Solid State Devices

Dr. S. Karmalkar
Department of Electronics and Communication Engineering
Indian Institute of Technology, Madras

Lecture - 6

Equilibrium Carrier Concentration (Contd…)

Today is the 6th lecture of this course and the 4th lecture on the topic of Equilibrium Carrier Concentration. What we did in the last class was we tried to give a qualitative model for this particular data we had shown in the beginning of the discussion on this topic.

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Solid State Devices

Lecture - 6

Equilibrium Carrier Concentration

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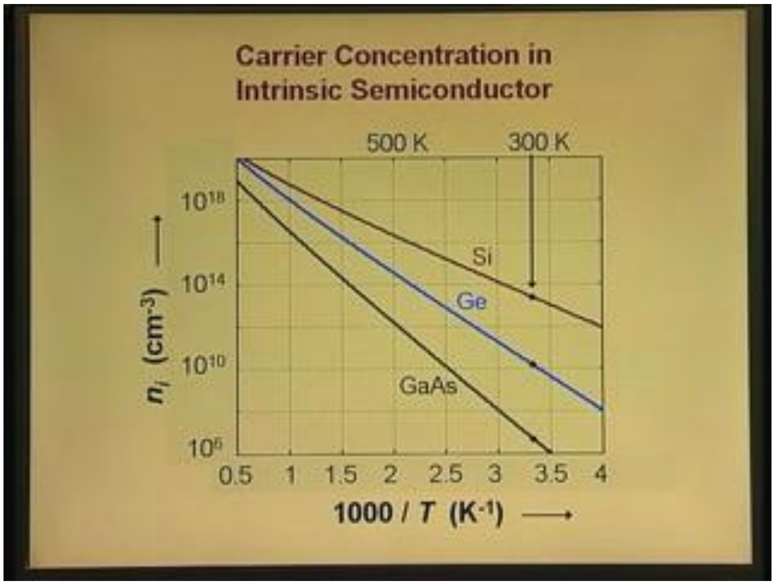

Carrier Concentration in Intrinsic Semiconductor

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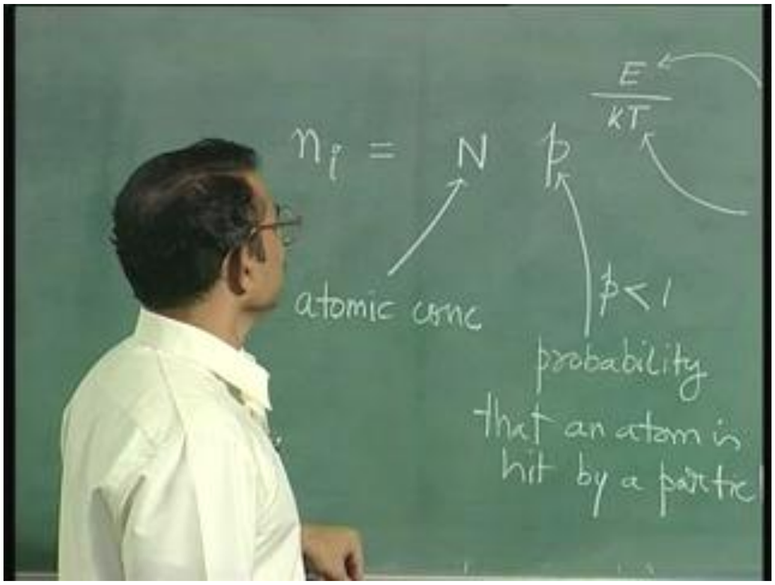

What we did yesterday can be written in the form of an equation:
n_i is equal to Np to the power E by kT where 'N' is the atomic concentration in silicon, 'p' is the probability that an atom is hit by a particle, 'E' is the bond strength and 'kT' is the average energy of the particle at temperature 'T' under equilibrium conditions. So E by kT represents the number of particles that must converge onto an atom so as to provide energy E equal to bond strength. So the entire discussion that we did can be summarized in the form of this equation. Here the probability p is lesser than 1, so if we were to write this equation using 1 by p here so that we get a quantity is greater than 1 then we can correlate this equation very well to the behavior that we have shown.

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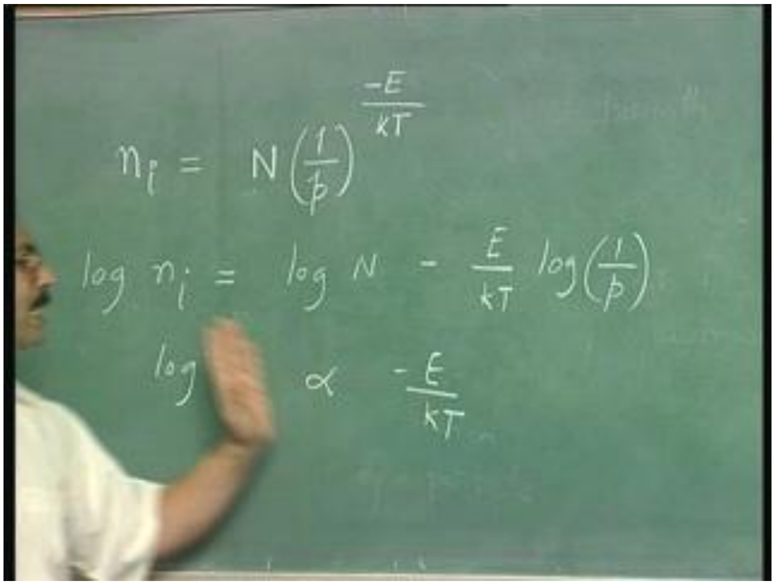

$$n_i = N\left(\frac{1}{p}\right)^{\frac{-E}{kT}}$$

$$\log n_i = \log N - \frac{E}{kT}\log\left(\frac{1}{p}\right)$$

$$\log \quad \alpha \quad -\frac{E}{kT}$$

So the same thing written in terms of 1 by P would look something like this. Now it is very clear that if I take the log of n_i, I will get $_{ni}$ is equal to log N minus E by kT log (1 by p), here 1 by p is greater than 1 so log of this quantity would be positive. So, according to this log n_i α minus E by kT. Therefore if you plot n_i on a log scale and (1 by T) a reciprocal of temperature on the other axis that is the x axis so log n_i is plotted on the y axis and 1 by temperature is plotted on the x axis then I will get a straight line. This is exactly what this slide shows.

Here the differences between the straight lines associated with silicon, germanium, and gallium arsenide can readily be associated with the changes in E for these three materials where E is the bond strength E 1.1eV for silicon, for gallium arsenide it is 1.42 eVs and so on. Thus the qualitative model is quite good in predicting the behavior. The problem here is that we do not really know what this p is? We have no way of calculating p in the model. What we can get is a broad behavior.

We cannot make accurate calculations but we can definitely show or rather we have shown using this model that n_i on a log scale varies as reciprocal of temperature and the behavior is linear when we plot log n_i v_s 1 by T which is not a small achievement at all. To get a more accurate description where we can make calculations at any temperature we must go to the Band Model which is the topic of discussion today.

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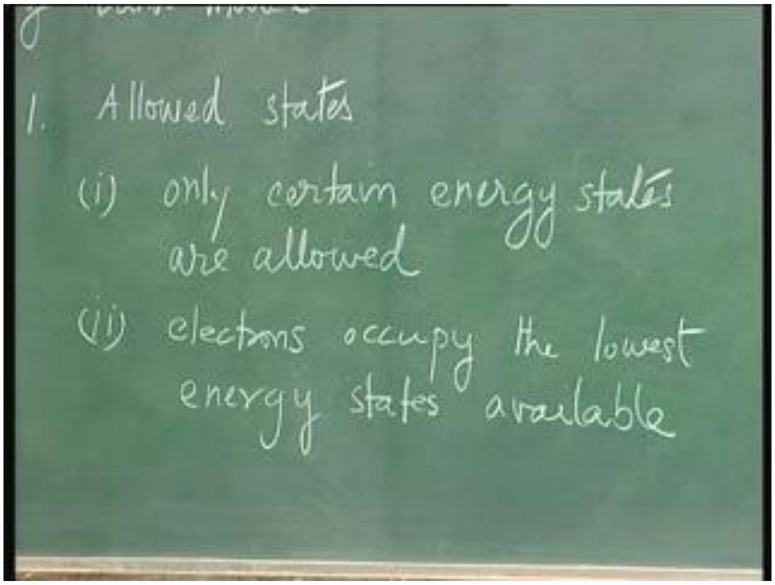

1. Allowed states

(i) only certain energy states are allowed

(ii) electrons occupy the lowest energy states available

Actually the band model means the energy band model. Many times the word energy is dropped. The energy band model tries to analyze the electron population in terms of the energies possessed by electrons. So more specifically what we are trying to do in this is, to see how the electrons are distributed over a range of energies at any given temperature. If we have some way of finding out this distribution then we can very easily separate that part of this electron population which is free and that part which is bound at any temperature.

The basic tenets of this model are three: The first one refers to the allowed energy states for electrons. Electrons are only allowed certain energy states. They are not allowed all energy states. This is the first important principle of quantum mechanics. Secondly, of the allowed states the electrons always tend to occupy the ones with lowest energy which are available. Electrons occupy the lowest energy states available.

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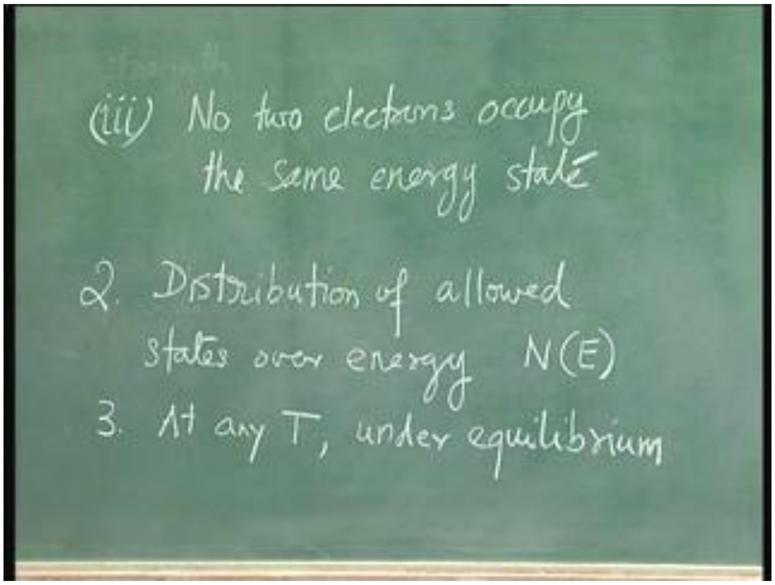

(iii) No two electrons occupy
the same energy state

2. Distribution of allowed
states over energy N(E)

3. At any T, under equilibrium

Third is the policy exclusion principle, it says that no two electrons can occupy the same energy state. This is the first important tenet of this energy band model, the allowed energy states. Next is, how many states are there and how these allowed states are distributed over energy?

Distribution of allowed states over energy:

This distribution is represented using a function N(E) which means N is a function of E. This is to say that all the states which are available for electrons to occupy are not necessarily distributed uniformly over energy. So we will have to see what is the exact distribution, what is the function in N(E).

Now the third and the last important tenet has to do with what fraction of the allowed states are occupied at any temperature, the fraction of states that are occupied at any temperature and energy. So electrons will not occupy all the states, only a fraction of the states will be occupied which obviously means the allowed states are very large in number much larger than the number of electrons so that is why the question arises as how are these states occupied?

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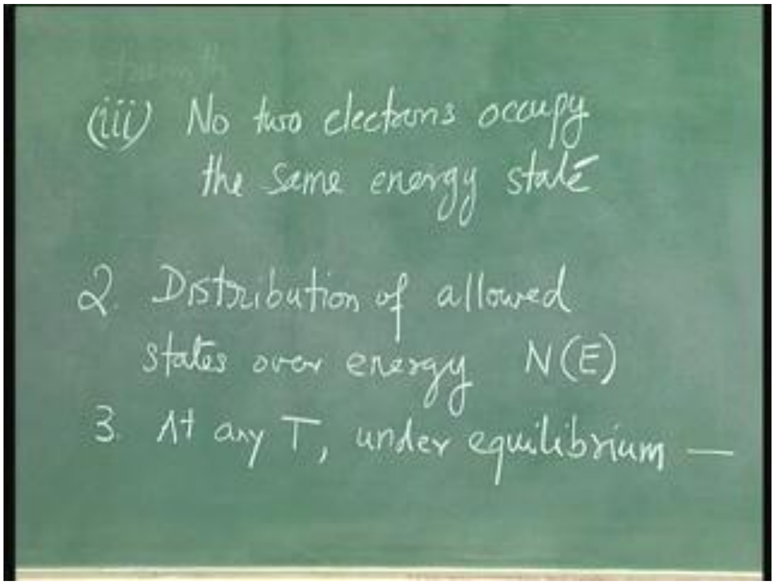

(iii) No two electrons occupy
the same energy state

2. Distribution of allowed
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3. At any T, under equilibrium —

Only a fraction of allowed states are occupied. This fraction is written as F(E,T). This fraction is a function of energy and function of temperature. This is normally called the Fermi-Dirac function. This function is derived from statistical mechanics. While the function N(E) the distribution of allowed states over energy is obtained from quantum mechanics and the first principle of allowed states also is a statement of quantum mechanics the last tenet or statement is related to statistical mechanics. The energy band model combines results from statistical mechanics and quantum mechanics and tries to put them together in a cogent coherent form.

Now let us take up each of these three tenets one by one. What are the allowed states for electrons in a crystal? What is the distribution of these allowed states over energy? What is the fraction of these states that are occupied?

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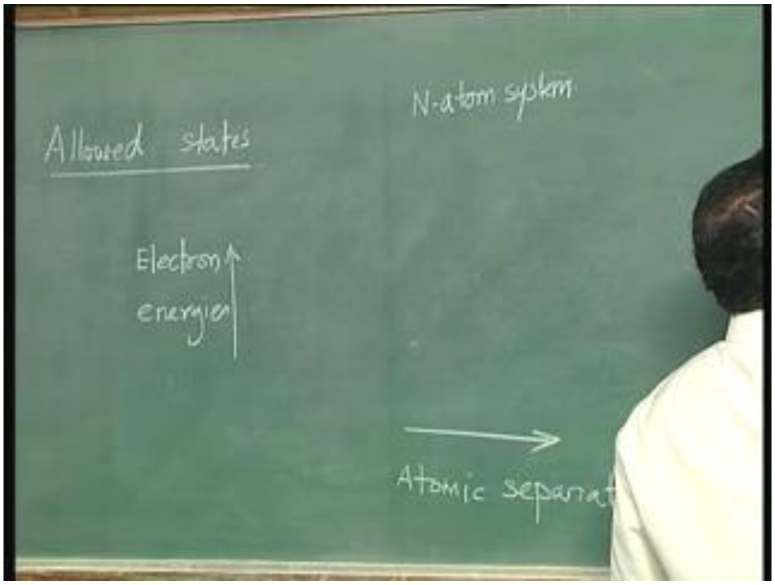

What are the allowed states? If we start with the picture associated with an isolated atom we will take silicon as an example. In isolated silicon atom what are the allowed energy states? Then you put together n atoms all regularly arranged and then you start reducing the inter atomic distance between the n atoms and bring it down to the distance that we have in the crystal. That is the way you try to see how the allowed energy states picture from an isolated atom progressively gets modified and then we get the picture for electrons in a crystal.

So, if you were to follow this approach, if I were to sketch on a diagram like this where the x-axis denotes atomic separation and y-axis denotes available energies or electron energies how will this picture look like? Let me build up this picture, we are trying to plot it for an n atom system where all n atoms are regularly arranged. You start with a very large or infinite separation. When the separation is infinite each atom is isolated, although it is still an n atom system but still in effect one atom is isolated from the other atom. Therefore we are starting with the picture for isolated atom at this right extreme. You know that silicon’s atomic number is 14.

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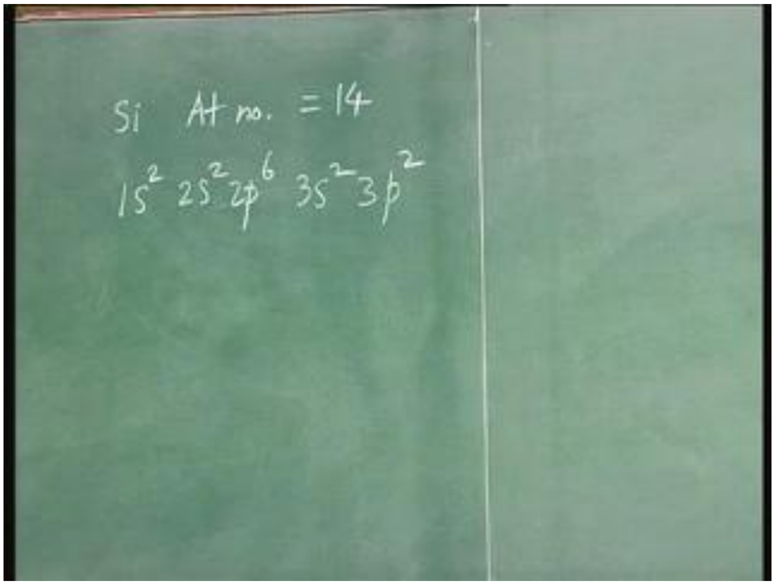

The distribution of these 14 electrons is written as 1S square 2S square 2p to the power 6 3S square 3p square in terms of the various orbital. Now you plot energies corresponding to this. So 1S square that is the energy of electron very close to the one S orbital is very close to the atom and progressively these correspond to energy states of electrons away from the atom. In this particular diagram the lower energies will correspond to electrons close to the atom and the higher energies will correspond to electrons away from the atom. If I were to show this it would look something like this for an isolated atom. We are not taking an n atom system you take an isolated atom then it would be something like this.

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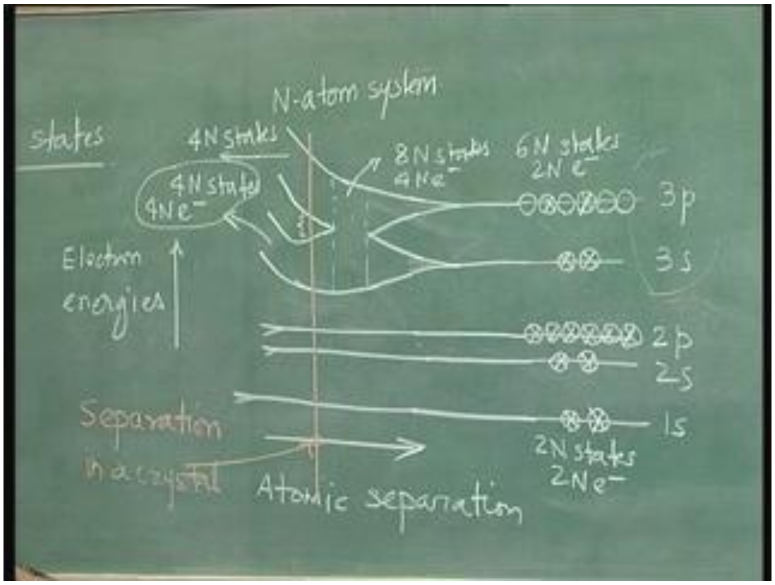

The highest is 3p, then below that you have 3s, then you have 2p, and 1s. Here I must mention that in this diagram the distance between various energies is not necessarily to scale. So 1s there are 2 available states, if you strictly use the polis athruzen principle, those two states of 1S orbital should be shown separately.

Similarly, for example if you take this 2p orbital there are 6 states and all the 6 states should be shown separately. But then if you do that the diagram becomes complicated so we use some simplification. What we assume is that, for simplicity both the states of 1s orbital are at the same level. I can show that by using two circles here the circle corresponds to a state and I will cross this circle to indicate that this state is occupied so 1S square then comes 2S square so you have two states available and both are occupied. Then comes 2P to the power 6 so there are 6 states and all 6 are occupied. There are 6 states but only two of them are occupied. Look at this 3p, only 2 electrons are there in this although there are 6 states available. In a 3p orbital there are 6 states. I will cross two of them to show only these two are occupied. So this would be the distribution of the 14 electrons in an isolated silicon atom over various energies.

Here, I have shown a line which means that over a range of atomic separation we are assuming these holes. Again this is strictly not correct because you are slowly bringing the atoms closer so we are assuming very high separation. So, in order to have some simplification in the diagram we can assume that for very high separations the picture is the same. This is the picture for isolated atom. If you have n atom system the only modification that will take place here is, for every atom there are 2 electrons and since each atom is isolated from the other atom the 2 electrons of all the n atoms in the 1S state would be at the same energy.

So, instead of 2 electrons now the picture here is 2N electrons. If you proceed like this here for this 3p state there are 6N states available for an n atom system. All the 6N states are at the same energy in our simplified model because the atoms are isolated. However out of this only 2N states are occupied. You just multiply this number by n so this is 2N states and 2N electrons. You can go on writing for this, but I will write for this end and for the other end.

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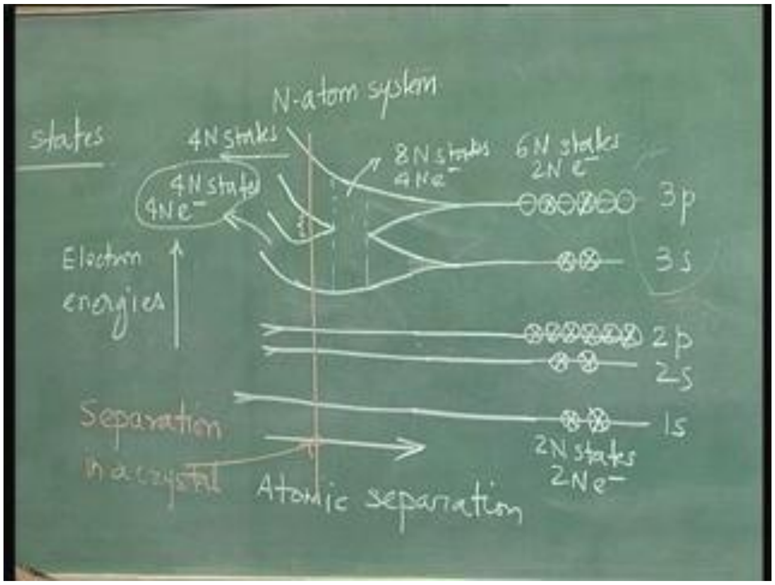

Here you have 6N states but only 2N electrons. Now let us see what is going to happen as you bring the atoms close. As you bring the atoms close the coupling starts between the various atoms. And now you again apply the polis athruzen principle, it says since no two electrons can have the same state each energy state is going to split into n states. When they are far apart this issue does not arise because there is no interaction between them but once the atom starts coming closer there is coupling and no two electrons in any system can have the same energy so there will be small changes in energy of each particular state. So as a result what happens is as you bring the atoms closer this 3S states will tend to spread into a range of energies. That is what is shown here by spreading of a single level into a band. Strictly speaking, in this band there are 2N states and 2N energies so I should show 2N lines that are separate and which is something like this.

But since the N is very large, for example in silicon we know that 5 into 10 to the power 22 atoms by cm cube is a very large number, so these various levels will be so close to each other and we can almost regard them as forming a continuous band. We do not show them as levels as discreet in this, it is as though they are spreading into a band, and similarly the same thing happens here. It tends to spread into a band. What is important to note is that the energy levels corresponding to electrons which are very close to the atom, for them the effect of the other atoms will come about only for very low atomic separations because they are shielded by the other electrons.

In terms of our energy band diagram what it means is that even though these outer levels are getting influenced by other atoms and therefore they are spreading into a band the inner levels here will not spread into a band so easily by this atomic separation. So you can simply so this as a discreet level at this stage. Now, if you proceed further, reduce the atomic separation further it turns in out that calculations indicate that these two bands merge for some atomic separation and if you go down further you have a single continuous band and you reduce the atomic separation this continuous band spreads into exactly two different bands. This is how the picture looks like for lower and lower atomic separation. For this particular 2P level the spreading begins only here and for 1S level it is even later.

Let us concentrate on these two because those are of interest to us. In fact the 4 valence electrons that we talk about are these 4 electrons in the 3p orbital. So in this case, there are not 4 but 4N electrons. How many states are involved if you take this particular level 3p and 3S together? The total number of states involved there are 6 plus 2 is equal to 8. What it means is the 6N states here are spreading and the 2N states here are spreading and they are merging together over this region. In this region, that is over this atomic separation you have 8N states but only 4N electrons because out of this 6N states only 2N are occupied. Out of this 2N states all 2N are occupied but here they merge so there are only 4N electrons.

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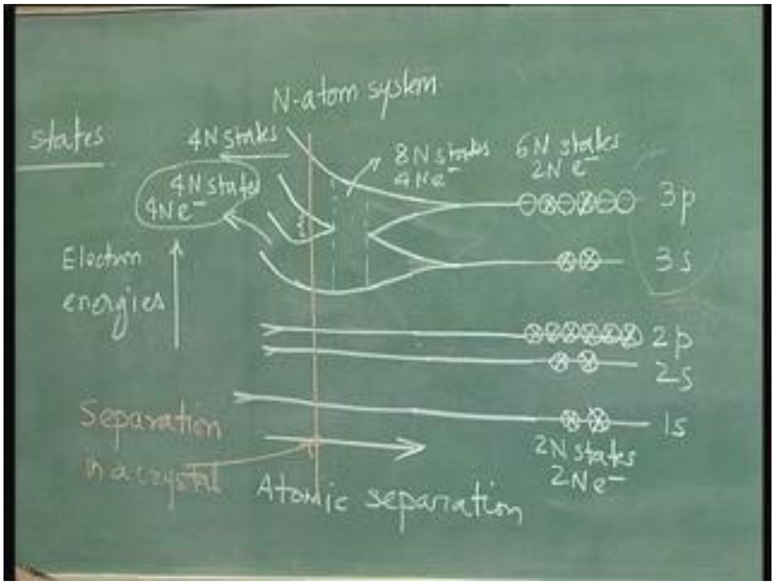

Now what will happen is, out of 8N states 4N electrons will occupy the lower states available. In other words, if you were to do a similar exercise for a metal you will find that the metal crystallizes in this atomic separation range. What we have drawn is for silicon, you can draw a similar diagram for a metal. Then for that metal also you will get similar behavior where you will find the atomic separation in the crystal will be in this range. That is why you have a continuous band of which only a part of energies are occupied. But for semiconductors for example in silicon it turns out that in the crystal the atomic separation is here.

What decides the atomic separation in a crystal? What should be the inter atomic distance in a crystal? This is decided by the fact that all the attractive and repulsive forces should cancel the lowest possible energy the total energy. If you use that criterion and find out the atomic separation it will turn over to be somewhere here for silicon. Now, this shows why at this atomic separation in the crystal you have one band separated by another band so this is the gap. These energy levels are not allowed. Further, calculations indicate that the number of states in this band is exactly 4N and the number of states in this band is also exactly 4N. So 4N states and here in this band also 4N states. But total number of electrons we know is 4N in this 8N states. So all 4N electrons will occupy these lower energies available so the upper band will be empty at kT is equal to 0K if there is no energy provided to the electrons.

So here you have 4N states and 4N electrons. Here 4N states but no electrons. This band is the so called valence band because all the valance electrons are occupying this energy band. And this band is the so called conduction band because when you provide energies to the electrons the electrons jump from the valance band to conduction band and when they jump the electrons which are in the upper band are free to move so therefore they are called conduction electrons.

Now, what is of interest to us in analysis of semiconductors is just the band picture at this atomic separation. Here let us write that this is the atomic separation in a crystal. What we are interested in is only the band picture along this line. So we can just draw that part of the picture and it would look something like this.

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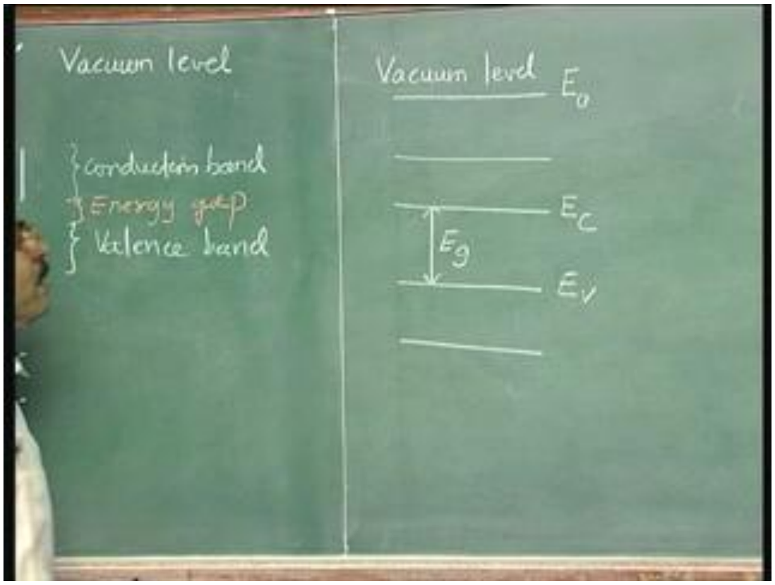

So on this axis you have electron energy and now you do not have to show anything on this axis because we bothered only about the band picture at the particular atomic separation. This is a band picture, the particular atomic separation, so this is one band of allowed energies then the energies are not allowed in this band then again you have another band of allowed energies then you really have a very small width of a band or almost a point. This point corresponds to 1S, this to 2S, this is 2p, this is a band corresponding to 3S and 3p which are merged and again separated. This is also a band corresponding to 3S and 3p which are merged in separated. This is the conduction band and this is the valance band.

We have not yet explained why the electrons which are in this band can participate in conduction that is something we will do later. Now I just want to tell you the name assigned to this band. This allowed band is conduction band, and this allowed band is valance band and this difference is the energy gap.

Now it turns out that the lower energies are not of interest to us because most of the properties of the semiconductor can be understood in terms of these two bands. Therefore one does not show these lower energies. Further it is of interest to note on this diagram which is the energy corresponding to an electron at infinity and this is totally separated from the crystal, that energy is somewhere here. Note that this entire range of electron energy indicates that range which corresponds to electrons within a crystal.

To have a reference, what is the energy of electron which is removed from a crystal and which is moved totally away from the influence of atoms? That will be somewhere here. This level is normally referred to as vacuum level or vacuum energy level. In practice now it is somewhat difficult to work with a diagram like this wherein the ends of this band are indicated as points. What one does is, for simplicity instead of a point you draw a line.

The representation that we will use for explanations would be something like this so vacuum level will be drawn as a line. At this level, the symbol used is E_0 so this is the vacuum level. And then the conduction band will be shown using two lines. The lower level of this will be represented by the symbol E_c where 'c' stands for conduction. The valance band will be shown below this and the top of this band is denoted E_v wherein 'v' stands for valance and this gap is E_g which is the energy gap.

As we will see, this represents the bond strength of the bond model, energy corresponding to the covalent bond. This gap between E_0 and E_C the difference between E_0 and E_C is called electron affinity usually denoted by the symbol chi. a Greek letter or alphabet. Please note that when the levels are drawn in this manner the x axis here does not indicate distance. You should not think that this indicates distance because as we have said strictly speaking this is the correct diagram because you are drawing the allowed energies at a particular separation. So here you should only have a point. But as I said it is difficult to work with this diagram so you are just drawing it like this. Instead of saying that the level is a point it is very difficult to show a point you draw a line so this is electronic energies 'e' stands for electronic energies.

Before we leave this topic of allowed levels let us try to understand why is it that when the atoms come closer the energy level of an isolated atom splits into different energies. When you have coupling between various atoms then the energy levels corresponding to the various atoms split and they are not the same. This is a very important point that one must note, it comes up at several places in Sciences, the splitting of energy level because of coupling between the systems or elements of the systems. We will illustrate this with example of an analogy.

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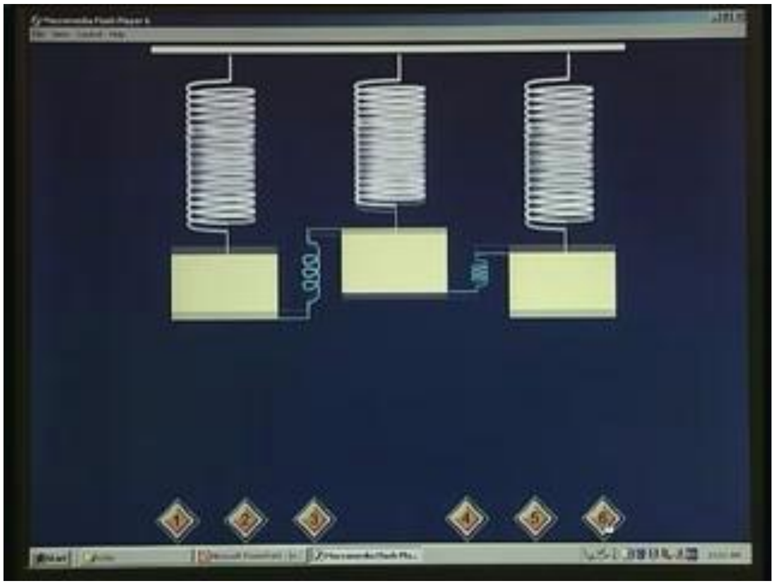

What is shown here is a spring mass oscillator. We will first have a discussion related to this oscillator and then I will indicate to you how the situation here is analogous to the situation we discussed for electrons in a system. Supposing I was to set this oscillator into oscillation it will have some frequency of oscillation which is given by 1 by 2pi square root k by m; k is the spring constant and ‘m’ is the mass. Now these three oscillators are independent and there is no coupling in this case. And what will happen is if I try to set the movement of oscillation it will have the same frequency as first oscillator. I can set 3 into oscillation and it will have the same frequency.

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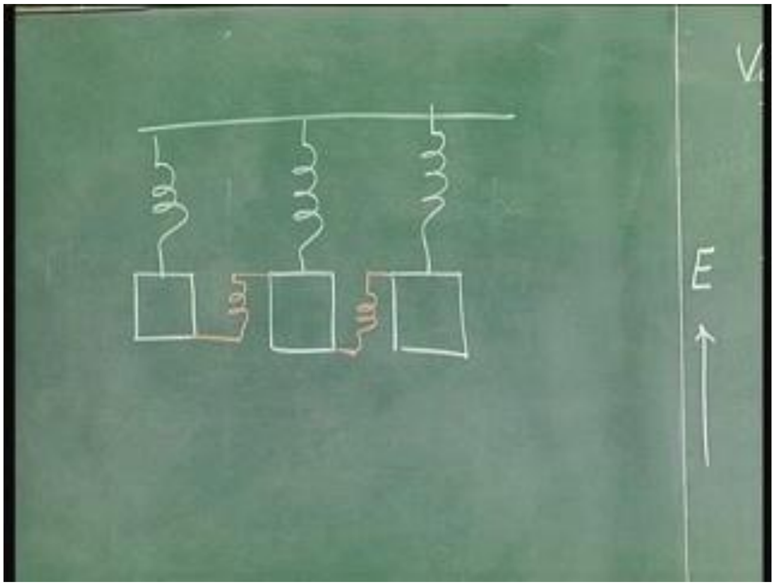

Suppose I was to couple these oscillators by a coupling spring as shown in this black board then we introduce a coupling spring as something like this so that the oscillators are coupled. Now what will be the frequency of oscillation of this system? Let us look at the frequencies of oscillation for this three oscillator system when they are coupled. One particular mode in which the three oscillator system coupled together can oscillate is this mode where all the three masses are oscillating in Unisom. In this case the coupling really has no effect, these frequencies are same as the frequency of an isolated oscillator. But now this is not the only mode in which the system can oscillate. For example, it can oscillate as follows: the central mass is stationary and the left and the right mass are oscillating in opposition.

The frequency of oscillation is now more than the frequency of oscillation when all the three were oscillating in Unisom. It is because now the effect of the coupling spring is also coming into picture. Effectively the spring constant ‘k’ has increased so the frequency is more and now you compare it with this oscillation, this is slower, so this is the second mode of oscillation. There is a third mode in which this particular system can oscillate. That is the centre mass is oscillating in opposition to the outer two masses and outer two masses are oscillating in Unisom, this frequency is even higher than the previous frequency where the center mass was stationary.

Let me play the three modes again. This is one mode of oscillation, this is another mode of oscillation the higher frequency and this is another mode of oscillation an even higher frequency. The three oscillator system has three different modes of oscillation or frequencies of oscillation when the three oscillators are coupled. One can easily extend this argument logically and if you put an ‘n’ oscillator system you can show that it will have ‘n’ different modes of oscillation and ‘n’ different frequencies.

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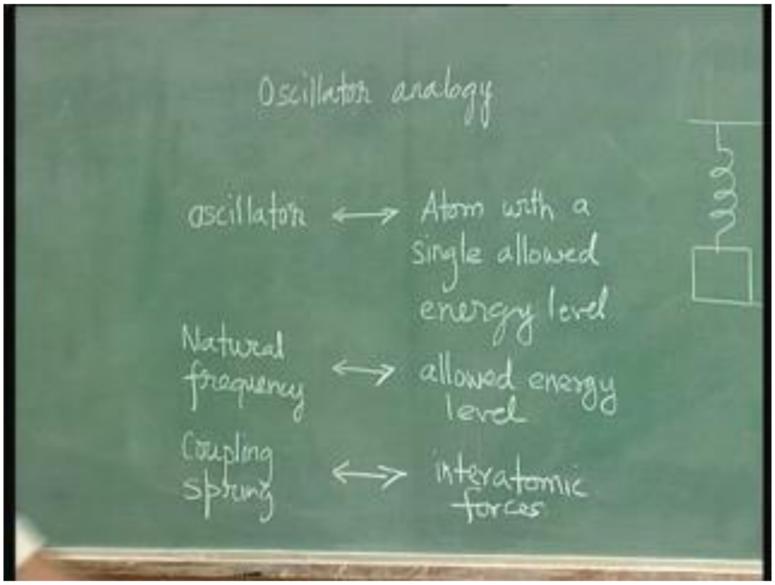

Oscillator analogy

oscillator ⟷ Atom with a single allowed energy level

Natural frequency ⟷ allowed energy level

Coupling spring ⟷ interatomic forces

Now let us come back to our discussion. In the oscillator analogy the oscillator is analogous to atom with a single allowed energy level. Further the natural frequency of oscillation of the oscillator is analogous to the allowed energy level which is the value of the allowed energy level.

Finally the coupling spring is analogous to inter atomic forces, the forces between one atom of silicon and the other atom of silicon. If you look at the analogy in this particular way then we will easily understand how a single energy level splits into more energy levels and equal in number to the number of atoms which are getting coupled. We will also understand that if in the oscillator for example if this coupling spring is very strong if you increase the strength of the spring or the spring constant 'k' then the separation between these three different frequencies that is $F_{0,}$ $F_{1,}$ and F_3 for the three modes of oscillation of this particular system will go on increasing.

Now you have F_3 is the maximum frequency, then you have F_1 and then you have F_0 and if you go on increasing the coupling between two oscillators or the strength of each of these individual springs then the difference between $F_{0,}$ $F_{1,}$ and F_3 will go on increasing, the separation between $F_{0,}$ F_1 and F_3 will increase.

Similarly, if you bring the various atoms close together in a system then the coupling between the atoms increases or inter atomic forces increase and in that case the separation between the various levels which have arisen from a single level that is the single level splitting into 'n' different levels for 'n' atom system the separation between these levels will also increase if the atoms are brought closer. In other words, if all these levels are very close then the separation of the single level into energy band the width of the band will go on increasing as you decrease the inter atomic separation. This is what we saw in our allowed energy level versus atomic separation diagram. Now let us summarize our energy band diagram.

We come back to this diagram that we have drawn. You know this energy level called the vacuum level, E_c is the lower edge of the conduction band, E_v is the higher edge of the valance band and this E_g difference between E_c and E_v is the energy gap this is equal to 1.1 eV for silicon and this chi, which is electron affinity the difference between E_0 and E_c is equal to 4.05eVs. Actually if you draw this band diagram to scale and try to show the conduction band and valence band then it would look like this.

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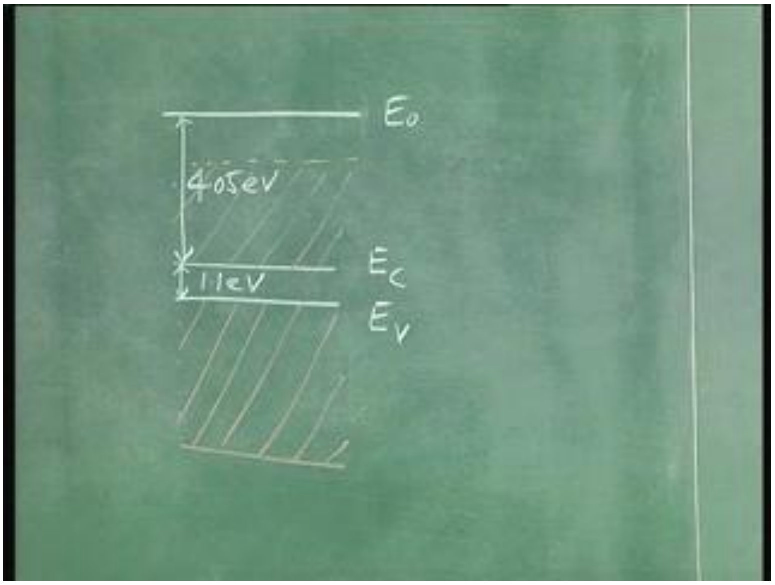

This is E_0, this is E_c and this is E_v. For silicon this is about 4.05 eVs, this is the electron affinity this is the energy gap and this is 1.1 eV. Now if you try to show the bands the valance band would be about 5eV 5 times this so your valance band would be this much. ~~S~~imilarly you will also have a wide conduction band. The energy gap is really small as compared to the width of the band, this is how the diagram looks when you draw it to scale so it is wide allowed energy bands separated by very narrow energy gap. It is always good to look at a diagram to scale because then we know the relative magnitudes of various parameters.

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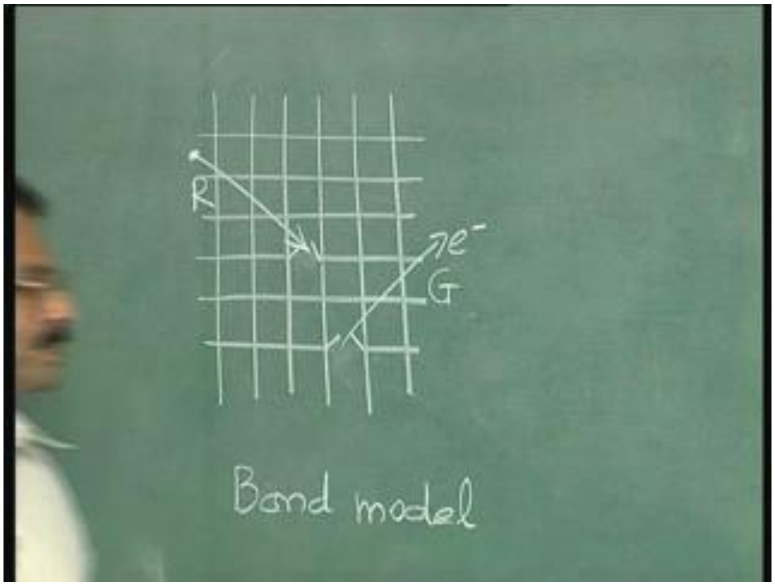

Let us see the correspondence between the band model and the bond model. The various events which are taking place in the bond models such as generations and recombination, how do they look like on the band model? An electron breaking the bond and becoming free to move about within the crystal undergoes a change in energy as shown in the band model.

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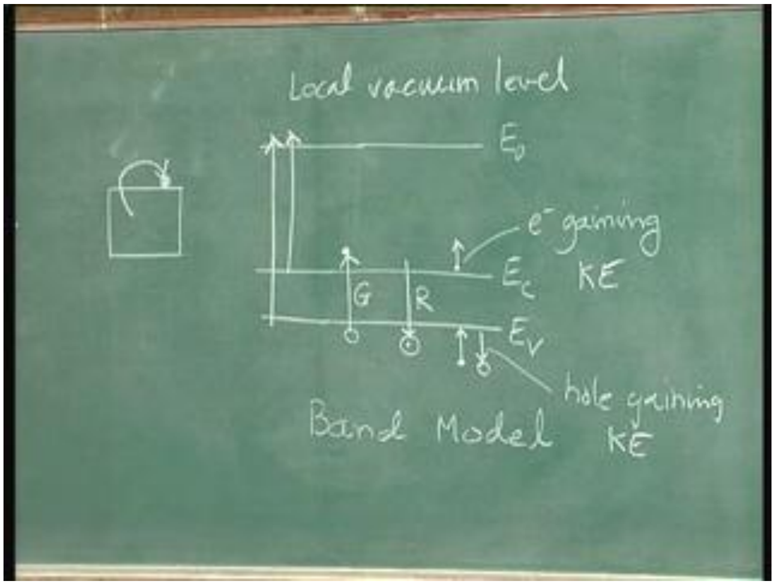

This is the process of generation in the band model. On the other hand, the recombination process that is a free electron jumping into the vacancy and getting annulated and establishing a bond, this is recombination and on the band model it will look something like this, the dot represents electron and the circle is hole, the electron has jumped into the hole so this is recombination where the electron jumps from conduction band to valance band.

Now what about a free electron gaining more kinetic energy? Its velocity is increasing, it is remaining within the crystal. This is equivalent to an electron jumping up in the conduction band, it is gaining energy. On the other hand, a vacancy or a hole gaining in energy, how will it look like? A hole getting in energy is the same as the valence electrons or bonded electrons which are moving through the vacancies gaining in energy. So this is equivalent to the valence electrons gaining energy or electron moving up in the valence band. You can also show this process as a hole moving down. Either an electron moving up in the valence band or the hole moving down because when an electron jumps up in the valence band the hole which was there comes down. This is hole gaining kinetic energy and this is electron gaining kinetic energy.

Finally let us look at another important transition, an electron jumping up from valence band to $E_{0.}$ What does this event shown on the band model represent? This is equivalent to a electron remaining within the crystal but taking part in a bonding process such as this. So this is a bond, there are two electrons where one is associated with this atom and the other associated with this atom and they are participating in a covalent bond. Now if this bond breaks and an electron is set free but moved out of the crystal, so the electron is coming out of the crystal then its energy transition would be represented as shown here as electron jumping from valence band to the vacuum level.

It is important to note that whether the electron is on the surface here or far away from the silicon crystal. Then energy of these electrons are the same because both these electrons are out of the influence of the atoms. This is true only if the silicon piece is uniform. Therefore the question arises that where is the electron which is at the vacuum level? Is it here or is it here? In our semiconductor Physics normally we take the electron to be on the surface.

There is a reason for this which will become clear when we discuss non-uniform silicon blocks or PN junctions and so on. This transition here represents an electron moved out of the crystal but the electron is localized on the surface of the crystal. That is why this inert is referred to as the local vacuum level. If the electron was a free electron then the transition would be something like this. So, free electron moved out of the crystal is equivalent to this transition. In the next class we shall discuss the remaining two tenets of the band diagram namely the density of states function, how the allowed states are distributed over energy and then what is the fraction of these states that are occupied at any given temperature and energy that is the Fermi-Dirac distribution function or the Fermi-Dirac fraction.