

Introduction to Semiconductor Devices
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Lecture - 04
3D Potential Well Model of Atom and Bohr's Model

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.

Hello, everyone, welcome back to Introduction to Semiconductor Devices. This is lecture 2 of week 1.

(Refer Slide Time: 00:17)

The slide titled "Recap - Quantum Confinement" illustrates the transition from a free electron to a confined one. On the left, a parabolic energy dispersion $E(k) = \frac{\hbar^2 k^2}{2m}$ is shown. In the center, two potential wells are compared: an "Infinite Potential Well" with discrete energy levels E_1, E_2, E_3, E_4 and corresponding wave functions, and a "Finite Potential Well" with a lower barrier height V_0 and discrete energy levels E_1, E_2, E_3, E_4 that are lower than those of the infinite well. On the right, a diagram shows a potential well of height V_0 and width L with a transmission probability $T(E, V_0, L)$ for $E < V_0$. The NPTEL logo is in the top right, and the presenter's video feed is in the bottom right.

In the last lecture, we understood the basic properties of semiconductors. We said how the conductivity is different in various semiconductors. And then we said that to understand the reasons why the conductivity is in that way, we have to understand a little bit of quantum mechanics. Then; we discussed about a free electron you know how the dispersion is in, parabolic shape and then if you confine an electron to a small dimension, for example, a potential well of dimension L .

Then you see, you saw that the energies are no longer continuous but they are discrete, you know. For example, energies are you know E_1, E_2 and so on. So, only these discrete states are allowed and corresponding to each of those states, you have a wave function. A wave

function is simply, you know it tells you the mod of $|\psi_s|^2$ will give you the probability of finding an electron.

So, you see that for various energy levels or energy states, you have different probability distributions of finding an electron. And then we said that an infinite potential well while it is a very simple problem to solve analytically, it may not be the accurate representation. So, we wanted to understand how a finite potential well behaves. And then, while it is possible to solve a finite potential well analytically, we did not do that, because it becomes a little bit more tedious than what is required in this course.

So, what we said was, we did this, we solve this problem using a numerical approach. And then, if you have a situation where the potential well has a depth V_0 ; this is the depth of the potential and we saw that there are these wave functions which look similar to the infinite case with some changes. And the important thing was that the wave functions are now penetrating into the barrier regions, especially the higher energy wave functions.

For example, this is a 6-wave function and that has significant amount of penetration into the barrier region. And this is not expected in the classical terms. The reason is, if you take a, let us say a cricket ball and throw it at a wall, would you expect the ball to go to the other side of the wall, you would not right, because the energy of the ball is very small, the barrier is very strong. But if you, do it with a great force, then it might actually break the wall. But that is an extreme situation.

A similar situation happens even in the microscopic scale. And I will just briefly mention a problem which is very you know similar to potential well which is basically a problem of a potential barrier. So, you could think of a potential barrier where you know you have a barrier of height V_0 in the region 0 to L and then everywhere the potential is basically 0. If a particle is incident on this, what happens?

So, if your particle has an energy E and if the energy is greater than V_0 , it simply goes, no problem. But if the energy is less than V_0 , classical mechanics tells us that there is no probability of finding the electron on the other side or particle on the other side, this is if you know, if you look at transmission probability. What is it? For example, if I have 100 particles

incident on the barrier from the left side, how many of them will actually get transmitted to the other side? That is the transmission probability.

So classical mechanics senses that you do not have any probability of finding the particles on the other side, but then quantum mechanically, there is a finite transmission probability. And you could actually solve it and get an expression. There is some function of E and then V_0 and then the size L and so on, you could get a function, but it is not important for us this moment.

But later on, we will actually come back to it when we discuss MOSFET and discuss how current flows through the gate oxide of a MOSFET. This finite transmission probability becomes important and we will actually discuss it in a greater depth there. But in any case, I would actually give you a problem in the homework, wherein I will try to ask you to compute a few transmission probabilities. So, this barrier case as well.

It is not difficult, you know, you have an equation and you will be able to do it very simply. Just try that in the homework. So now let us get back to what we were discussing.

(Refer Slide Time: 04:26)

The slide is titled "Atom as a 3D Potential Well" and features a list of bullet points on the left and a diagram of a potential well on the right. The diagram shows a potential well with a central nucleus and energy levels E_1, E_2, E_3 . The potential is labeled $V(r) \propto \frac{1}{r}$ and the well depth is $V=0$. The diagram also shows quantum numbers $l = 0, 1, 2, \dots$ and $m = -l, \dots, 0, \dots, l$. The NPTEL logo is in the top right corner, and a video feed of a speaker is in the bottom right corner.

- Electrons orbiting atoms experience a spherically symmetric potential well with $1/r$ dependence on radius
- The depth of potential is finite
- Radial confinement is captured by the quantum number n
- Additional quantum numbers l and m are introduced to capture the azimuthal and polar symmetries
- $l = 0, 1, 2, \dots$ and $m = -l, \dots, 0, \dots, l$

You know, this potential well, the 1D potential well looks like a toy problem, right? It is quite simple to solve. How does it help us? That is a question that must be in your minds right now. But I would argue that this is a simple problem, but it actually captures quite a lot of essential features of what happens in atoms. If you think about an atom, an atom is simply consisting of a nucleus and electrons which are orbiting the nucleus.

So, there is a columbic attraction between the electrons and nucleus. So, if you had a charge q , how much is a potential around the charge? You could calculate it. We could have done it in electrostatics, if you simply put, the potential is going to be proportional to q by r . So, all around the nucleus, you have a potential of the form $1/r$. And what is this potential doing? It is essentially causing the electron to be confined near the nucleus.

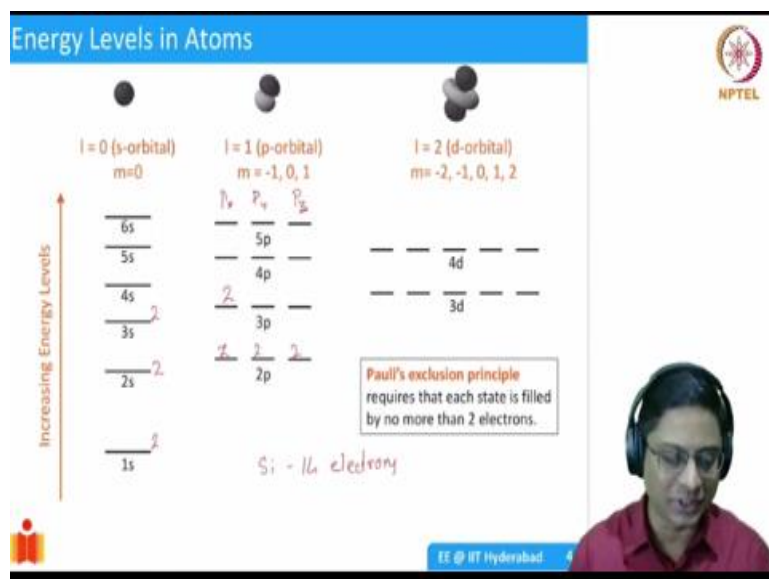
So, what is the dimension of an atom? It will be maybe, let us take it to be 1 or 2 angstroms; 1, 2 angstroms. The lattice constants are usually 3 to 4 or 5 angstroms. So, the size of the atom is smaller than that. So this potential, $1/r$ potential, which is surrounding the nucleus is causing your electrons to be confined in this region. So, what happens in that scenario? Well, in the 1D case, we saw that there is this discretization happening.

In a 3D case also, something similar happens, because now the potential is different; the potential well is actually a 3-dimensional potential well, so you have, you know, all the r directions, the radial directions, you have this potential well, which causes the energy to be discretized. And you have this quantum numbers, you know, n equal to 1, 2, 3, and so on, right?

Similar thing happens and you have energy levels, E_1 , E_2 , E_3 , and so on, which are actually occurring within the potential well. This can actually be calculated analytically, but it becomes a little bit tedious. And we do not want to do that for this. For the purposes of this course, it is enough you know, if you understand this sort of quantization happens. Well, it is not that simple, because we have one more step. We have a 3-dimensional potential when compared to 1 dimension.

So, we have additional quantum numbers. n is one quantum number which we have already seen. Now, the other quantum numbers we have introduced, which are called as l and m . These are initial quantum numbers that come in because of the symmetry in the azimuthal direction and in the polar direction. And there is going to be some variations of probabilities. Well, actually, you know, I am sure all of you have seen this in a different form already.

(Refer Slide Time: 06:58)



When you studied electronic configurations in your plus 2, you would have seen that there is this s orbital, p orbital and d orbital. Well, those are essentially probability distributions in space. And that can be exactly calculated by the technique I just described. I mean, if you go through the math, you would actually get these shapes, you know, in the 1D case, you saw that the probability was varying as a function of x .

In a 3D case the probability will vary as a function of x , y and z . So, we have this quantum number n , which is actually capturing the confinement in the radial direction, because of which you have 1, 2, 3 and so on, states and the quantum number l can have 0, 1, 2 and so on. When l is equal to 0 essentially, you would have understood this as s orbital which means that you have probabilities uniform in spherical direction.

In all directions, the probability of finding a particle is uniform. Whereas, if you put l equal to 1 and solve that, you will see that the probability has this dumbbell shape which you would have studied as p orbital. And what is more? You know, whenever you have l equal to 1 and n can take 3 values, you know, it can go from -1 to +1. So, in this case, it will go as -1, 0 and 1.

And these are the 3 levels, quantum numbers which are allowed, which result in 3 energy levels at the same energy, I mean, there are 3 levels at the same energy. We call as degeneracy. So, you have this you know, p_x , p_y and p_z . These are essentially energy levels, you know we have the same energy, but then there are 3 distinct levels and we call them as degenerate levels.

Similarly, if you go to l equal to 2, we have a d orbital, which is again having m from -2 to +2. So, there are 5 degenerate levels in the case of d orbital and because of that, you have these energy levels which you get. For example, you know s, you have 1s, 2s, 3s and so on and p, you have 2p, 3p and so on. And d, you have 3d, 4d and so on. And the corresponding energy levels are drawn to scale in this picture.

And so, in your chemistry class or, in the plus 2 level, they will tell you to actually say that we remember the electronic configuration, right 1s, 2s, 2p, 3p, 4s and so on. You just remember the sequence. The reason that sequence comes about is because of the energy, the way the energies are distributed. And we already know from Pauli's exclusion principle that each of these energy level cannot be occupied by more than 2 electrons.

Most you have 2 electrons, right? If you have no electrons or one electron or 2 electrons like most right. So, how does this help us? Well, if you think of silicon, take an example of silicon. Silicon has an atomic number of 14. That means it has 14 electrons. How are these electrons distributed? Well, we start filling the states from the bottom, because the bottom most levels have the highest probability of being filled.

So, you can assign 2 electrons in the 1s state, 2 electrons in the 2s state and then there are 3 of these 2 p states that 3-fold degeneracy. So, you can assign 2 electrons to each of this. And then so we have filled up 10 electrons and you have 4 more. So, you will fill 2 in the 3s state and then 2 in the 3p state. So, this is how electrons are distributed. And this has very profound implications on how the energy bands form that is why I just wanted to review this.

(Refer Slide Time: 10:27)

Bohr Model Representation of Silicon

Figure 3.4 | Schematic of an isolated silicon atom

- Electronic configuration $[\text{Ne}] 3s^2 3p^2$
- Valance Shell – 8 available states, 4 filled
- Core electrons (1s, 2s, 2p) are tightly held by nucleus and do not contribute to conduction

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So, what you see is, you could also think about it in the Bohr's picture right, you know, in a Bohr's model kind of representation, you could think about it. So, this is how it looks like. The previous case was the energy level representation. This is a physical representation. So, what you see is that in a silicon atom, you have the nucleus which has these you know, protons, which are you know, in the nucleus, so +14 charges.

And you have first shell consisting of 1s. First shell means, n equal to 1, so 1s, it has 2 electrons. And the second shell is consisting of 2 s and 2 p, which has again, in total 8 electrons, because 2s is 2 and then 2p has in total 6 electrons. So, 8 electrons in this. And then you have the third shell, which is n equal to 2 where you have s and p orbitals. The s orbitals are filled up 2 of them, but the p orbitals have 6 allowed states. This is important. This makes a big difference.

So, they have 6 allowed levels in the p orbital, because we have 3 px, 3 py, 3 pz and out of which there are only 2 of them, which are filled up. So, what is the total number of available states in the outermost shell? It is basically having 3s and 3p. So, this has 2+6, total 8 available states. 8 states are available; out of which 4 are filled. So, this is very important.


And we actually give this you know, special name, we call the outermost shell as a valence shell. To just emphasise that, you know, the spelling is, I think is wrong here. But anyway, valence shell, which is basically having 8 states and 4 are filled. So, it is exactly half filled. And the inner shells, the n equal to 1 and n equal to 2 shells are really very close to the nucleus and they do not play much role.

So, they are not really that important. So, we call this as a core. This entire thing inside, we call this as a core. This does not really play much role in the electronic properties. But the outermost shell creates a huge amount of difference. So, but you know, this is still a single atom. And you are almost never going to look at atoms individually.


You are going to look at collections of atoms. So, how does, how do we understand collections of atoms? To do that, we have to understand a little bit more.

(Refer Slide Time: 12:49)

Lattice structure of Silicon



(a) Crystalline (b) Amorphous (c) Polycrystalline



- Diamond lattice – 4 nearest neighbors for each Si
- Lattice constant 5.43 \AA ($5 \times 10^{-10} \text{ cm}$)
- Density $5 \times 10^{22} \text{ atoms/cm}^3$
- Miller indices define crystal orientation

Source: Solid State Electronic Devices, Streetman and Banerjee (Top)
<http://www.ece.utexas.edu/~mqs/ee360/> (Bottom)

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