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Lecture - 08 Direct and Indirect Bandgap Semiconductors

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So, well, you know, we have talked about band gaps. We have talked about electron holes in semiconductor. So, now, we will go back to the original you know the first question, you know, the classification between metal semiconductors and insulators and that time, we simply said that the conductivities such and such number, but, now, we are in a position to actually go a little bit more.

You know, we can provide a deeper explanation to that. So, if you look at an insulator, it turns out that an insulator is basically a material whose valence and conduction bands are separated by large energy band gap because, when you did all these bands and all that we never really took the type of atom. Any atom can have a band provided it has a crystalline structure.

So, a glass also has some sort of, you know, it can form an amorphous and also quartz which is crystalline form of glass. And diamond, of course, it can be crystal. So, when you have these

things, you have a large band gap. So, the band gaps are shown in the figure here. This is about 9 eV for glass and 5.5 eV for diamond. So, when you have this large band gaps, then we already saw the difficulty in producing electron hole pairs. So, what happens?

Simply, your, you know depending of course, you have to look at the periodic table and elements and all that, but it turns out that the this band will be full. This valence band is full. The conduction band is empty. There is no possibility of generating electron hole pairs. So, they cannot conduct. Larger the band gap, the better insulator it is. So, why is the band gap large?

I will leave it to you right now. We think about it is not hard. You can apply the analysis from particle in a box and analyse it. Then what are semiconductors? Semiconductors are those materials which have intermediate band gap is what we said. So, here are a few numbers; energy, the band gap for silicon 1.12 eV; band gap for germanium is 0.66 eV and band gap for gallium arsenide is 1.42 eV. These are calculated using numerical approaches.

Why this numbers? I mean, it becomes difficult to analyse without you know intuitively, but you could still think about it. Just compare silicon and germanium, they have the same lattice type, same you know lattice type, diamond lattice, diamond cubic lattice. So, go back and look at lattice constants of these 2 materials. Just type Wikipedia search for germanium, it will show you.

The Wikipedia page shows you the lattice type. Same for silicon. So, you can analyse, try to see if the lattice constant is somehow related to band. And if you apply the same analysis to gallium arsenide, it will not work. The reason is, it has a different lattice type. So, this is not possible. Well, anyway, you take a look. And by the way, temperature plays a major role in band gap.

We never really considered that you know. In our intuitive picture, we simply said this bonds, you know, because they have these bands happening and then bands interact and form bands. Sorry, the energy levels will interact and form bands. Why? You know, why should the band gap be dependent on temperature? That is an interesting question. If you think about it, what happens when you increase the temperature?

You are transferring energy to the lattice. As you increase energy, what happens to the lattice? Lattice, the material expands right. When the material expands, it is actually the lattice which is expanding. So, lattice constant is increasing. Whenever lattice constant increases, what happens to band gap? Go and think about it in the from the particle in a box analogy.

Whenever your size of the box is large, the spacing between the energy levels reduces. And after all, all your bands are originating from those discrete energies in the particle in a box. So, from that, you can understand that the band gap should lower. So, there is an empirical relation usually given for each semiconductor, how much it changes with temperature, it is not necessary for us in this course.

It is a little bit more of a detail, but it is enough if you understand that temperature has a dependency on; has an impact on the band gap. The last class of materials are basically metals. So, what happens in metals? Well, it turns out that the band gap is very small. And if the band gap is very small, electrons can easily jump into the conduction band. And if they do that, they are available for conduction.

And that is where the conductivity of metals is large. This is one scenario. Some of the metals might actually have even more extreme case wherein the bottom of conduction band or CB is actually below the top of VB. So, if this happens, then because of this overlap of bands, lots of electrons are present in the conduction band and they can conduct. So, because of that metals are very, very good conductors of electricity.

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So, there is also another interesting aspect that, you know, you can understand, I do not know if you have thought about it, but well, if you, how does a piece of silicon look like. This is what are called as, these are what are called a silicon wafers. These are essentially you know, about 525 micron thick, half a millimetre thick wafers. That is a typical number. It could even be 750 microns in the latest technology. But anyway, so 525 about 8 inch wafer. This was used in the past.

Nowadays, we use 750 micrometre thick and then 12 inch. So, these are the wafers. This is basically a very, very smooth. If you look at the surface, it is shiny. It is shiny because it is atomically smooth. If we measure the roughness, it is going to be 1.2 nano-meters. It is very, very smooth surface and that is silicon. You have this perfect pure material of silicon, which is fabricated to this wafers.

You could also do similar thing for glass. So, glass is silicon dioxide. But if you look at it, glass is transparent. I mean, we see that. Silicon does not look like it is transparent. Why is this difference coming from? The difference, it turns out, it comes from the band gap. Glass has 9 eV band gap. When you have a 9 eV band gap and we saw that if you take a visible light photon, we will take the smallest wavelength.

So that we have the highest energy. The smallest wavelength is 300 nano-meters, let us say in the visible range. The corresponding energy is basically I think we will do 1.24 divided by 0.3, so multiply by 3. So, it will be about 3.7 something, let us take it as 3.7. So, when you have this photon incident, can it make an electron jump from the valence band into the conduction band? Well, it turns out that this cannot happen.

The reason is, there is no state available at that energy. The band gap is 9 eV. So, there is no state available at the 3 eV also. So, we cannot make this transition happen. So, the photon goes through glass. Whereas if you look at silicon, the same photon, silicon has a band gap of 1.12 eV. So, when you shine photon, the similar energy 3.7 eV photon, then of course, you know electron will jump into the conduction. And that is why you have EHP generation.

And because of that the photon gets absorbed and highlighted. And you have these electrons which are flowing. And this is a very, very important process. You know, if you think about a solar cell, what happens in a solar cell? Well, you have light shining, when light shines, it is

creating electron hole pairs and those electron hole pairs will move. There is a little bit more to it, but we will talk about in the last 2 weeks on the lecture.

But then how a photon interacts with a semiconductor is a very, very important part of optoelectronics, LEDS, lasers, solar cells and so on. We will look at it later.

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The last thing I want to do today is talk about direct and indirect band gap semiconductors. So, this is a E-k diagram for gallium arsenide. It is more complicated than what you saw with the Kronig Penny model. The reason is that you know, it has additional, it is actually showing you the E-k diagram in 2 different directions in the same plot. So, this, just accept it right now.

This basically is one direction, you could say, this is one direction in the lattice. And this is another direction in the lattice. These, you know 100 and 111, Miller indices, but we said that we would not want to go into the details page, you know, showing you all the direct, I mean, all the major directions, they are showing you in a single picture that is all. You have to remember.

So, now what it is showing you is that you do not have that simple parabola. You know, if we took a Kronig Penny model also, it would have been a parabola, some sort of a parabola, because, but now it turns out that it has a little bit more complicated shape. And why that happens? It is done because of, there is a lot more theory behind it. And these are calculated using what is called density functional theory and all that which is important for us.

So, the only thing I want you to focus is that there are 2 bands. One is the valence band which is basically in this way and the conduction band which is on the top separated by a band gap. Usually the top of the valence band is denoted by energy E equal to 0 here just for reference and then it does not really matter. So, now, the band gap of gallium arsenide is 1.42 eV and that is what is shown here this distance Eg is 1.4 eV.

And now and another small thing to note that future is bands are parabolic near extrema. We will use that fact later on. So, now you have this. Why do we call gallium arsenide a direct band gap semiconductor? We call it a direct band gap semiconductor because this is bottom of conduction band and it coincides with top of valence band. Well, they occur at same k basically. This is important.

So, whenever this happens, we call it a direct band gap. Now, we have to look at one more step in this. We have to look at energy conservation. Because what happens is if you shine a photon on the direct band gap semiconductor what happens? Let us try to write out the energy conservation law, conservation energy, conservation of energy. What do we do in this?

$E_i^e + hv = E_f^e$

The top energy has to be in the conduction band. You might ask why does not energy you know from what below the, you know, if, why not an electron go from this point to this point, that becomes more complicated. It does happen in some certain situations, but let us not worry about it right now. So, this is energy conservation. You can write it like this. It is simple.

So, what this tells you is that what is the bottom of the conduction band. This is basically E_C right and the top of the valence band is, put it this way. This is E_V . So, this turns out to be hv. Basically, hv is equal to Eg. Whenever this happens, you have the absorption taking place the conservation of energy is satisfied, but if you have a photon of a lower energy, then there is no state available here. It cannot get absorbed.

So, this is again the same story repeated in a different way. So, this is direct band gap semiconductor. In addition to this, we have what are known as indirect band gap semiconductors.

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In the indirect band gap semiconductor, you have the E-k diagram which looks slightly different. In this case, the top of the maximum of valence band does not coincide with bottom of conduction band. This implies, we call this, whenever this happens, we call it an indirect band gap semiconductor. So, but you know, still the energy is the same thing.

You know, the band gap is always defined as the energy gap between the top of the valence band and the bottom of the conduction band that story is still the same, but the position at which this occurs is different. And because of which there is basically this difference, what essentially it means that there is a difference in the momentum, with a difference in the momentum.

So, we know from our classical physics, there are 2 conservation laws. One is conservation of energy and the other one is conservation of momentum. So, will the conservation of momentum be satisfied? Conservation of momentum, what happens to it if it is satisfied or not. If it is not satisfied that, transition is not likely to happen. So, how do we write conservation of momentum?

We have to write basically, you know we can refer to k as a momentum, $P=h\times k$. We saw that. So, we will say k I mean, we will just write in terms of, taking all this multiply by h cross.

$$K_i^e + K_{photon} = K_f^e$$

Now, from the indirect band gap semiconductor, we are seeing that the initial momentum of, let us say, the electron was at the top of the valence band and in this diagram, it is shown as k equal to 0. So, let us say, this was 0. And k final, let us say, this is k, I do not know, k 0, we

call it just for reference. So, the bottom of the conduction k CB, we call it k CB. k CB means basically the momentum is at least the minimum of the conduction band occurs. So, this is k CB.

Now, will this relation be satisfied or not? How do we decide that? To decide that, we have to know what is the momentum of the photon. What is the momentum of proton? Momentum is m times v, mass into velocity. And we have all studied that photon is a mass less particle. So, momentum is 0. Well, that is not exactly accurate, because photon is a relativistic particle and whenever you have a relativistic particle, you have to use different expressions for calculating momentum.

$$p = \frac{h}{\lambda}$$
$$E = \frac{hc}{\lambda}$$
$$E = pc$$

So, if I take like for example, I will take a 1 eV photon,

$$p = \frac{1.602 * 10^{-19}}{3 * 10^8} = 5.4 * 10^{-28} \frac{kg m}{s}$$

If I take like for example, I will take a 1 eV electron,

$$E = \frac{p^2}{2m}$$
$$p = \sqrt{2mE} = 5.4 * 10^{-25} \frac{kg m}{s}$$

So, what is the conclusion? The conclusion is that momentum of a electron is much, much greater than momentum of a P of a photon. or rather since we use k in the top. Let us say, k electron is much, much larger than a photon. That means if you have an indirect band gap semiconductor, so I mean, I can also in other words, I will also say that momentum of photon is negligible.

When I say this, I mean negligible in comparison to electrons, sometimes k could, photon as momentum, I will say. that is a very shorthand way of saying that it has negligible momentum compared to the electron. So, when you have photon momentum to be very small, can this relation be satisfied? This relation right, this is what conservation of momentum is right and this be satisfied, no, it cannot by itself.

So, optical absorption process in an indirect band gap semiconductor is less efficient. Optical absorption in indirect Bg let us short form here, because I do not have space, indirect band gap is less efficient. If you write out the same conservation rule for a direct band gap semiconductor, you saw that the k initial at k final was at the same k. So, negligible momentum of photon was actually good.

I mean, the conservation law was satisfied. So, direct band gap semiconductors are efficient light absorbers or even emitters that is whenever you see lasers and you know, LEDs and all that, they are all made of direct band gap semiconductor materials. And that is where most of them are usually in 3, 5 materials which have direct band gaps. Whereas indirect band gap materials are not very efficient.

I mean, there are ways to beat around that there is a lot of latest research, which you know place to work around it. But even today, we do not really have a silicon laser. We have a laser sort of gallium arsenide,, indium phosphide and stuff like that. But we do not have out of silicon. That is the reason for this. So, how does can absorption occur at all? I only said it is, I did not say that it is not possible.

Generally, you know, if you have a conservation law, which is violated, you would say that it is not possible. But I am only saying that it is less efficient. The reason is that you can have a, what is called as a second order process. So, if you shine a photon, here on an indirect band gap semiconductor, let us say I will shine a photon of energy equal to band gap. Then electron can go only here, because photon has no momentum. It cannot change k, it only can make a vertical transition in the E-k diagram, not a horizontal transition.

So, a photon can make this happen. And then for actually the electron to go into the final state, it requires help from a different type of particle, which we call as for phonon. A phonon is simply a unit of lattice vibration, nothing, you know. Let us not get into that. So, it requires an additional passing particle called as phonon. So, a combination of these 2 can actually make a transition occur.

So, if these two occur simultaneously, then you can have transition possible. So, the conservation law will be satisfying. Of course, you have to rewrite this conservation. You have to put a photon moment of, you have to write a vector, some of them, but anyway, it is not necessary right now. So, it is just that the second order process we call it and that is less efficient, that is why indirect band gap semiconductors are not good, like, absorbing or emitting materials.

So, typically, you know, most of our, the popular semiconductors are all indirect band gap, unfortunately. So, this is silicon. Silicon is an indirect band gap semiconductor. So, it is germanium. You might ask, why is silicon the most? It looks like it is less efficient. So, why is it the most popular semiconductor? Well, it turns out that it is actually cheaper to make, it is more widely available.

Gallium arsenide is much more expensive. So, but it still works for us. You know, silicon works that is enough. Of course, you know, gallium arsenide has better properties in some senses. So, there are electronics made out of gallium arsenide and other semiconductors, but those are more expensive and they are useful for specialised applications. For routine applications, we use silicon. So, this is where I would like to stop.

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