Solid State Chemistry

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Lecture – 59
Band Gap and Optical Properties

Now, I will go to the 4th lecture of this last week of this course. And in this lecture, I will show how to use the band structure to understand some very basic optical properties of materials. In particular, I will be looking at what is the condition on the band structure in order to have materials that can be used for optical emission like light emitting diodes or for optical absorption like solar cells. So, these two are very important modern materials and we will be looking at the optical properties of these materials. So, we will go to week 12, lecture 4 will be Band Gap and Optical Properties.

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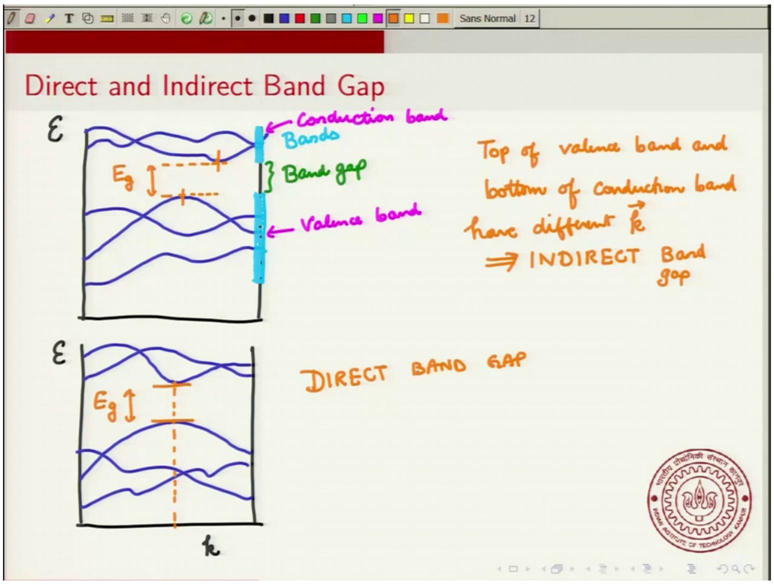

Direct and Indirect Band Gap

Top of valence band and bottom of conduction band have different $\vec{k}$ ⇒ INDIRECT Band gap

DIRECT BAND GAP

Now, the most important concept that decides the optical properties is the nature of the band gap when whether it is direct or indirect. So, we will look at materials that have a band gap, and we will ask the question is the band gap direct or indirect. So, what is the meaning of a direct band gap? So, if you have a band structure let me draw band structure do not I mean this is some wave vector axis, and you have a you have the energy as a function of wave vector ok, this is k along some direction ok. And the band structure will have let us say it has various bands and ok. Let us look at a band structure like this. And, now we see that in this structure, there is a band gap ok, there is a possibility of a band gap in such a material. And the band gap you see that we see that in all through this region, all through this region, there are bands ok, all the way from here to here ok, you have some band ok.

So, if you go all the way down here, you have this band, then you have these two bands you have one or more bands in this region. Similarly, you have one or more bands for these set of energies ok. Then show you have, so, this would be a these are two bands in the material ok. And this is the band gap ok. When we analyze this a little further ok, when we analyze the bands are little further, then we get some more information about these bands, about the different bands. And often we see that the bands here, for example, they are sometimes refer to as the valence band, and these are refers to as the conduction band and so and then there is a band gap in the material. This is very common for lot of the semiconducting materials ok.

And so, the semiconductors or insulators at have a band gap ok. Often, this above the band gap the states are called conduction bands. So, this band is called the conduction band, and this is called the valence band ok. Typically this is a very common feature of the structure of lot of materials ok. Now, we would not go into the details of why this is called valence band and why this is called conduction band, but essentially we these materials typically have some band gap, and there is a conduction band and a valence band ok.

Now, this point, this point ok, this is a lowest energy in the conduction band. This point is refer to as the bottom of the conduction band ok and this point is refer to as a top of the valence band ok. And, this band gap is basically the energy of the band gap is the energy difference between this state and this state. So, this is the band gap and it is denoted by the symbol E g ok. So, the band gap is denoted by E g.

Now, we notice that the top of the conduction band and the top of the valence band are not located directly below each other ok. So, you we see that they are located at different, different k ok. So, this case, when the top of valence band and bottom of conduction band have different k ok, different, let me put a vector. So, different wave vectors this is refer to as an indirect band gap ok. Now, you could have another material, you could have another material where things are slightly different. So, again the e versus e versus k ok, you might have a relation now that looks ok.

And now, the top of the conduction, the bottom of the conduction band and the top of the valence band are directly below each other. So, they are at the same k ok. So, now, such a band gap is called is called a direct band gap. Direct band gap is nothing but the opposite of the indirect band gap, where the top of the where the top of the valence band and the bottom of the conduction band are directly, they are at the same wave vector ok. Now, what is the implication of this ok, what we will see is that if you want an optically active material that can be used for optical devices, you need a direct band gap ok.

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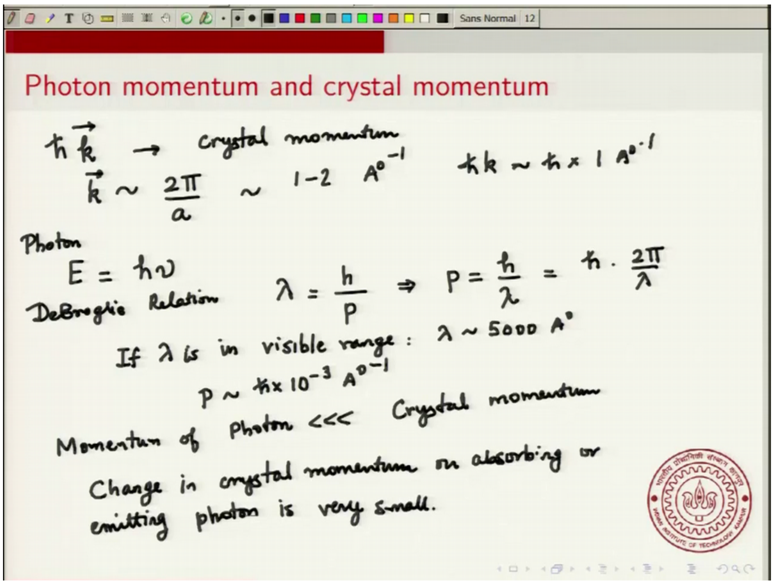

Photon momentum and crystal momentum

$\hbar \vec{k} \rightarrow$ crystal momentum

$\vec{k} \sim \frac{2\pi}{a} \sim 1\text{-}2 \ A^{\circ -1}$ $\qquad \hbar k \sim \hbar \times 1 \ A^{\circ -1}$

Photon

$E = \hbar \nu$

DeBroglie Relation $\quad \lambda = \frac{h}{p} \Rightarrow p = \frac{\hbar}{\lambda} = \hbar \cdot \frac{2\pi}{\lambda}$

If λ is in visible range : $\lambda \sim 5000 \ A^{\circ}$

$p \sim \hbar \times 10^{-3} \ A^{\circ -1}$

Momentum of Photon <<< Crystal momentum

Change in crystal momentum on absorbing or emitting photon is very small.

And see we will see why that should be the case ok. Now, we said earlier that that k, k vector is refer to as the crystal momentum ok. And the typical range of values of k in the first Brillouin zone, the typical value is of order 2 pi by a; a is the lattice parameter ok. So, this is the typical value of the crystal momentum ok. And if a is typically a few Angstroms ok and so this will be about depending on the value of a it will be about 1 to 5 Angstrom inverse ok, depending on what the value of a is ok, maybe 1 to 2 Angstrom inverse ok. So, a is typically about 3 to 6 Angstroms, and 2 pi is around 6, so it is about 1 to 2 Angstrom inverse is the typical value of the crystal momentum.

So, what that means is that now if there is a if there is a photon, if there is a photon ok, now the energy of the photon, so for a photon ok, the energy of the photon is given by

Planck's constant times of frequency of the photon. So, photon of frequency nu has energy h nu. And there is another relation called the De-Broglie relation which says that the wavelength of the photon or is the Planck's constant divided by the momentum of the photon ok.

So, this implies that the momentum of the photon is the Planck's constant divided by the wave length of the photon ok. And so if you divide the momentum by the, so I should emphasis that it is not just k that is the crystal momentum, there is a h bar in this ok. And I will just say that k is of order is of this is the typical size of k ok. So, coming back to the momentum of the photon ok, so this is h by lambda ok. And, so if you take, if you look at this value ok, so typical photon has I mean if you look at let us say visible light ok. So, if lambda is in visible range in visible range ok and let me write this momentum in a slightly different way.

So, I will write this as h bar into 2 pi by lambda ok. So, if in lambda is in visible range, then the basically lambda is of order of you know visible range is about 500 nanometers that is about 5000 Angstroms ok. And what you can see is that P for the photon that is h bar times 2 pi by 5000 ok. So, it is h bar times something like 10 power minus 3 Angstroms ok. So, this is the typical value. So, it is not equal to, so it is of order h bar times 10 power minus 3. It is a 2 pi by 5000 ok, 2 pi is about 6, so 6 by 5 is of order 1, and you have 1 by 1000 that is 10 power minus 3 Angstroms inverse ok.

Whereas for the crystal momentum ok, so h bar k is of order h bar times about 1 Angstrom, 1 to 2 Angstrom inverse, Angstrom inverse ok. So, basically what we conclude? The conclusion we have is that momentum of photon is typically much smaller than momentum of crystal ok, the crystal momentum. So, I should not say momentum of crystal, I should call it the crystal momentum. So, momentum of photon is much smaller than the crystal momentum ok.

And this has an implication. If there is an electron that is there in the in valence band ok, and it observed the photon and it goes to the conduction band ok then basically the change in momentum is very small ok. So, change in momentum on going from the conduction band to the valence band is typically very small ok. So, that means, change in momentum in crystal momentum on absorbing or emitting photon is very small ok, that means, photon an absorption or emission of a photon is not going to change the crystal momentum ok.

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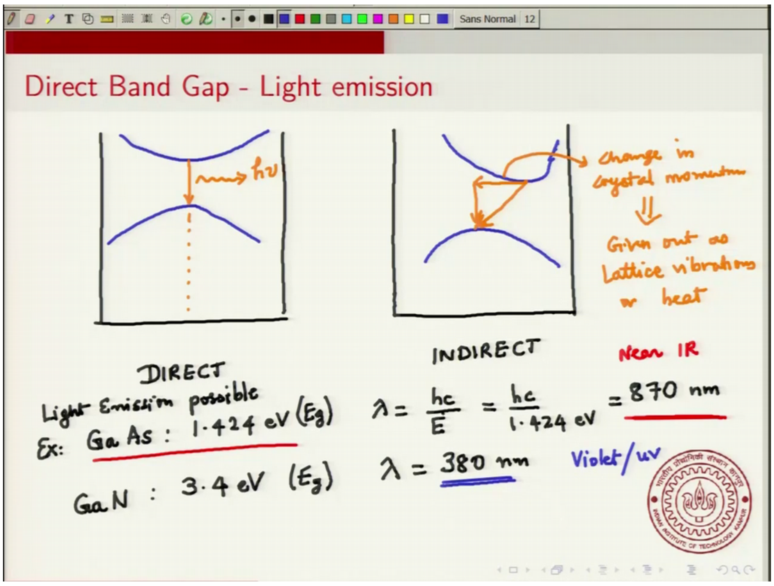

Direct Band Gap - Light emission

change in crystal momentum

⇓

Given out as Lattice vibrations or heat

DIRECT

INDIRECT

Light Emission possible

Ex: GaAs : 1.424 eV (E_g) $\lambda = \frac{hc}{E} = \frac{hc}{1.424\text{ eV}} = 870\text{ nm}$ Near IR

GaN : 3.4 eV (E_g) $\lambda = 380\text{ nm}$ Violet/UV

So, what does is imply that implies that if you have a material with a direct band gap ok, so I will just focus on the band gap. So, I will just focus on this part of the of the band structure. And if it were to emit the; if it were to, if it were to make a transition from the bottom of the conduction band to the top of the valence band ok, then it would emit some light ok.

Now, this what we said is that this transition does not change the momentum ok. So, if it emits light, it is not going to change its momentum. So, if it has a direct band gap ok, so then it is then it can actually emit this light. Whereas on the other hand if it has an indirect band gap, if you have a material with an indirect band gap, its, and so now if there is a transition from the top of the conduction band to the bottom of the valence band ok, now this involves a large change in crystal momentum ok. So, this is a large change in crystal momentum ok.

And so there is a large change in crystal momentum on going from the top of the from the bottom of the conduction band to the top of the valence band ok. And large change in crystal momentum ok, so this is given out as lattice vibrations or heat ok. So, that means, light will not be emitted during such a process; during such a process there will be a large because the crystal momentum is changing a lot, there will be large lattice vibrations and lot of heat will be generated ok, or lot of heat, yeah lot of heat will be generated during this process, but you will not get any light emission.

Whereas, in this case, in this case there is no change in the case of a direct band gap ok, there is no change in the crystal momentum ok. So, in this case there is possibility of light emission ok. So, light emission is possible in this case possible ok. So, the typical light emitting materials ok, the typical light emitting materials are or materials that have band direct band gap; one example is gallium arsenide ok. This has a direct band gap. The direct band gap of gallium arsenide is 1.424 electron volts. So, gallium arsenide has a band gap of 1.424 electron volts now.

So, if an electron makes a transaction from the bottom of the conduction band to the top of the valence band ok, then it will emit a photon ok, the wave length of the photon will be given by the energy divided by it will give being a h c divided by the energy ok. And this energy is an electron volts, when you put the values when you put the values of the Planck's constant, the speed of light and the energy in Joules converted to Joules, you will get a wavelength of well let me write it explicitly.

So, if you have 1.424 electron volts ok, this works out ok. If you if you work out the answer, you will 870 nanometers. So, for gallium arsenide ok, so for gallium arsenide, gallium arsenide works can work as an LED that emits light at 870 nanometers and this is near IR ok. So, the visible range is about 380 to 640. So, 870 is in the IR range, in the infrared range ok. On the other hand, if you look at gallium nitride that has a large band gap that is 3.4 electron volts ok. So, this is the band gap. So, the band gap is 3.4 electron volts. And now if you calculate lambda ok, you will get something like 380 nanometers ok.

And this is in the this is very close to the violet or just in the UV region. So, this is violet slash UV region ok. Now, and by manipulating these materials you can get you can get light emitting diodes of the entire spectrum of light. And, these are used in everyday applications including all the computer screens, all the smart phones screens etcetera. So, what we see is that light emission is usually done by materials like gallium arsenide and gallium nitride. And by manipulating them you can get the whole visible range ok.

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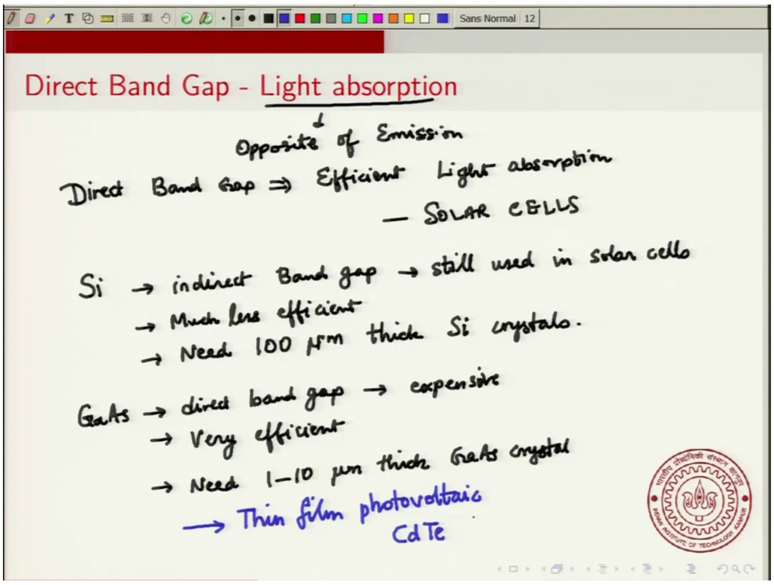

Direct Band Gap - Light absorption

Opposite of Emission

Direct Band Gap ⇒ Efficient Light absorption

— SOLAR CELLS

Si → indirect Band gap → still used in solar cells

→ Much less efficient

→ Need 100 μm thick Si crystals.

GaAs → direct band gap → expensive

→ Very efficient

→ Need 1–10 μm thick GaAs crystal

→ Thin film photovoltaic

CdTe

Now, what about light absorption? So, light absorption is the exact opposite of emission ok. And, usually direct band gap materials are most efficient implies efficient light absorption. And this is used in solar cells ok. Now, if you look, now it turns out that for commercial reasons ok, silicon ok, this has an indirect band gap is often used in solar cells ok, still used in solar cells because of its large availability still used in solar cells. Mainly because it is available everywhere since silicon is an abundant material. So, it is cheaply available, and it is still used in solar cells ok.

Now, it is much less efficient much less efficient ok. And so typically if you want to make a photovoltaic cell using silicon ok, you need 100 micro micrometers thick's thick silicon crystals are needed. In fact, for photovoltaics mostly the polycrystalline silicon is used, but you needed to be a least 100 micrometer thick ok.

Now, gallium arsenide on the other hand ok, this is a direct band gap ok. It is very efficient, but it is expensive gallium is not under a abundant material ok. So, it is quite expensive and very efficient ok. And for the same for the same light absorption efficiency, you need only 1 to 10 micrometer thick gallium arsenide crystal ok. So, the light absorption efficiency of gallium arsenide is much better than that of silicon, but nevertheless silicon is still used because it is so widely available.

However, if you are making if you are making like thin film photovoltaics ok, so if for some application you need a very thin film photovoltaic then you used the materials like gallium arsenide, there are other materials also like cadmium, telluride and so on ok. So, these are materials that are used in very special cases where you need thin film photovoltaics ok, but by and large silicon is still widely used in solar cells.

So, with this I will conclude this lecture. This is the 4th lecture of week 12. In the next lecture, I will summarize what we learned in this week, and then do a few practice questions.

Thank you.