{d}{dx}[\mathrm{erf}(x)] = \frac{2}{\sqrt{\pi}} \exp(-x^2)$$

$$\frac{d^2}{dx^2}[\mathrm{erf}(x)] = -\frac{4}{\sqrt{\pi}} x e^{-x^2}$$

$$\int_0^z e^{-y^2} dy = y - \frac{y^3}{(3\times1)!} + \frac{y^5}{5\times2!} - \frac{y^7}{7\times3!} - - - -$$

Error function x is, has a definition in maths, 2 upon root pi, it is an integral 0, 2 upon root pi, 0 to x, e to the power minus alpha square. Alpha is any other parameter, variable. So you can write y, you can write z, any parameter. So e to the power minus alpha square d alpha. This is the definition of error function, plots I have already shown you. If you see this integral which is shown bottom, please see the last line, 0 to z, e minus y square dy.

If I expand them in series, it will be y minus y cube by 3 into 1 factorial, y5, plus. 5 into 3 factorial minus y to the power 7, 7 into 3 factorial and so on and so forth. So this series is essentially e to the power minus y square dy, 0 to z, whichever it is. I should not say z, I should say y only. So this expression is a series but I know this is the expression I need and this is 2 upon root pi, 0 to x, e to the power, this is called error function. Error function at 0, you can take from me. When it is 0, all ys are 0, so what is the sum? 0.

So one can say error function 0 is 0. You say from the series, everyone has x term, so x, 0, 0, 0, 0, 0, 0, everywhere 0. So error function x is equal to 0 is always 0. Error function x equal to infinite is very important. 2 upon root pi, 0 to infinite, e to the power minus alpha square d alpha, now this integral 0 to infinity e to the power minus alpha square d alpha, mathematically can be derived as for series some of this is root pi by 2, is root, this is a slightly diverging series and difficult to sum up. But 1 minus t kind of equivalence can be done and you can sum it up.

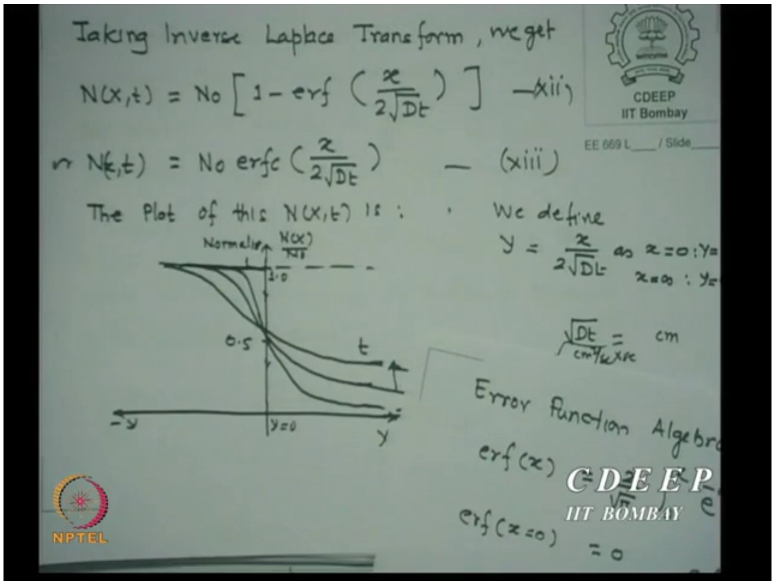
So it gives you root pi by 2. 0 to infinite, e to the power minus alpha square d alpha is root pi by 2. So if I put here this 2 by root pi into root pi by 2, means exponential, sorry error function infinity is 1. And that graph was shown to the 1, it will go to the 1 always, maximum.

Okay, there is few more terms. We actually our profile which we are going to get is 1 minus error functions and that is called since 1 is the infinite part, so you subtract rest is compliment to that. So complimentary error function, erscx, this is remember, error, infinity minus error function x, error function infinity is 1, this term. So 1 minus error function x, is called complimentary error. You can think like this, in integral 0 to x, x to infinity. So that is essentially doing the same job.

If I differentiate error function, it is 2 upon root pi, exponential minus x, this is the most important differential really because it is essentially, which is this term coming? Exponential minus x square kya define karata hein? It is a normalized x as of now. We have defined, it is a Gaussian profile. So aap error function se Gaussian mein jayenge, that is what exactly we are going to see this in the next time. Similarly if I take second order differential, then error function as x is, iska differential karo. Minus 4 upon pi, x e to the power minus 2 x square.

These are the error function terms which you note down because I will be assuming that you know error function algebra, so we substitute whenever any differential second order, first order comes or infinite 0 comes. We can just substitute there as it is. Is that okay?

(Refer Slide Time: 75:08)



Taking Inverse Laplace Transform, we get

$$N(x,t) = N_0 \left[1 - \mathrm{erf}\left(\frac{x}{2\sqrt{Dt}} \right) \right] \quad \text{— (xii)}$$

or

$$N(x,t) = N_0 \, \mathrm{erfc}\left(\frac{x}{2\sqrt{Dt}} \right) \quad \text{— (xiii)}$$

The Plot of this N(x,t) is :

We define

$y = \frac{x}{2\sqrt{Dt}}$ as $x = 0 : Y =$

$x = \infty : Y =$

$\sqrt{Dt} = $ cm

$\sqrt{\mathrm{cm}^2/\mathrm{sec} \times \mathrm{sec}}$

Error function Algebr

$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int e$

$\mathrm{erf}(x=0) = 0$

So we have found from our diffusion equation before we quit that Nxt is N0, complimentary error function of x upon 2 root Dt. This is the diffusion profile which I got, for which case? Which is the case I discussed today? Constant source or infinite source whichever book we are using, some use infinite source, some use constant source. This will give always complimentary error function profiles.