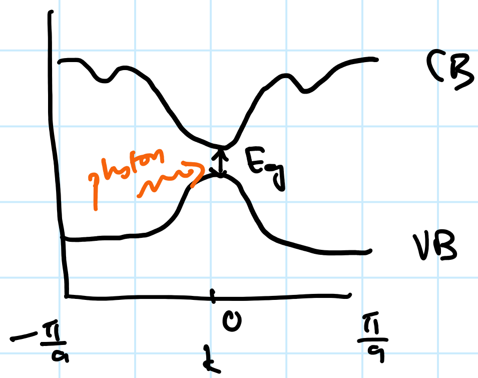
Section 6: Absorption (Solutions)

Sunday, October 24, 2021 11:29 PM

I. Optical Absorption

a) Direct Bandgap



Direct gap: lowest minimum in conduction band lies directly above highest maximum in valence band.

Need to satisfy conservation of energy <u>and</u> conservation of momentum.

$$\Delta E = 0 \Longleftrightarrow \Delta\omega = 0$$

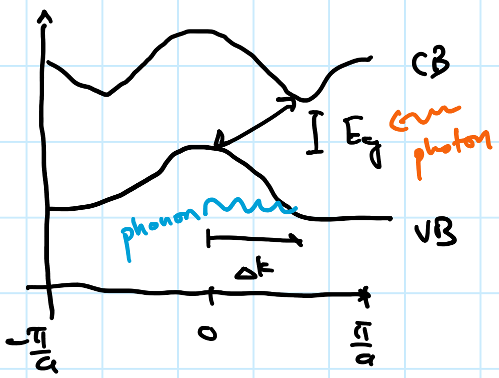
$$\Delta p = 0 \longleftrightarrow \Delta k = 0$$

Note: photons — $p = \hbar k \approx 0$, $E = \hbar\omega > 0$

<u>phonons</u> (lattice vibrations) — $p = \hbar k > 0$, $E = \hbar\omega \approx 0$

Hence, direct bandgap semiconductors can directly absorb a photon with can directly absorb a photon with energy $E_{ph} \approx E_g$ since $\Delta k = 0$ already.

b) Indirect Bandgap



Indirect gap: lowest minimum in conduction band does **not** lie directly above highest maximum in valence band.

Hence, indirect bandgap semiconductors do **not** directly absorb a photon with energy $E_{ph} \approx E_g$ since a phonon with appropriate k is needed as well (and phonons follow a statistical distribution of energies/momenta).

(II) Direct vs Indirect Bandgap Exercise

Consider two materials, Semiconductor A and Semiconductor B. A has a direct bandgap, while B has an indirect bandgap.

a) Which material has a larger absorption

a) Which material has a larger absorption coefficient α? You can assume the incident light is above bandgap for both.

b) Suppose you want to make a solar cell. Both materials are available, but only in one thickness, $t = 525\ \mu m$. Which would you use if you want to extract as much energy from the light as possible?

c) How would you improve the absorption of an indirect bandgap material in general?

d) It turns out that Silicon is an indirect bandgap material, while other options like GaAs are direct. Why is Si the main solar panel material then?

a) A, because it has a direct bandgap. No phonons are needed to assist the conservation of momentum requirement.

b) For fixed thickness, A will have larger absorption.

$$I_f^a = I_0 e^{-\alpha_A t}$$

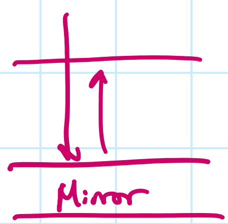
$$I_f^b = I_0 e^{-\alpha_B t}$$

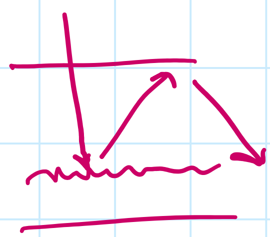
If $\alpha_A > \alpha_B$, $I_f^a < I_f^b$

If $\alpha_A > \alpha_B$, $I_f^a < I_f^b$

c) Make it thicker.

More esoterically, you could put a mirror at the bottom of the substrate (rear mirror) or roughen the bottom surface. This leads to a light trapping enhancement, with the fundamental limit being $4n^2$ (Yablonovitch, JOSA 1982)





Rough argument:

[i] Intensity enhancement: $I \sim n|E|^2$

$\Longrightarrow I_{mat} \sim n^2 I_{inc}$

[ii] Reflection: effective doubling

$\rightarrow 2n^2$

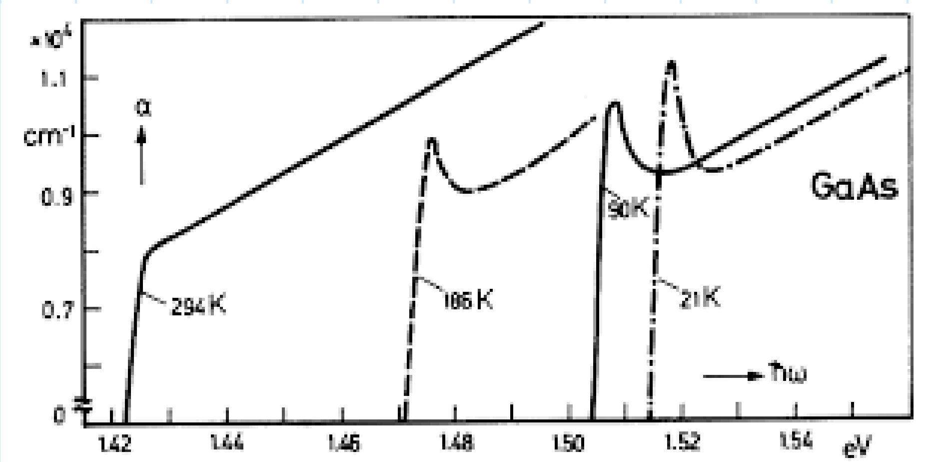
[iii] Angle-averaging (need to look at the original paper more, but its something like an average over the solid angles over which the light is scattered)

$\rightarrow$ extra factor of 2 for bulk,

$4n^2$ absorption enhancement

d) Silicon is cheaper and nontoxic. For the most part, you can get better absorption by simply making it thicker, as in part c. It also has a very stable native oxide. However, for the most part it's because of cost.

III. GaAs Absorption Spectrum



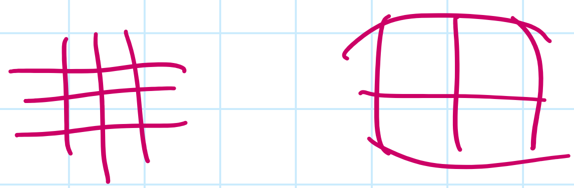
a) Let's look at the room T (294 K) absorption spectrum first. Again, GaAs is a direct gap semiconductor. How would you expect the plot to change if GaAs was indirect?

b) The spectrum clearly changes as the temperature changes. Do the changes make sense?

c) What do you think those peaks at low temperature are?

a) Absorption edge should get "smeared out" because you need phonons to maintain momentum conservation.

b) Main change is absorption edge goes to higher energy as temperature decreases. This makes sense — bandgap should decrease with temperature.

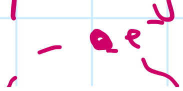


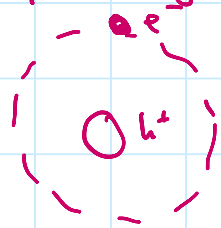
low T — "more orbital overlap"

high T — "less orbital overlap"

$$E_g^{low} > E_g^{high}$$

c) Excitons! Bound electron hole pair, "hydrogen-like"





Typically, binding energy is very small compared to E_g — so $k_B T$ usually overwhelms it. Hence, excitons are typically observed at low T. However, recent work has found that certain 2D materials like monolayer MoS_2 have excitons w/ quite large binding energy, so they are excitonic at room T! I will talk about this in more detail in hopefully a future section.