Introduction to Semiconductor Devices
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Lecture - 06
Energy Band Formation

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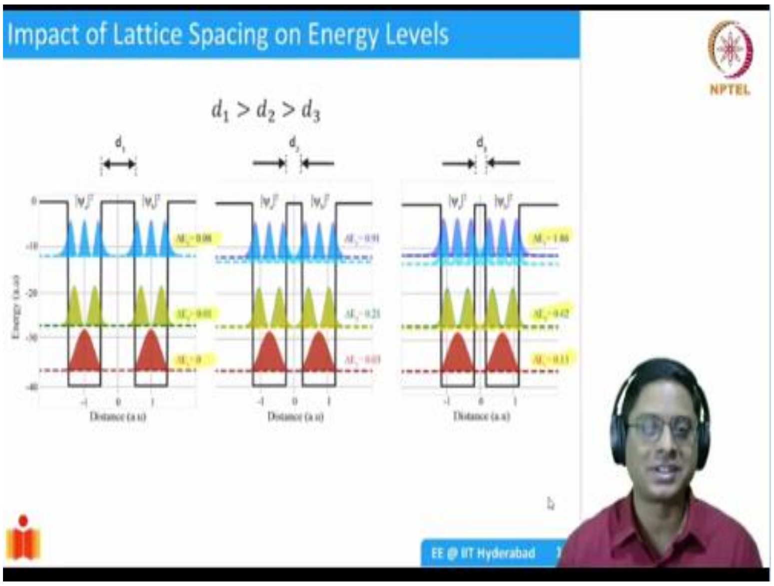

Impact of Lattice Spacing on Energy Levels

$d_1 > d_2 > d_3$

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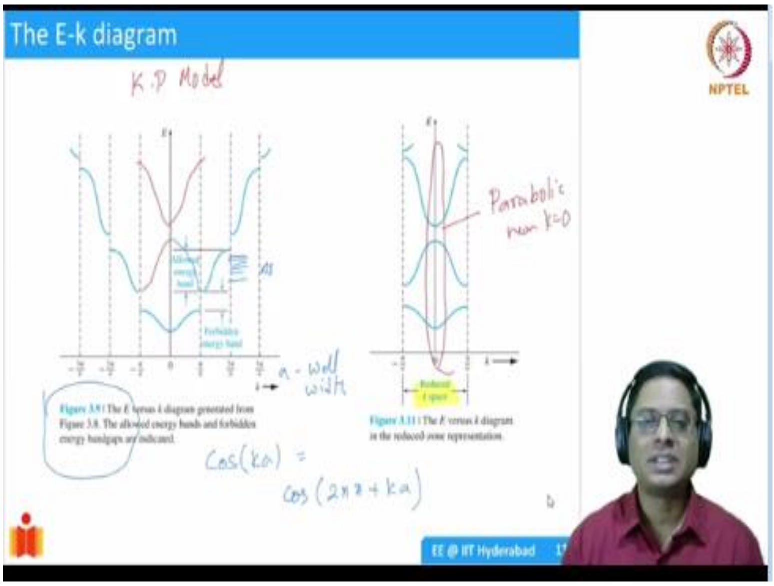

The E-k diagram

K.P Model

Figure 3.9 | The E versus k diagram generated from Figure 3.8. The allowed energy bands and forbidden energy bandgaps are indicated.

Figure 3.11 | The E versus k diagram in the reduced-zone representation.

$\cos(ka) = \cos(2n\pi + ka)$

So, now how does this still help us? Again, we have to come back to know what it is. The reason it helps us is if you do all that. And now I am going to again tell you the end of the story, I am telling you the conclusion of the story without telling you how the thing is solved. Remember this Kronig Penny model. When you have the K P model, Kronig Penny model, we had the series of potential wells.

I will say now, it can be solved. When I say that, it essentially I mean, it involves a lot of mathematics. So, we want to, do not want to do it. So, it can be solved. And if you solve it, you will start seeing that you know, you have corresponding to, you saw that in the previous case, corresponding to each level, you have 2 levels. The ΔE was there. Now, if you have N levels, what you will start seeing is you will have N levels which are allowed.

Again, there is a gap. Again, there will be N levels, which are allowed, alright. So, if you plot the energy versus k relation for this Kronig Penny model, you will start seeing that it is sort of behaves in a similar way to the traditional you know, parabolic dispersion that sort of shape is there overall. But, in addition to that, what you see is that you have some first band of energies which are allowed.

So, when they are allowed, you have the blue curve right here. You have this allowed bands and forbidden bands. So, in between, there are some solutions, which are not allowed that means you cannot have an electron having that particular energy. So, that is it turns out that it comes out to be this. So, because you have N levels and basically each of this is consisting of very, very, very small levels.

And all of them essentially, the gap is so small that you can consider them to be a band of continuous levels that difference ΔE is going to be you know, negligible in the physical case. So, again, there is one more small thing I just want you to, you know, in some sort of, you know, accept it. So, the solution here has a form, you know, a function, which is basically $\cos(ka)$ well. This is from the textbook, you know.

Whenever I show you the figures, with this caption here, like in this form, caption is written, It is from the textbook, I am just, you know, it is from Donald Neamen’s textbook, you please, you can go back and refer to that particular figure, and then you can read a little bit more, that is why I just want to leave those figure captions in the place. When I do not provide any references, you know, whenever I take it directly from the textbook, I am not providing references.

But you know, the caption should tell you that you can go back and look in even if you want to understand the details. So, this has, you know, the textbook, in the class I have used; in the lecture, I have used l as a width of the well; in the textbook, they use a. So, basically a is a well width that is why it is coming like this, but essentially the same thing as you know, we use l. So, it turns out that they have a dependence of $\cos(ka)$

And we know that this is equal to $cos(2n\pi + ka)$ That means, if I put, you know, +2π and -2π if I add and subtract, it is not going to change. So, what happens is this dispersion, you know, it becomes complicated for us to just draw it all the time. So, what we do is, we take this particular location, you know, this branch, this is allowed state. So, and this is you know, 2π here, this is a peak.

I will shift it by 2π basically. If I shifted by 2π, this, I can push it to like this and this guy, I can shift it by 2π. So, if I do that, I will get another branch like this. And similarly, this one, I can shift it and I can bring it to close this one. And this is again shifted going to like this. So, in effect, because if you shift this, it is not going to change the energies. So, we can actually represent in a simple way in what they call as reduced k space as this space.

So, basically, you have series of bands like this, each of them is parabolic. So, this is, if you look at around 0, they are all parabolic. If you go to higher case, this is parabolic near k equal to 0. So, what is happening is, you have this series of allowed bands and you know forbidden regions and this particular diagram is called as E-k relation. I promise you this is the summary of it.

Even if you do not understand the entire process, it is okay right now. What I want you to take away is you can represent the allowed energies in a semiconductor using this E-k relations. In the next class, I will again talk a little bit more about E-k relations, but we will use that to identify what is direct and what is indirect semiconductor. We will do it in the next class.

For now, I just want you to accept or you know understand that basically, if you had a free electron, it had a parabolic dispersion. And then if you had a confined electron, you had discrete levels. But the moment you get multiple atoms interacting with each other, then you get this small you know, bands of energies which are allowed and bands which are forbidden.

So, you have this range of energies which are allowed and that can be represented as in E-k relation. So, there are 2 forms of band diagrams. One is what we call as a Fourier space, E-k and the other one is what I will discuss now, you know, in the physical space.

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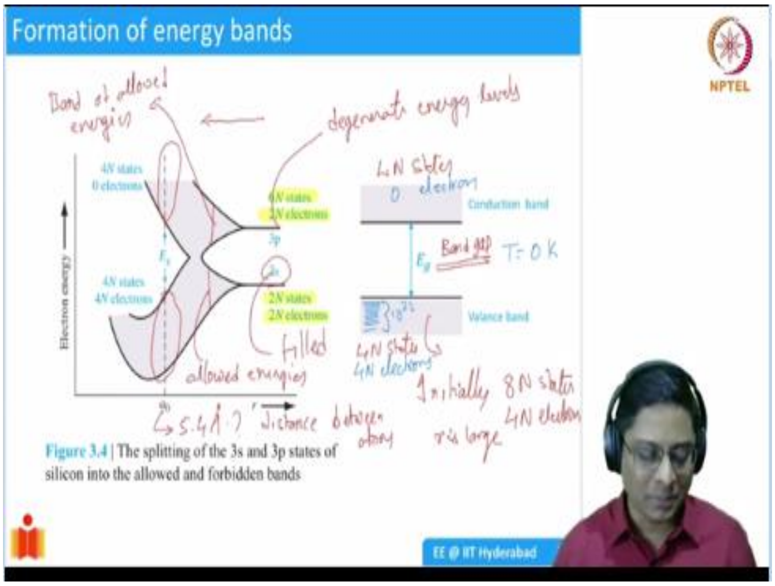

Formation of energy bands

Figure 3.4 | The splitting of the 3s and 3p states of silicon into the allowed and forbidden bands

So, we refer to each, I mean any of them you know, we can use refer to either of them depending on a convenience. So, this is a very, very important picture. And I think if you understand this, you understand how the bands are forming. So, this is basically a graph showing you how the you know distance between you know atoms r. This is basically distance between atoms. This is distance between atoms.

If the distance between atoms is large, what happens to energies? Well, we are not really interested in the core electrons you know, 1s, 2s electrons, 2p electrons, we do not care. We are interested in the 3s because a valence is what; I said will contribute to the electronic properties. So, what are the valence orbital? We have 3s and 3p. So, we see that 3s has how many states available ?

So, each atom has 2 3s states. And if you have N atoms, you will have 2 N states. Each of the atoms has 2 states and you have N atoms, so, 2 N states. And we saw that the 3s states was fully filled. So, you have 2 N electrons, which are there in those states. So, basically, this is completely filled. The 3s is filled. What happens to 3p? We saw that the 3p energy level is higher than 3s.

And you had, how many states, 6 states. Each atom will have 6 states, because you know, there is 3 fold degeneracy. Each of them can take 2 electrons. So, there are 2s, 2 electrons states available. So, 6 N states are available, but only 2 N electrons because each of those 3p has only 2 electrons. So, totally it has 2 N electrons. This is what happens when the atoms are far apart.

Now, as you bring the atoms close, what happens? As you bring the atoms closer, as you reduce r, in this case, all the states are actually degenerate, like, right, states are degenerate. I will call it degenerate states, degenerate energy levels. Because all of them have the same energy, because the interactions are not there. It is very, very; atoms are very, very far apart, the interactions are not there. So, there is degeneracy.

But the moment you start reducing the distance between the atoms or, between the atoms, you start you saw that as you bring them, potential wells moves closer and closer, there is a lifting of degeneracy. And there is a small gap that is appearing ΔE. So, because of that, what happens here is as you bring the atoms closer, you will see that there is this energy levels of forming a band., this is a band of energies, band of, well, band of allowed energies.

Similarly, for the 3s states, you have allowed energies alright. So, this continues when you get to the exact lattice constant. This is the lattice constant. For silicon, it was I think 5.4 something. We just check it out 5.4 Angstroms, 443 maybe. So, you have the lattice constant when you exactly get to that point which is the more stable you know that is why silicon lattice is stable.

In the energy, total energy is minimised that is why stable lattice points. So, when the lattice is stable, then you have basically 2 branches. The energy levels have interacted and they have split into 2 branches. One is the bottom branch,, which we call as a valence band and the top branch which we call as the conduction band. So, that is what I have shown here.

Basically, this branch is basically represented here and this branch is represented here. The energies are exactly, I just took the line. So, what you see is that how many states are there in this branch? Initially, they were 2N states here and 6N states here. So, initially, there were 8N states. Initially, 8N states are there out of which 4N are filled, 4N electron are there that was the initial condition when you know, r was large r is large.

At this point, it is like that but as you brought the atoms closer, this band split up into 4N states in the upper; here you have 4N states and here you have 4N states. You have a band of energy allowed in the lower valence band and upper one is called conduction band. Now, which of them is filled up? Total number of electrons was 4N electrons. So, all of them will be filled up in the; all of them go into the 4N electron are here.

So, the valence band is completely filled up whereas the conduction band has 0 electrons. We have 4 N states available but no electrons in them. Of course, just remember this is at T equal to 0 Kelvin. I will talk about what happens when the temperature changes tomorrow or in the next lecture. So, what you see is that because of this interaction, bands are forming; bands of energy levels.

So, if you look at these bands closely, it will be like very, very; you know, how many atoms are there in a silicon lattice? We said for every cm^3, there are 10^{22} atoms. So, there will be 10^{22} levels here. Each of them is so close to each other. So, it is like you know that ΔE will be like$10^{-18}, 10^{-19}$ something like that. So, it is negligible for our purposes. So, we call it a band.

But physically, there is still some energy you know, small differences, but that is insignificant that is beyond negligible, I do not know what you can call it. So, you have this valence band and conduction band. So, valence band is completely filled up with electrons; conduction band is completely empty. And separating the two is basically what we call as band gap. This is your band gap, Eg.

So, this is where we can, in principle, start I mean, you know, you can talk, start talking about semiconductors from here, you know, you can say that, there are this valence band, a conduction band and you can go forward from there. And you will understand the rest of the material quite well. But I wanted to give you a very strong intuitive foundation. This is probably you know, what is not typically done in a traditional curriculum.

I have taken a very non-traditional route. I have done a little bit more detail than what I would do it.

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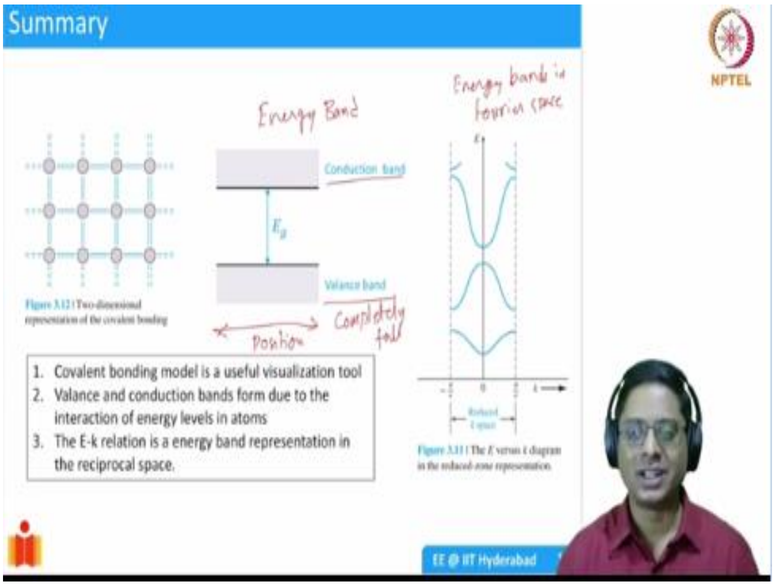

Summary

Figure 3.12 | Two-dimensional representation of the covalent bonding

1. Covalent bonding model is a useful visualization tool
2. Valance and conduction bands form due to the interaction of energy levels in atoms
3. The E-k relation is a energy band representation in the reciprocal space.

Figure 3.11 | The E versus k diagram in the reduced-zone representation

But I think, it is essential to have a strong foundation, at least you need to be aware of where the physical origin is. So, I did this. So, in summary, what we did in today's lecture now. From all that I want you to remember 3 things. If you remember these 3 things, you will fine for the next lecture. What are those? The first step is: as I want you to go and review the covalent bonding model; I said this visualisation 2 dimension visualisation. So, go back and review what this is; this is what. It is a very useful thing.

And in the next lecture, I will start talking about you know, what happens, you know, if you remove one silicon atom and put something else there. So, essentially what we said was, each of these grey areas represent a silicon atom. And each of the lines represents a covalent bond. So, each silicon atom is connected to 4 silicon atoms in the, you know, it has 4 nearest neighbours and it has 4 electrons.

So, because of the covalent bond, it basically shares 4 electrons with the neighbours and then formed a stable you know, it fills up the valence shell. Because of it, it forms a stable compound which we can use. So, this is what is the 2 dimension visualisation. I want you to go back and review it if it is still unclear to you. And the second thing, I want you to remember is: we had all this discretization which are coming in and then you have this bands forming.

Finally, in silicon, you have basically, the most important thing is a valence shell, we do not have to worry about the core electrons; in the valence shell, when the electrons interact, you end up getting a valence band and a conduction band. This is the valence band and the conduction band. This is completely full. You cannot add more electrons, especially at 0 Kelvin. And conduction band is completely empty.

And then there is an energy gap between the two., this is the energy band representation. Energy bands. This, I mean, this is basically in some sense position. I did not mention it, because, I mean, it is not easy to put a dot. But later, we will start drawing band diagrams wherein we will draw energy bands as a function of position. That is one thing. And you can also represent energy bands in the Fourier space. Energy bands in Fourier space.

I am sure, this will not be that clear to you at this point of time, but unfortunately, you would have to do, if you know a little bit of Fourier transforms, you will understand that you know, there is an analogue, you know, if you take the signals course, you would have seen that time and then frequency or Fourier variable, I mean, you can look at Fourier transform from time to frequency and frequency to time. You can do that.

Similarly, between space, you can do from X to k and k to X. It is a kind of Fourier transform pair. This is called as spatial frequency. k is called as spatial frequency sometimes. Anyway, so, you can have energy bands in the k space and they are called as E-k diagrams. These are useful for identifying what is a direct and indirect band gap semiconductor. For that purpose, I use it next time after that.

You know, we do not really use it much except for a couple of occasions where we talk about the mobility and things like that effective mass and things like that. We will talk but I just want you to accept that there is a E-k relation. The E-k relation is essentially the dispersion you know, I also called dispersion. The free electron had parabolic dispersion.

Whereas, if you have a you know, bands, it takes a little bit more complicated shape because there is discretization and each of those discrete levels are actually forming bands because of interactions and all of that can be represented in the form that is shown in the graph on the right here. So, we will again study it in a little bit detail. It is not possible if I want to go, we have to go in a lot of depth, which is not necessary for this course at this level.

But I just want you to be aware that there is these two types of band diagrams; one is as a position of x, other one is as a position for your E-k basically, the Fourier space. So, these 3 things, if you remember from today's lecture and understand them, you will be ready to go for the next lectures. Alright. With that, I would like to stop. Thank you very much for your attention. We will meet again in the next lecture. See you then, bye.