ME 432 Fundamentals of Modern Photovoltaics
Homework Assignment #3, Fall 2020
Due Friday Oct 2

Please note: You may attach Excel spreadsheets, Matlab code, Mathematica, etc. However, if you use external software, please write out the formulas or methodology you used to calculate your answer. Your logic flow/thought process should be described clearly.

Question #1: Optimal Band Gap for a Photovoltaic Absorber.
Now that you have practice working numerically with the solar spectrum from HW1, we'll calculate the optimal band gap for a photovoltaic absorber here on earth, considering losses due to non-absorption of photons and thermalization. You should make a plot of efficiency vs. band gap, and see where the maximum is. Efficiency is (energy out/energy in), and you calculated the denominator in HW1,Q2. Your work in HW1,Q3 can help with the numerator. Use the following considerations:

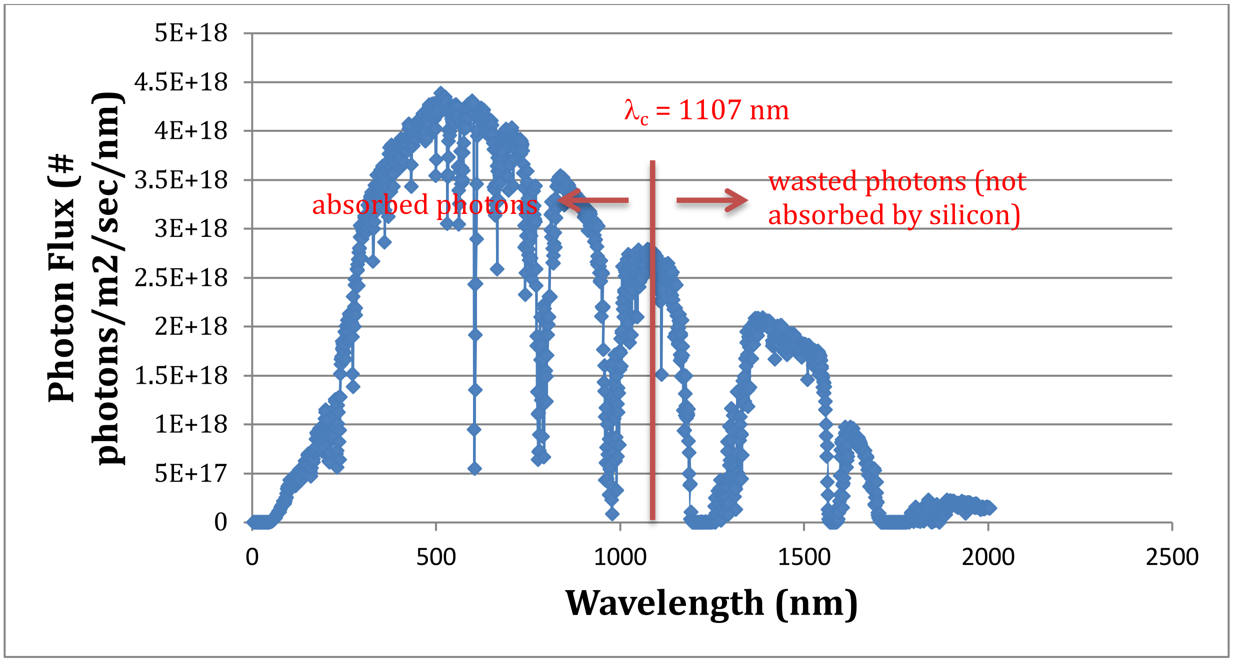
(a) Photons from the solar spectra with energy below the band gap energy ($E_{ph} < E_g$) will not be absorbed (they are simply wasted).
(b) Photons with energy above the band gap ($E_{ph} > E_g$) are absorbed, resulting in electron excitation from the valence to the conduction band. However, the excited electrons will lose some of their energy (E_{ph}-E_g) to thermalization (heat, or lattice vibrations) and only contribute E_g to the collected energy.

Your goal is to make a plot of efficiency vs. band gap. On this plot, mark the efficiency limits of the following materials (you will need to look up their band gaps (Wikipedia)): Si, GaAs, CIGS, CdTe, amorphous Silicon, Ge, ZnO, quartz (SiO_2).

Note: Some of you may be familiar with the Schockley-Quiesser limit for solar cell efficiency vs. semiconductor band gap. (If not, don't worry, we'll talk about it in class). The calculation that we are doing is similar to, but not exactly the same, as the Schockley-Quiesser model. The shape of your curve will look quite similar. The only difference is that we are neglecting a basic thermodynamic limitation: namely, we are assuming that every photon that is absorbed and thermalized to the band edge is going to contribute to electric current. This is not in fact the case – thermodynamic restrictions tell us that a certain fraction of the excited electrons must drop back into the valence band before we can collect them (radiative recombination). If we considered this in our model, we'd have exactly the Shockley-Quiesser limit.

To solve this problem, we need both "energy out" and "energy in". The "energy in" refers to the total power flux incident from the sun at the surface of the solar cell – that is, the integrated AM1.5G spectrum for which you should have obtained around 900 W/m^2 from the first HW assignment. This number is, of course, independent of the band gap – it is just the total power flux provided by the sun, whether it is absorbed or not by the solar cell.

The numerator, "energy out", is a little more tricky. This parameter now depends on the band gap. You can make this problem easier by using the photon flux diagram that you prepared in HW 1. There are two things to consider. For a semiconductor with band gap E_g, the cutoff wavelength for absorption is λ_c=1240/E_g. For wavelengths longer than this, the photon energy is smaller than the band gap, and the semiconductor cannot absorb (is transparent). The diagram below illustrates this conceptually for the case of silicon, with a band gap of E_g=1.12 eV and a cutoff wavelength of λ_c =1107 nm. All wavelengths $\lambda > \lambda_c$ are not absorbed by the solar cell, and wasted.



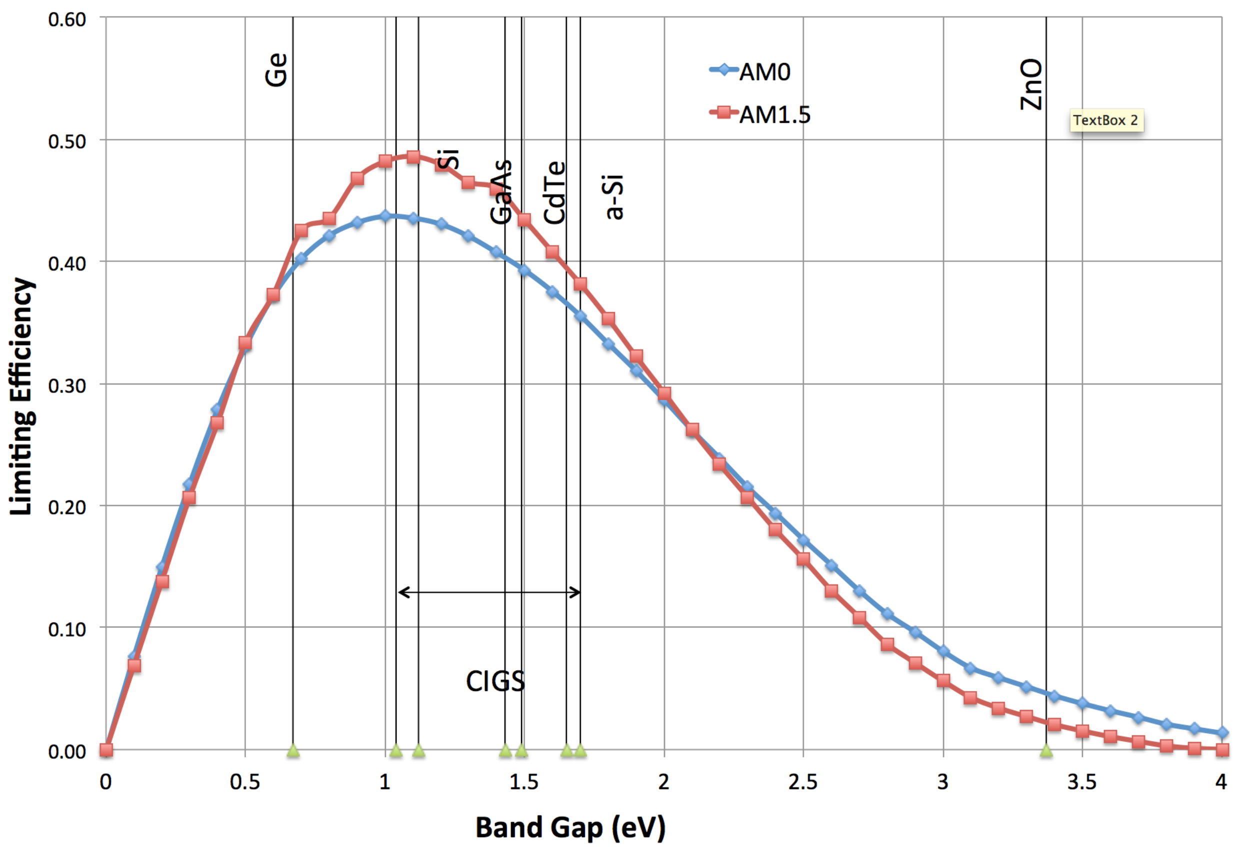
Thus, if we integrate the photon flux from all wavelengths from λ = 0 nm to $\lambda = \lambda_c$ nm, we'll get the total number of photons absorbed by the semiconductor per sec per m^2. Note that this number will be different for semiconductors of different band gaps.

$$\frac{\#\,photons}{\text{sec m}^2} = \int_{\lambda=0}^{\lambda=\lambda_c} (\text{photon flux})\ d\lambda$$

Now we have the total number of photons absorbed (per sec per m^2) as a function of the band gap, but to get "energy out", we need the energy produced by these photons. This is straightforward – because of thermalization losses, we know that each photon ultimately produces an electron/hole pair that sit at the band edges, and thus stores an energy of E_g. This is true, regardless of the initial energy of the photon E_{ph}. Of the photon energy E_{ph}, we lose a certain amount (E_{ph}-E_g) to thermalization, and store the remainder (E_g). Thus, the "energy out" is simply the integral expression above, multiplied by the band gap:

$$\frac{energy\ out}{\text{sec m}^2} = E_g \times \int_{\lambda=0}^{\lambda=\lambda_c} (\text{photon flux})\ d\lambda$$

Note that you will need to calculate this expression several times – for the different possible band gaps. Both the integral and E_g depend on the band gap. This is most easily done with some software such as MATLAB/Mathematica (or, I suppose, MS Excel). Be sure to keep our units straight – if you used (901 W/m^2) for "energy in", then you should use the same for "energy out" (not eV/sec/m^2). Alternatively, you can put "energy in" and "energy out" in terms of (eV/sec/m^2). In either case, your final plot should look like this:

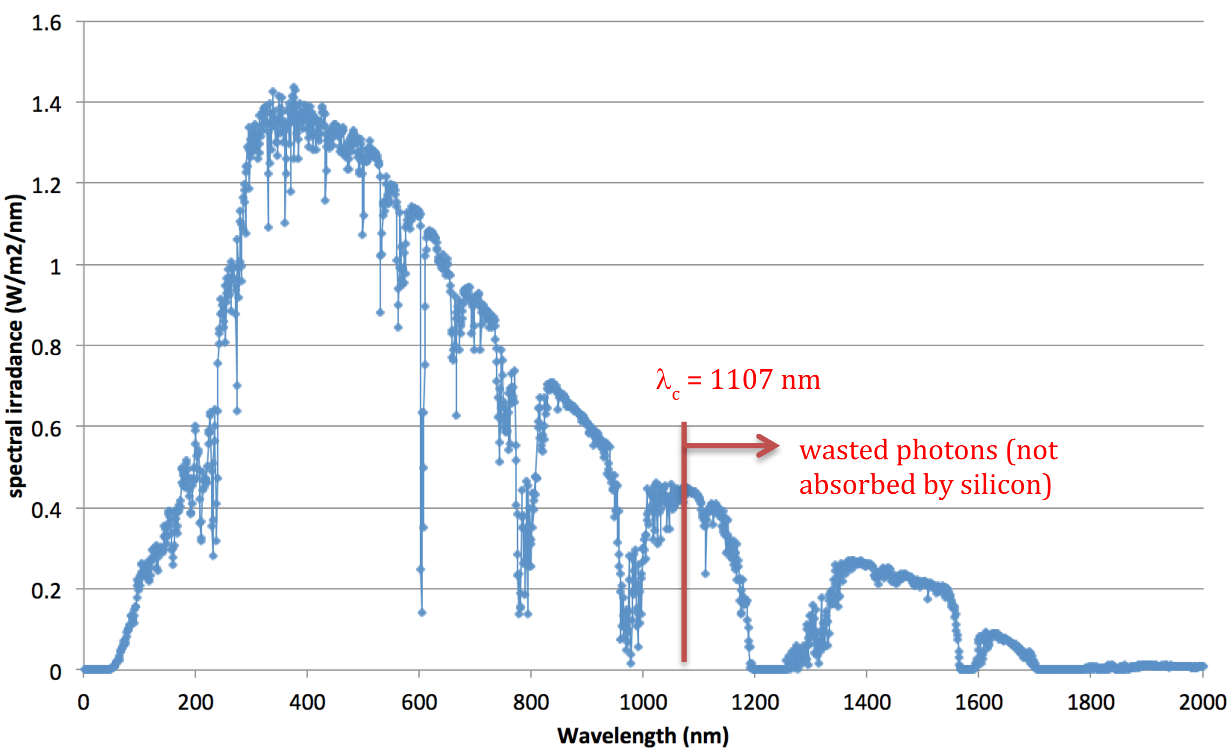


We see that the highest possible efficiency for a single semiconductor photovoltaic is close to 50%, and occurs for band gaps near 1.1 eV (silicon is near perfect, according to this model).

Question #2: **Comparison of thermalization vs. non-absorption losses.**
We know that for vanishingly small values of the band gap, all photons can be absorbed but thermalization losses result in no cell output. On the other hand for the largest band gaps thermalization losses are minimal, but non-absorption of photons results in no cell output. At the optimal band gap that you found in Question 1, what percent of the incident solar spectrum is lost to non-absorption? To thermalization?

We'll say that the optimal gap occurs around 1.1 eV (silicon), with an energy conversion efficiency around 48%. Again, we have around 900 W/m^2 incident on the surface ("energy in"). Our "energy out" is 0.48*900=432 W/m^2.

That means that 900-432=468 W/m^2 are lost. Some of that loss occurs because photons are not absorbed in the first place, and some of it is lost because of thermalization. To figure out how much is not absorbed, we can integrate the solar spectrum (now as a power flux, rather than photon flux) overall all of the non-absorbed wavelengths.



We can integrate to find the total amount of the incident energy that is not absorbed at all:

$$\frac{energy}{\text{sec m}^2} = \int_{\lambda=\lambda_c}^{\lambda=\infty} \left(\text{spectral irradiance}\right)\, d\lambda$$

This gives about 190 W/m^2. Thus, of the 468 W/m^2 of the incident solar spectrum that is lost, 190 W/m^2 is not absorbed in the first place, and 468-190=278 W/m^2 is lost to thermalization. Overall, this means we lose 190/900 = 21% to non-absorption, and 278/900 = 31% to thermalization, leaving us with 48%.