Solid State Chemistry
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Lecture – 58
Metals, Insulators and Semiconductors

Now, I will go to the 3rd lecture of week 12. And in this lecture I will talk about the relation between the band structure and the density of states and the electrical properties of materials that is I will talk about Metals or conductors Insulators and Semiconductors ok. So, week 12 lecture 3 will be talking about metals insulators and semiconductors by metals I mainly refer to conductors ok.

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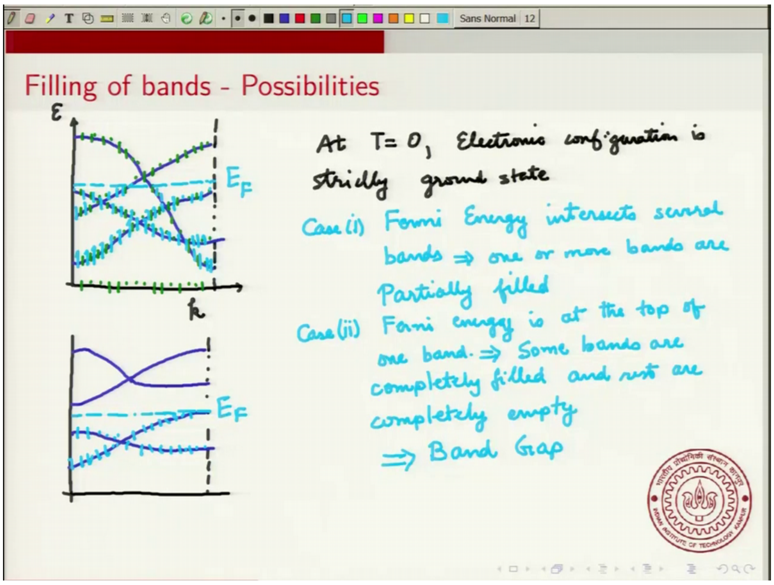

The whole idea of electrical properties of materials is based on the band structure and the possibilities that you get from filling of the bands ok. Now, if you recall what we said in one of the earlier lectures was that the way we calculate the electronic structure of the materials is to first make the band structure ok. So, this band structure has E as the function of k. So, you first calculate the band structure and I will just again for simplicity, I will show the one dimensional picture, but you can do this in higher dimensions.

So, let say this is the range of allowed values of k and you have a band structure that could be something like this ok. And what we said is that once you have the band structure you look at all the possible states ok. So, these are the possible states. So, basically the states correspond to different values of k.

So, if you look at the k axis, you can tell how many states are there again these the number of states is given by the Bond von Karman boundary conditions ok. So, you keep you have all these states you have all these possible states ok. The and in some states even for this map, then what you do is once you have these states you start filling electrons into band. So, you count the total number of electrons and you start filling them into the bands.

So, depending on the number of electrons you start filing them I am showing only one ok. So, you can think of it as a spin state or you can think of these lines as 2 electrons and you start filing from the lowest energy onwards. So, you keep filling and let say you have lot of electrons you have lot of bands also ok. So, you keep filling them and again you fill from the lowest energy onwards. So, you have to fill you have to look very carefully how you fill the electrons into the bands, but when you are done with this exercise, then you see the you are left with some the electrons you keep filling bands up to some energy ok. This is the highest this is the energy of the highest band that is filled highest state that is filled ok.

Now, this approach that we took is 0 temperature approach in the sense that in the sense at T is equal to 0 electronic configuration is strictly ground state ok. That means that if you start filling from the bottom and you fill only up to the highest available states and this energy call the Fermi energy E F ok. So, the Fermi energy is the highest occupied state at T is equal to 0 that is called the Fermi energy ok.

Now, there are different possibilities ok. Now in this particular case your Fermi energy in this case ok. So, this is case i Fermi energy intersects several bands one or more bands it is does not matter one or more bands. So, basically one or more bands are partially filled are partially fills. So, if you see this band it is only partially filled it is only filled up to here where as this band is completely filled similarly this band is completely filled ok. This band is partially filled ok.

So, one or more bands are partially filled the second case you could have a another case I will just show it schematically below here. Now in this case let me I will draw slightly different let me take a solution in the band structure ok, but let me consider the case now where the Fermi energy is right here so; that means, all these bands are completely filled well ok.

I want to change that little bit. So, I had I do not want to this line sorry I will just change this a little bit. So, what I want to show is something like this and let me say this goes somewhere here. So, now, what you find is that, these two bands the 2 bands at the lower 2 bands are completely filled ok. So, the Fermi so, they are filled all the way all the states are filled or occupied where as the upper 2 bands are completely empty. So, this is a second case Fermi energy is at the top of 1 band implies some bands are completely filled. So, I emphasize the word completely and rest are completely empty ok. Now in this case ii there is clearly a band gap ok.

There is a band gap in this case because there is a difference in energy between the last filled band and the first vacant band and so there is a band gap ok. In this case they are may or may not be a band gape in the band gape, but clearly you see that the Fermi energy at least intersects several of the bands ok. So, now, we can see that these two cases; case i where the Fermi energy intersects several bands and case ii where the Fermi energy is high is at the top of the band these two will have fundamentally different electrical properties ok.

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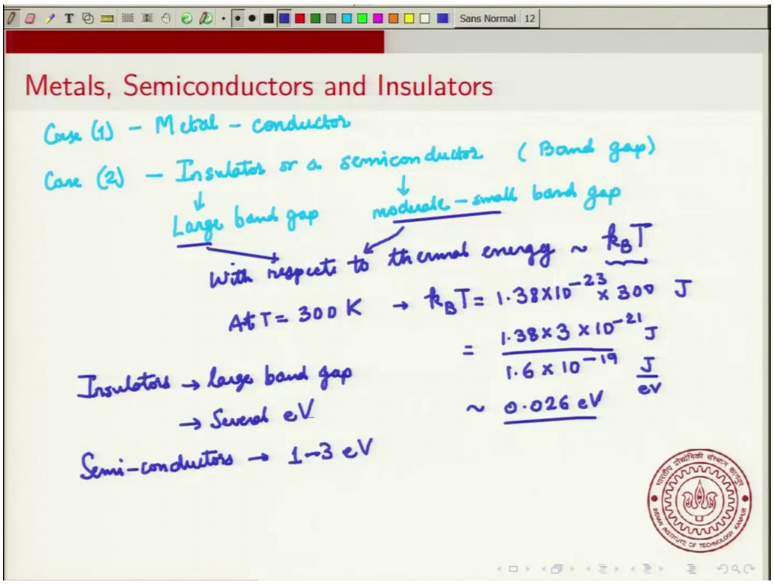

So, now let us now look at the electrical properties. So, the 1st case that corresponds to a metal, one is a metal or more precisely it is a conductor. The 2nd case can be either or insulator or a semiconductor. A semiconductor is, so, in this case you have a band gape ok. So, in this case we have already seen that is band gap ok.

Now, an insulator has a large band gap whereas, semiconductor has a moderate or small band gap ok. Now when we use the word large or small, you should ask immediately what is large with respect to what ok. So, this word large and moderate small are with respect to thermal energy ok. Now thermal energy a measure of the thermal energy is actually the Boltzmann constant times the temperature ok. And when we look at this value this, so, at T equal to 300 Kelvin which is about room temperature you have k B T is equal to 1.38 into 10 raise to minus 23 into 300 Joules.

Here the unit of Boltzmann constant is Joules per Kelvin ok. Boltzmann constant Boltzmann's constant is 1.38 into 10 raise to minus 23. So, k BT is so, many Joules and I can write this as into 3 into 10 raise to minus 21 divided by 1.6 into 10 raise to minus 19 Joule per electron volt ok. So, this will give me the value of Boltzmann constant in electron volts and this works out to about 0.026 electron volts ok. So, the thermal energy in electron volts is typically of the order of 0.026 electron volts ok. So, usually if your band gape is so, typically insulators have band gaps much higher than 4 or 5 ok. So, insulators have large band gaps this is several electron volts semiconductors have lot of the order of 1 to 3 electron volts ok.

Now, what; that means is that with sufficient thermal energy or semiconductor can actually conduct ok. Now if you see this is 0.026 is still much less than 1 or 3 electron volts ok, but semiconductors can use another property called doping which is use to increase the number of charge carriers ok. I will not be discussing that, but just in terms of band gap we see that insulator should have a much larger band gape, but if you have a band gape of the order of 1 to 3 electron volts then you would call it a semiconductor. If you have much larger than 4 or 5 electron volts then you would call it an insulator.

Metals of cores do not have a band gap, metals or conductors do not have a band gap and so, this is the basic picture of electrical conductivity of solids.

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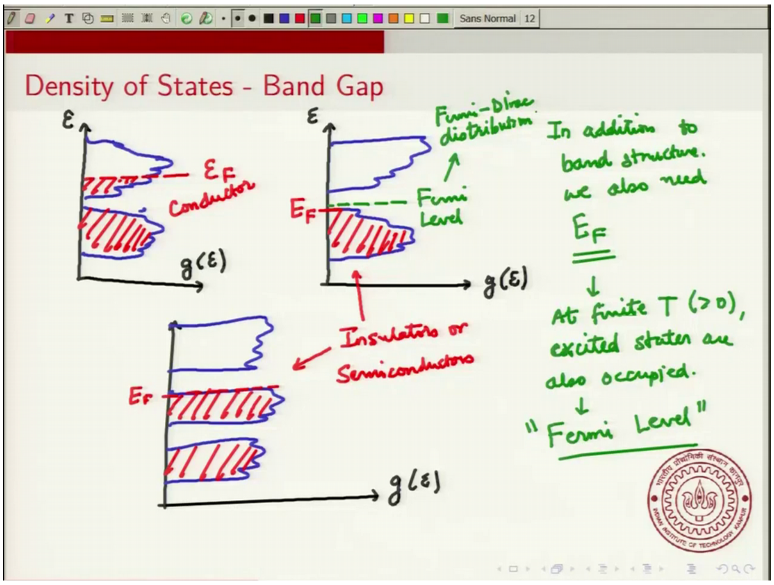

Now let me let now, look at the density of states and what that implies for the case of the band gap ok. If you look at the density of states I will just schematically draw the density of state for a metal. So, for a metal you will have; you will have some density of states again I will use the same, I will plot g of f g of epsilon on this scale and epsilon on this ok. You will have some density of states what is interesting where the Fermi level is.

So, the Fermi level will be let me. So, it is slightly differently just to emphasize the few points, I will get I will have I could have states like this ok. Now the Fermi energy could be will be somewhere here that is in between some set of density of states ok. Now this is a direct consequence of the fact that is the Fermi energy intersects several bands. So, it will be in one of these big bands ok.

In the case of; in the case of an insulator now, your g of E will look like this and now the Fermi energy will be right here at the top of some set of bands and there would be a band gap, I am showing this I mean you could have again you could have several you could also have things like you know having lot more structures. So, if you look at the g of E you could have you; could have things that look like this ok.

You could have multiple bands here I am just showing 2 bands you could have; you could have things like this and you could have; you could have Fermi energy somewhere here E F ok. Then what you will say is that all these bands are all full these all these energies these are states corresponding to these energies are fully occupied states corresponding to these energies are occupied. In the case of the conductor you would say something like this that all these states; all these states are fully occupied.

Now, the states corresponding to these energies are actually partially filled ok. In this case you will just have a all these states being occupied these are insulators ok. So, these two are either insulators or semiconductors depending on the size of the band gap, where as this would be in conductor ok. So, a lot of information about the nature of the material the electrical properties can be got by looking at the band structure.

Now, notice that in addition to band structure this is the very important points. So, I am just going to emphasize this, that in addition to band structure. So, we also need E F ok. So, you need the Fermi energy ok. Now at 0 Kelvin we just do the we just find the Fermi energy by looking at states by filling states from the bottom states ok. At finite temperature actually this you know some of the there can be some excitations. So, at finite temperature there is a probability that even the higher excite even the more excited states are also possible ok.

So, at finite that is nonzero temperature this is greater than 0 excited states are also possible are also occupied and you define something called Fermi level which is basically this is something; this is something that is slightly different from the Fermi energy. So, the Fermi level that usually if the Fermi energy is in this case you have a Fermi energy here, but there can be excitations. So, some of these higher states might also be occupied ok.

The Fermi energy is some sort of it is some level this is the Fermi level ok. And this I am not going to this in detail, but the Fermi level is concept that is useful at finite temperature and this has to do with something called Fermi Dirac distribution; Dirac distribution ok. And I am just mentioning this ok, but I will not expect you to know this and I just expect you to know the Fermi energy at T is equal to 0.

But the Fermi level is a useful concept at non zero temperatures that has to do with the Fermi Dirac distribution and the Fermi level is where the Fermi Dirac distribution takes a value of half the occupation number of a state is equal to half, but again we are not going describe that in detail, but just this is just for your information that at finite temperature, you can define the equivalent of a Fermi energy which is called Fermi level ok.

But again for this course I just expect you to know the Fermi energy and how do you understand the difference between semiconductors between conductors and insulators. So, with this I will conclude this lecture the third lecture of the last week of this course and in the next lecture, I will use the same band structure and the band gap to talk about the optical properties of materials. So, whether how what should be the property of the band structure in order for a material to absorb light, what should it be for it to emit light and so on ok.

Thank you.