Introduction to Semiconductor Devices
Dr Naresh Kumar Emani
Department of Electrical Engineering
Indian Institute of Technology – Hyderabad

Lecture - 05
Covalent Bonds and Inter-Atomic Interactions in Silicon

This document is intended to accompany the lecture videos of the course "Introduction to Semiconductor Devices" offered by Dr. Naresh Emani on the NPTEL platform. It has been our effort to remove ambiguities and make the document readable. However, there may be some inadvertent errors. The reader is advised to refer to the original lecture video if he/she needs any clarification.

How the matter is arranged? So, matter comes in you know, predominately 3 forms. You could think of it like. So, essentially you can have a perfect regular arrangement of silicon atoms, which we will call as crystalline state in which the inter-atomic distances are exactly fixed. So, you can have this perfect regular order which is perfect order, this is basically important. We call it as crystalline state.

In another state, you could have a situation where there is no order. Basically, there is no long range order we say. Basically, I mean there is not even short range order here actually. So, the atoms are randomly distributed and this is called as amorphous state. And then we have a third state, which we will call as poly-crystalline state wherein you have small domains.

So, these domains you know, in each pattern, domain having short range order that means the relation between atoms is fixed that the distances are fixed perfectly, then makes a short range.

You have a shortage domain, but then if you go to long ranges, there is no order. They are all randomly aligned. So, that is called as poly-crystalline and it is consisting of many, many small crystals. So, this is a poly-crystalline state.

And it makes a big difference whether you know, material is in which state. So, for example, silicon that we use in our electronic devices is always in the crystalline state. We like the crystalline state most. Sometimes, we use poly-crystalline silicon, but that we will talk about later, but, we like crystalline state, so much so, that it is a very, very highly pure form of silicon.

Now, we will take in our electronic devices silicon which is 99.9999 times basically pure. This is a percentage of purity. If you look at 1 billion atoms, there might be 1 single impurity in that that is the level of perfect purity we use for an electronic devices. So, if I have this state, but how are they arranged that makes a big difference. If you look at silicon, it forms what is known as a diamond lattice.

A diamond lattice is simply represented here. So, you have a cube and in the cube, you have silicon atoms which are present. For example, you have 8 silicon atoms at the corners here. So, in the corners of the cube, you have 8 silicon atoms and then you have 6 silicon atoms at the centre of the face. The cube has 6 faces side, top bottom and so on. So, you have 6 faces.

In the centre of each of those faces, you have a silicon atom and then there are 4 atoms which are in the interior in the diagonals, along the diagonals of the unit cell. This particular thing is called as a unit cell and this length is basically called as lattice constant which is equal to 5.43 Armstrong as given here. So, this is a lattice constant. So, this is how silicon atoms are arranged in a crystal. So, this makes a big difference for us.

And one important point you should note is that every silicon atom is actually connected to 4 nearest neighbours, think about it. If you look at 1 silicon atom here, it is connected to 4 atoms. And this atom also is connected to 4 atoms. The ones which are in the corners, they are also connected to 4 atoms, but from the neighbouring unit cells, you know one already you know, there is one connection here.

And then there is one connection here, one connection here, there will be another from the neighbouring atom, neighbouring unit cell. So, that will have 4 connections. So, there are 4,

exactly 4 nearest neighbours for each silicon atom. And you could actually compute, you know, what is the density of silicon here. It is not very difficult. I will put it in the homework, but basically, it turns out that the density of atoms in silicon is about 5×10^{22} atoms/cm^3.

I want you to keep this in the back of your mind. This is a very important number, because when we talk of doping in silicon, we have to use this as the reference. So basically, it tells you that if you have 1 cm^3 of silicon, it has 10^{22} atoms. It is a very, very large number of atoms. And this is going to play some role. And finally, the electronic properties are going to depend on what is the face of silicon.

For example, if you have a crystal, what we said is you have this unit cell which is actually having these atoms and now, if you take a bulk piece of silicon, it is essentially consisting of these unit cells, which are arranged in this form in 3 dimensions. So basically, this exact unit cell will repeat many, many millions and millions of times that is essentially a crystal. So, you have exactly the same distances.

It is like you know, you build a Lego block or something like essentially that. So, this unit cells are built you know in 3 dimensions. So, it becomes important, what is the arrangement of atoms in the top of silicon. You know, if you take a top surface of the silicon, bulk silicon, it becomes important. For example, it is the arrangement of atoms in this fashion wherein you have 5 you know, 4 atoms in the corners and then centre, one atom.

Is that the orientation? Or is it the orientation this way along the diagonal? You have many, many more atoms along the diagonals. So it becomes important and there is a lot of, you know, in the textbooks, if you look at it, they will talk of what is known as Miller indices to denote what is the crystal orientation? And I really think that that is not really that important for us. So I just not going to talk about it much. It is there in your textbooks.

If you are interested, you can actually do a little bit more of studying, but I do not think it is that important for the purposes of this course. It is something that you can study. So, essentially, this Miller indices define and we are not going to get into that. But what we would like to understand is, how does this, how do you think of energy levels when there are atoms close to each other like this?

When you have a silicon which has 4 atoms close to it, how do you think about the energy levels? That is something we need to understand.

(Refer Slide Time: 06:38)
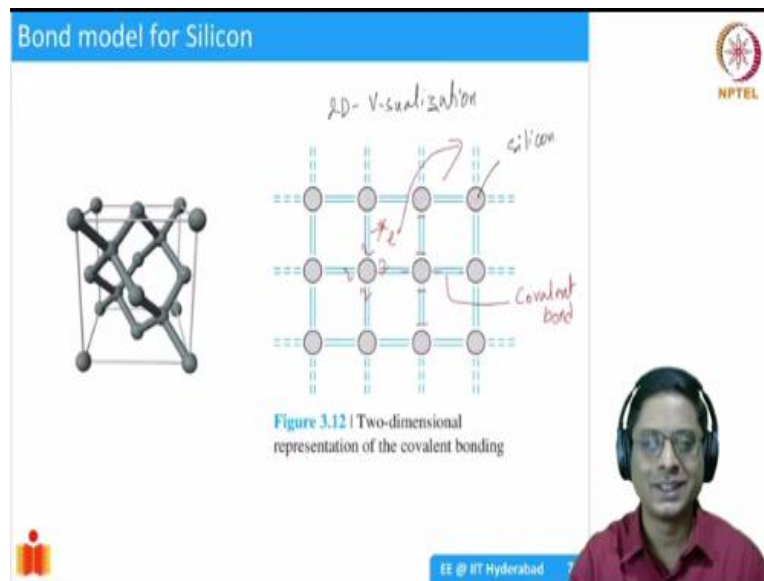
And to do that will actually not simplify because it is not very easy for us to think of this diamond lattice all the timeline. It is somewhat complicated. So, what we do is we represent, you know, this is basically a 2 dimensional visualisation. this is not really the accurate picture. So, if you want to accurately think about each silicon atom is connected in 3 dimensions like tetrahedral, the corners of a tetrahedron as silicon atoms, so the centre is what you have.

So, it is difficult to think about it. So, what we will do is we will see present in a 2D picture like this. So, what we are doing here is each of this is basically a silicon atom. And it is connected to 4 silicon atoms. For example, this you know, if you take this silicon atom, it is connected to 1, 2, 3 and 4, 4 silicon atoms on the 4 sides. So, this is again, it is sort of a representation of what is happening.

And what did we see? We saw that silicon atom has in the outermost shell 4 electrons, there are 8 available states, but 4 electrons and that is not really a stable form. We know from our basic chemistry that the atom always tries to have the fully filled shell that is a more stable form that is the Neon is, Argon is you know very, very stable. So, silicon also tries to get 8 electrons in the outermost shell. How does it achieve that?

So, if we want to represent I can maybe represent like, you know, I can put a minus here to denote electron, there are 4 electrons in this silicon, but it has 8 states. How does it get 4 more

electrons? Well, it shares with the neighbour. So, this guy has a 4 electrons. This guy has one, this has one electron, one electron, one electron. So, these 4 electrons from the neighbours are shared and they form a covalent bond.

And the covalent bond is represented in this picture by this lines. These lines are representing your covalent bond. So, once this covalent bond happens, because of the sharing, you see that each atom of silicon has 8 electrons. For example, if you count here, there are 2 lines here, there are 2 lines here, 2 lines here, 2 lines here. So, each atom of silicon has 8 electrons.
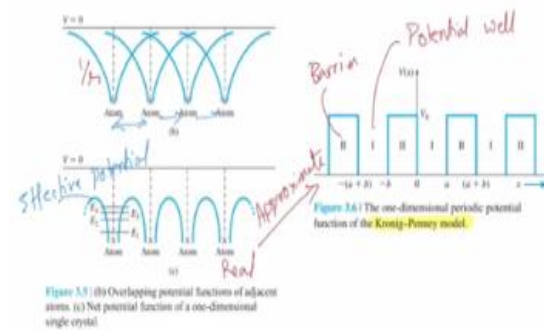
So, it is in a stable situation, stable configuration. So, this is a simple 2D visualisation, it is not exact picture. Exact picture here to talk about the diamond lattice. But for us, you know, later on, we will try to remove one silicon and put something else that we call us doping. And then what happens if you actually break one of these bonds. Because you know, this, let us say this bond is broken, what does it mean?

The bond breaks that means your electron can go somewhere else. It is not bound to the lattice, but it can freely move about. So, this is again an important thing, we will talk about it in the next lecture. But for now, let us complete the understanding of how to get energy bands. So now, we understood individual silicon atoms. We said that, there is this discrete energy levels which are formed and then you can call it 1 s, 2 s and so on and all that. That is fine.

But what happens when I bring 2 silicon atoms close to each other? Is it the same thing? It turns out that well.

(Refer Slide Time: 09:59)

Figure 3.6 | The one-dimensional periodic potential function of the Kronig-Penny model.

Figure 3.5 | (b) Overlapping potential functions of adjacent atoms. (c) Net potential function of a one-dimensional single crystal.

It is not that simple, but before I get into those details, I would like to tell you how a silicon lattice can be represented. So, we already saw this you know, when we said that each silicon atom has the potential of the form 1/ r. So, this is 1/ r and then you have silicon atoms which are arranged in a arrangement, some arrangement. Basically it could be some distances depending on the face of the you know, which face we are talking about, they will be different arrangements.

But in effect, we have a perfect order this distances are known to you. So, you have these atoms, each of which is essentially a potential well and all of them are essentially next to each other. When you have such a scenario, what happens is, these are very strong potentials, but then because of the interactions, the effective you know potential becomes like this, effective potential due to silicon atoms, neighbouring silicon atoms you have this.

So, this is sort of, you know, similar to basically a series of potential wells. For example, here this region II basically is a barrier. Region I is basically a potential well. So, what we are saying is, of course, you know, this is the real situation, real how the petition will look like. But if you want to solve this, it is going to be very, very tedious and you have to do it using a computer, you cannot do it manually.

So, we approximate this real potential using basically a series of barriers and wells. And this, we call as Kronig Penny model. So, you see the beauty. So, we know how to solve a finite potential well. And now, simply this is a series of potential well that is all. We have to solve for this. If you are able to solve for this, we can predict how electron moves in a crystal.

So, even though seemingly complicated $1/r$ dependence with you know, millions of atoms that kind of trend get reduced to this. So, again, this is solved in your textbook, but I do not think, it is essential for you to right now look at how the problem is solved, will just tell you the conclusions of what it is, what happens after the Kronig Penny model, but I will try to give you an intuitive picture in the next 5 minutes or so.

So, for the purpose, I would like to get to understand how the origin is happening. You should be intuitively convinced about what we are doing. That is all I want you to do. You do not have to remember these things. But you just have to be clear how the thought is going from infinite potential to finite potential one. And then a series of potential wells that is the flow of thought here.

So, now we have the series of potential wells. But how do we understand what happens in the series of potential wells?

(Refer Slide Time: 12:54)

To do that, maybe, we will take a simple scenario. Consider a finite potential well, I am only showing you this, this is a finite potential well, with, let us say, some depth. It is not important for right now. And I am only showing you one particular state, you know, it can have many, many states, but I am showing the ground state in the first state. So, you saw that you know, the potential basically has some sort of a, you know, you will have maximum probability of finding an electron in the well.

But then there is some small leakage of wave function into the barrier regions. This is what we saw. Let us call this wave function as Ψ_a. This is for one potential well. And now, let us think of another potential well, another atom essentially, which is at some distance away from this. So, let us call this as Ψ_b. It has a wave function also. And because we are talking about the same atom in the same environment, you know, if they are far apart, like when this you know, distance is large,.

Let us call this distance as d. When d is large, few microns, let us take it I mean, there is no harm. When d is large, it should be that Ψ_a should be equal to Ψ_b. There is nothing else like. I mean, it has to be you know, similar potential similar you know, everything. So, it has to be a similar way function. So, that means what is the energy if you want to call as E 1, energy of the first potential well and then E 1, let us put superscript a.

Just to denote that it is energy level of the first well and then you have energy level, E 1 of the second one. What will be the energies? What will the relation between these 2 energies? Well, because they are very, very far apart, these energies are going to be equal.

$$E_1^a = E_1^b$$

So, we will call this as basically degenerate energy levels. Now, if you have 3 potential wells, what happens?

Well, you will have 3 degenerate levels. If you have 4 potential wells, if you have a, you will have 4 degenerate levels. And if you have n potential wells, implies you have an n degenerate energy levels. Well, I am only showing you one particular state E 1 that is you can have similar things like E 2, E 3 and so on. Each of these energy levels will be n-fold degeneration. We will have a n-fold degeneration that is a term we use technically, alright. So far, so good.

But what happens if I start reducing the distance d, then I reduce the distance d, you know then d reduces, there is interaction of wave functions. Is not it? Because these are finite potential wells, there is some penetration of the wave function into the barrier region. And then, as you bring these 2 things closer, there will be more and more interaction. So, what happens because of that?

Well, to understand that we have to think about what is, you know what is the most important thing in the practical world, the probability of finding an electron is important. So, since we

said, this is the Ψ_a. So, Ψ_a has a probability of $|\Psi_a|^2$. Will minus Ψ_a satisfy? If I consider minus Ψ_a, will it satisfy the Schrodinger equation? Of course it will.

So, what happens is, when you start having this 2 potential wells, the overall wave function is going to be a superposition of individual wave functions. There will be a linear combination of wave function. So, I will say, my overall wave function Ψ is going to be $C_1\Psi_a+C_2\Psi_b$. This is a linear combination of wave functions. Now, what can happen is, you can have a situation where both these wave functions are positive.

So, I can have a situation where this is you know, I will say this is positive and this is positive that is one solution that is allowed. You can also have a situation where this is positive and this is negative. You can have other combinations as well, right now, let us just stick to these 2 states. So, when you have these 2 combinations, you will have wave functions, which turn out to be in the form that is shown the green one, we will call it as symmetric wave function.

And this is additional detail, I mean, it is not really necessary for you right now, but anti symmetric wave function. So, as the d reduces, the probability, if your d is large, the probability you know, let me call it Ψ_{sym} and Ψ_{anti}. Let us call it these 2 functions, the shapes are different right. When d is large, the probability of $|\Psi_{sym}|^2$ like I mean, the probability of finding an electron in this way, is equal to $|\Psi_{anti}|^2$. There is no difference when d is large.

But when you have the distance reducing, then they will start interacting. The probability will slightly with different, because of which, you will have 2 energy levels, which are having a small difference in energy. So, this, I am running out of space here. So, I will just show the energy levels here. I will call this as ΔE. So, what we are saying is, as d reduces, ΔE increases.

There is more and more difference you know, as you bring the wave functions closer, there is more interaction, because of which the probability $|\Psi_{sym}|^2$ is not equal to $|\Psi_{anti}|^2$. So, I can say, the energy levels as basically ΔE is basically E anti symmetric minus E symmetric. So, as d reduces, ΔE increases. This is what physically you would expect it to happen.

So, one level essentially has become 2 non-degenerate levels. So, in the first situation, let me try to add a page here.

(Refer Slide Time: 20:07)
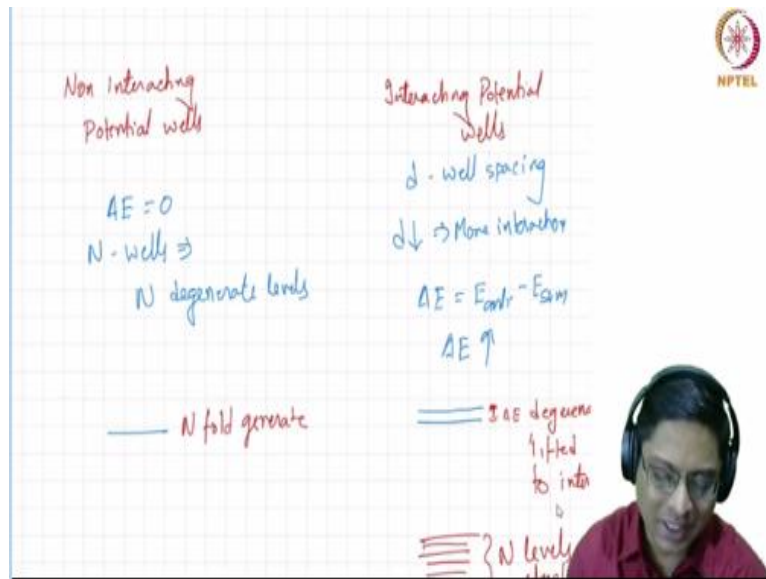
So, in the first situation, you had independent or you know non-interacting that is a better work out, non-interacting potential wells. When you have non-interacting potential wells, you have basically ΔE is equal to 0. I mean, there is no difference in energies. So, basically you have, if you have N potential wells. N potential wells, N wells imply N degenerate levels.

So, basically the energies are all same. They have the same energy level. But if you have interacting potential wells, then if your interaction is strong, the interaction is basically given by what is d the distance the well spacing. If your well spacing d reduces that is more in, implies more interaction, more interaction. If interaction is more, then ΔE which is simply E anti symmetric minus E symmetric is going to increase.

ΔE is going to increase that means, instead of having you know, in this case, you had single energy levels. In this case, you will end up getting sorry I should actually draw it on the same line. There are 2 levels basically. This is a level energy n- fold degenerate. This case would see that energy levels are very small lifting of degeneracy. This is your ΔE due to basically, now you do not have degeneracy basically.

Degeneracy lifted due to interactions. So, what happens if you have n atoms or n potential wells which are coming close to which you will have. In the non-interacting case, you have N-fold degeneracy, but in the interacting case, you will end up getting N levels closely spaced. That is what happens. So, know, it is okay. If you are you know, I am sure that you will not understand it fully in the first time, please revisit it.

And if you have any questions, you know, we will try to have a interaction one to one. Please schedule a interaction whenever the course is running in July. So, we will discuss it in greater detail. So, do not be confused, if you do not be upset if you are not understanding in the first time. I am actually taking a little bit more of giving you, a little bit more of details to actually feel the intuitive picture.

So, well, it takes you some time to understand; maybe when the first offering of the course, it will not be clear, but later if you if you see, if you do research in electronic devices later on and you come back, I am sure you will find this you know very, very important. So, let us come back.

(Refer Slide Time: 23:50)
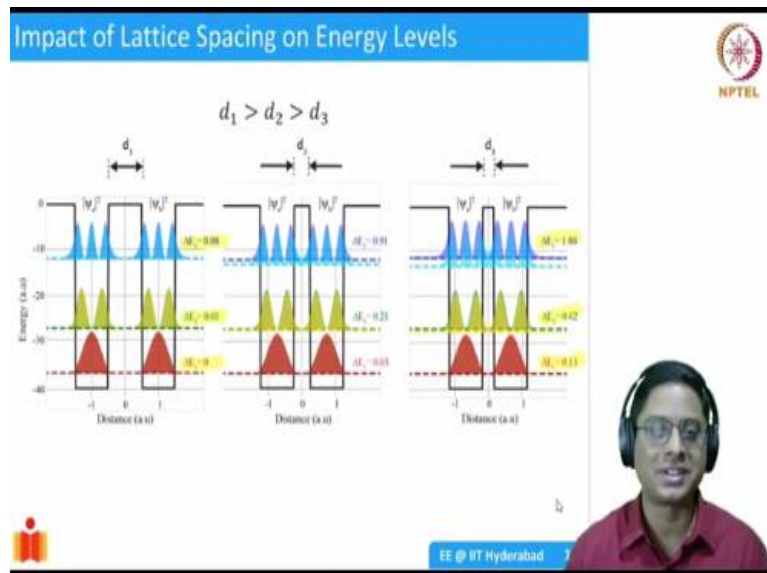
So, this is essentially you know, that is the intuitive picture of what is happening. I just you know, find one more step ahead and then actually we will calculate these things using the software and we are showing the results. So, when your d is large, we said that now there are 2 wells and the probabilities are looking like this.

As you decrease it, you will see that the energy levels are actually having small gaps. So, this is represented by ΔE here. So, in the lowest energy level, it was zero. The second level, it is 0.01 very, very small gap difference in energies and here it is 0.08. But the moment you actually make it very close to each other, you see that there is significant amount of splitting between the levels.

This is just you know, I mean, just if you are curious, you know, it is just an additional thing, but it actually happens. It is not just you know, hand waving, it actually happens if you calculate it fully, numerically, accurately. You will see this okay.