An introduction to modeling solar cells

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April 3, 2019

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Foreword

Solar energy has recently become the cheapest source of energy in many areas of the world[], as the prices of solar energy continue to plummet[], it is widely expected to out compete (and replace) most other forms of energy, including coal, oil and gas. It is therefore becoming increasingly important for Engineers and Scientists, to understand the basics of solar energy technology. This workbook, aims to teach you the basics of how solar cells work, what limits their efficiency, and how their efficiencies can be boosted with improving technology. The workbook consists of a part A and a part B. Part A, asks you to perform a short literature review on various types of solar cells; and part B) guides you through simulating a solar cell using a CAD package. The idea of the simulations is to give you a real practical feel for what is really going on in a solar cell, and what governs it's operation. Don't be afraid to play around more with the software, or use it in your projects/research. I think the best learning is done by playing.

I wrote this workbook for a class of general engineering students in 2017 and revised it in 2018. The class contained a very broad selection of students and lasted only a couple of hours. As such, this workbook gives you enough information to get going with gpvdm, and guides you through solar cell simulation in an hour or two. To enable me to do this, I've glossed over topics such as mobility as a function of trap filling/carrier density. If want a more detailed discussion of solar cell physics either see the manual or the papers associated with the model.

Assessment

If you are taking the module H14REN at Nottingham, you will be required to submit a single report containing both the literature review and the simulations. You should submit a **single pdf**, not a MS word document. The first half of the report should contain the literature review and the second half should contain, the answers to the questions which appear in the boxes throughout the work book. The literature review, is not really a literature review, I don't want you to spend your time writing beautiful English sentences, but a series of questions to make you go and read some literature. You should answer all parts of this workbook the same way you would answer an exam question (i.e. short to the point answers), this is to avoid the need for significant amounts of writing.

1 Part A: Short literature review of solar cells 40%

In no more than a total two pages minimum size 12 font, (excluding references), answer the following questions. Try to cite one journal article in answering each question (web pages do not count ;)):

- What are the advantages of organic solar cells over other types of solar cells (focus on the manufacture)?

- What are the drawbacks of Perovskite solar cells?

- Discuss the benefits and drawbacks of multi-junction solar cells.

- Do you think concentrator solar technology, will out compete silicon solar cells?

- Discuss Swanson's law in relation to Si solar cells, and what this means for emerging PV technologies.

- How intense is solar radiation and what does this mean for solar energy generation.

- Discuss Keeling curve and what its implications are for the human race.

- Discuss with a diagram (your own diagram), the importance of the band gap for solar energy harvesting materials.

- Discuss the major losses in whole PV systems.

- Which type of solar cell do you think will dominate the market in 50 years, will it be one technology or multiple technologies?

2 Part B: Simulating solar cells 60%

In this part of the coursework you will be using a CAD tool called gpvdm (General-purpose Photovoltaic Device Model) to simulate and understand solar cells. Your write-up, to this section should not exceed 4 pages, marks will be deducted for longer reports. No appendix is allowed. The first task is to download and install it.

2.1 Downloading and installing gpvdm

If you are going to carry out the simulations on your own laptop, you can install gpvdm using the windows installer which can be found at: `https://gpvdm.com/download.php`. If you are using a University computer, you will have to install the software manually as you don't have administrator rights to the computers. I have tested the software on the University computers, and it works, I can not however guarantee it will work on your home computer.

2.2 Installing gpvdm on a University computer

If you follow these instructions exactly gpvdm will work on a University Computer: Download the zip file containing gpvdm from `https://gpvdm.com/windows_other.php` , make sure you use the latest version. The web site will ask you for a password, it is username:user and password:password. Once you have downloaded the zip archive, open the zip file and extract the folder *pub* to $c : \backslash$. Then rename the folder $c : \backslash pub$ to $c : \backslash gpvdm$. Once you have done this run the executable $c : \backslash gpvdm \backslash gpvdm.exe$ (see figure 1)
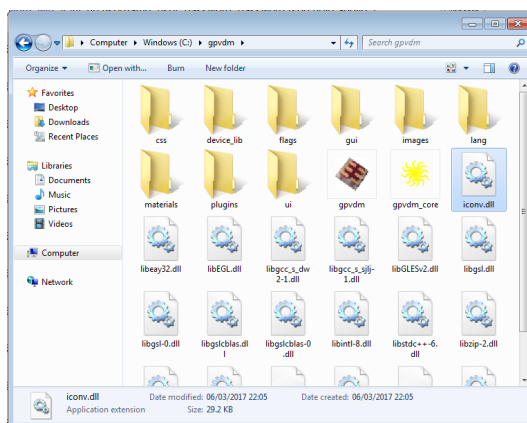

Figure 1: Running and installing gpvdm. Double click on the gpvdm icon to run the model.

This should bring up the gpvdm interface which looks like this (see figure 2):

2.3 Making a new simulation

Click on the *new simulation* button. This will bring up the new simulation window (see figure 3). From this window select the *Organic Solar Cell* option and click
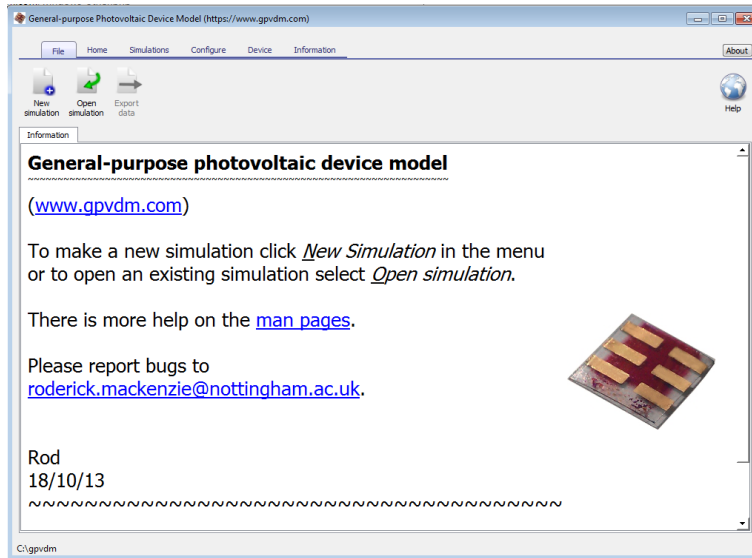
Figure 2: The main gpvdm simulation window, when you start the software

next. If you are in a University computer room, I suggest you save the simulation to your desktop (which is on the c: drive), not a USB stick or the Z: drive. Gpvdm dumps a lot of data to disk and the z: drive/usb stick drive will be far too slow for the simulation to run. [Note: Once University computers are shut down, they are wiped clean. Therefore it is important to move your simulations from the desktop to the z: drive before you log off(!).] Once you have saved the simulation, the main gpvdm simulation window will be brought up (see 4)
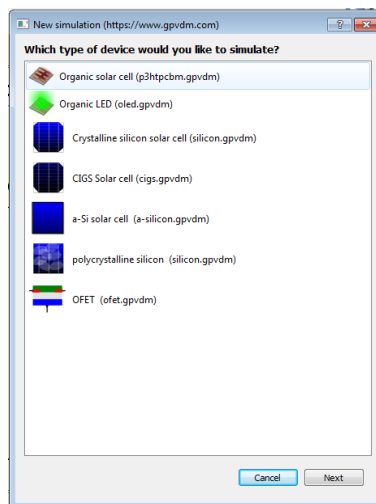

Figure 3: New simulation window

You can look around the structure of the solar cell, by dragging the picture of the solar cell with your mouse. By hitting 'z' you can make the solar cell spin around. [Note: If you don't have the correct drives for your graphics card installed you will only get a 2D image of the solar cell. If this is the case, don't worry, it will not impede your ability to do the course work.]
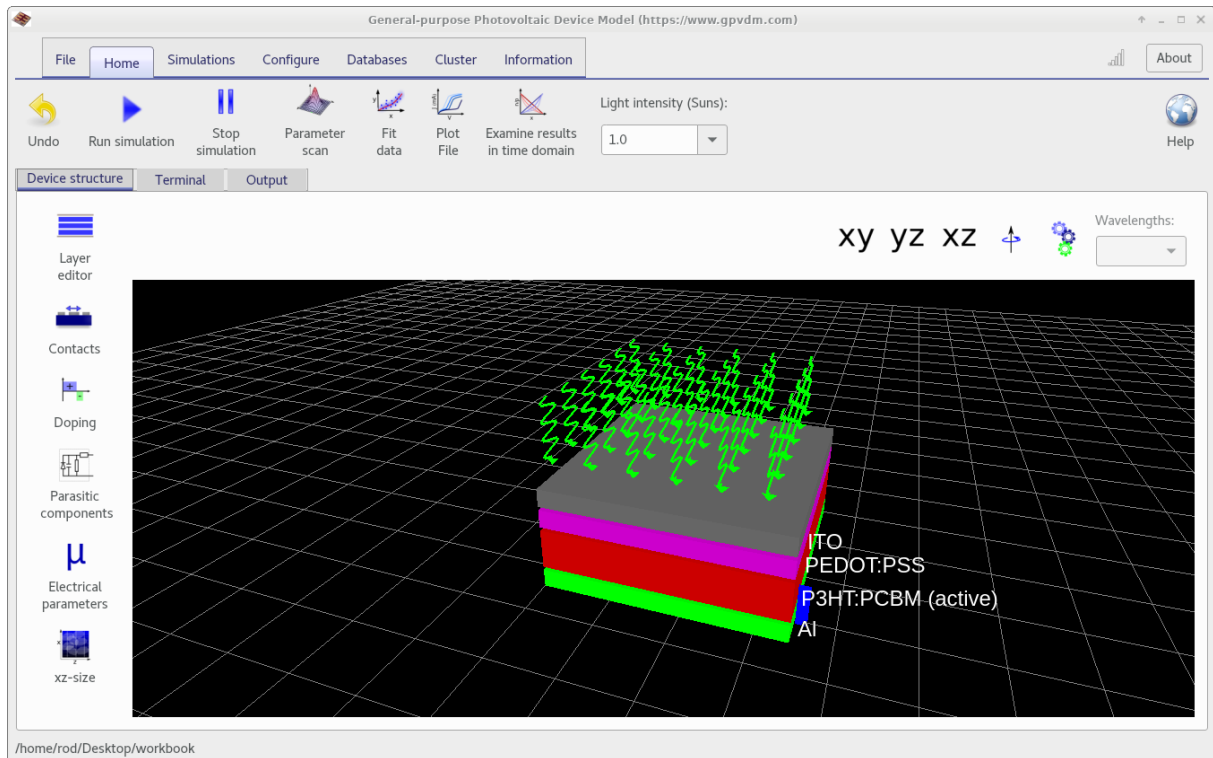
Figure 4: The main gpvdm simulation window

Question 1: If you look at the image of the solar cell, you can see that it is split into 4-5 layers. Each layer has a name associated with it (ITO/PE-DOT:PSS etc..). Write down, what does each layer of the solar cell does and what do the initials stand for? Where possible find images of the chemical structures and place this information in your report. You will be able to find this information in the internet.

2.4 Running your first solar cell simulation

Hit the *Run simulation* button, and the simulation will run. On slower computers it could take a while. Once the simulation is done, click on the *Output* tab (see figure 5), there you will see a list of files the simulation has written to disk. Open *jv.dat*. This is a plot of the voltage applied to the solar cell against the current generated by the device. These curves are also sometimes called the 'charistic diode curve', we can tell a lot about the solar cell's performance by looking at these curves. Hig the 'g' key to bring up a grid. Place this result in your report, [Hint: you can use ctrl+c to copy the plot to the clipboard.]
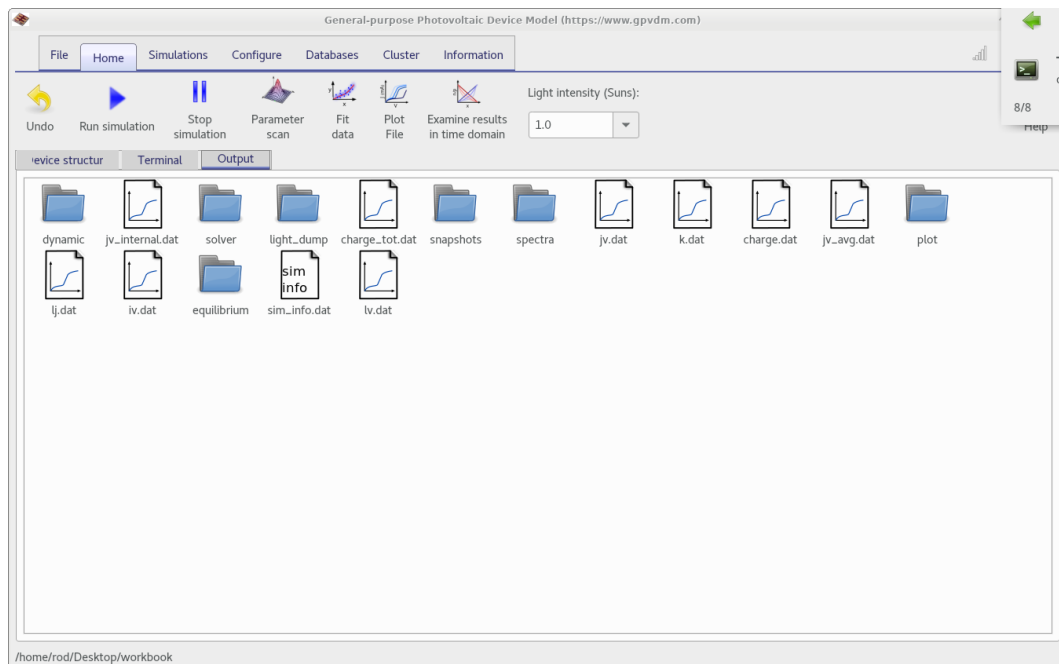

Figure 5: The output tab

Now open up the file *sim_info.dat*, this file displays information on the performance of the solar cell, such as the Open Circuit Voltage (V_{oc} - the maximum Voltage the solar cell can produce when iluminated), efficiency (η - the efficiency of the cell) , and short circuit current (J_{sc} - the maximum current the cell can produce when it is illuminated). Figure 6, shows where you can find these values on the JV curve.

> Question 2: What is the J_{sc}, V_{oc} and Fill Factor (FF) of this solar cell? How do these number compare to a typical Silicon solar cell? (Use the internet to find typical values for a Silicon solar cell.)
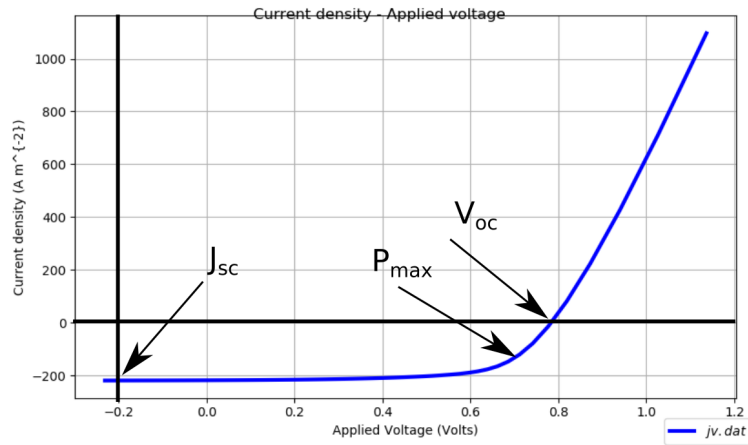
Figure 6: The output tab

If you look back at figure 4, the main gpvdm simulation window. Look at the left hand side of the window, you will see a button called layer editor. Click on this button and it should open a new window (see figure 7). Within the window is a table which describes the structure of the device. The column *thickness* describes the thickness of each layer. The P3HT:PCBM layer is the layer of material which converts photons into electrons and holes, this is commonly called the *active layer*. An active layer thickness of $50nm$ is considered very thin for an organic solar cell, while an active layer of $400nm$ is considered very thick (too thick for efficient device operation). Vary the active layer between 50 nm and 400 nm, for each thickness record the device efficiency (I suggest you perform the simulation for at least eight active layer widths).
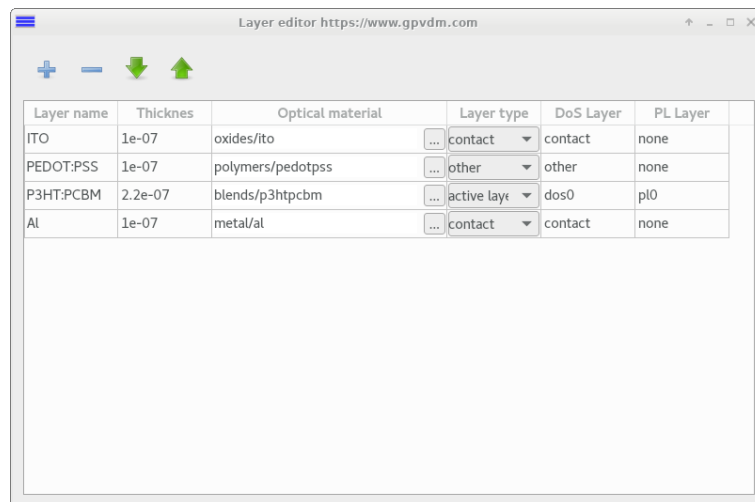

Figure 7: The layer editor

Question 3: Plot a graph (using excel or any other graphing tool), of device efficiency v.s. thickness of the active layer. What is the optimum efficiency/thickness of the active layer? Also plot graph V_{oc}, J_{sc} and FF as a function of active layer thickness. J_{sc} is generally speaking the maximum current a solar cell can generate, try to explain your graph of J_{sc} v.s. thickness, [Hint, the next section may help you answer this part of the question.]

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2.5 How do solar cells absorb light?

2.5.1 What does the sun's spectrum look like?

In this section we are going to learn how a solar cells interact with light. Firstly, let's have a look at the solar spectrum. Sunlight contains many wavelengths of light, from ultraviolet light, though to visible light to infrared. The human eye can only see a small fraction of the light emitted by the sun. Gpvdm stores a copy of the suns spectrum to perform the simulations. Let's have a look at this spectrum, to do this go to the *Database* tab, the choose *Opticaldatabase*. This should, bring up a window as shown in figure 8
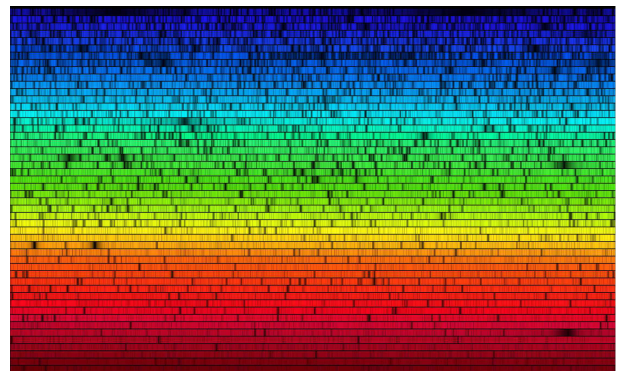

Figure 8: The optical database viewer

Double click on the icon called, *sun*, this should bring up a spectrum of the sun's spectrum. Have a look at where the peak of the spectrum is. Now close this window, and open the spectrum called *led*. Where is the peak of this spectrum.
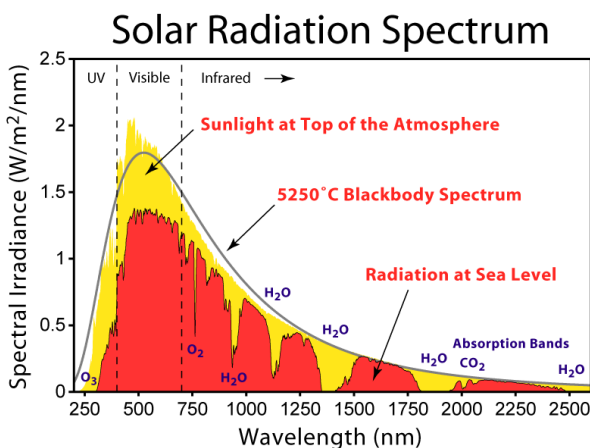
Figure 9: a: A plot of the entire solar spectrum. b: The image below shows the solar spectrum at 392 nm (blue) to 692 nm (red) as observed with the Fourier Transform Spectrograph at Kitt Peak National Observatory in 1981. R. Kurucz

Question 4: Describe the main differences between the light which comes from the LED and the sun. Rather than referring to the various regions of the spectrum by their wavelengths, refer to them using English words, such as *infrared*, *UltraViolet*, *Red*, and *Green* etc... you will find which wavelengths match to each color on the internet. If you were designing a material for a solar cell, what wavelengths would.

2.5.2 Light inside solar cells

As you will have seen from when you fist opened the simulation, the solar cells are often made from many layers of different materials. Some of these materials, are designed to absorb light, some are designed to conduct charge carriers out of the cell. The simulator has a database of these materials, to look at the database, click on the *Database* tab, the click on *Material database*. This should bring up a window as shown in figure 10, once this is open navigate to the directory *polymers*, and double click on the material *p3ht*, in the new window click on the tab *Absorption* (see figure 11). This plot shows how light is absorbed in the material as a function of wavelength.
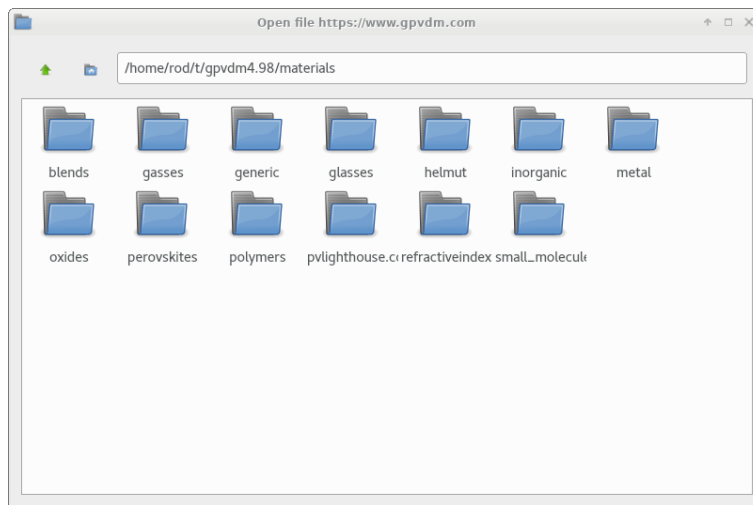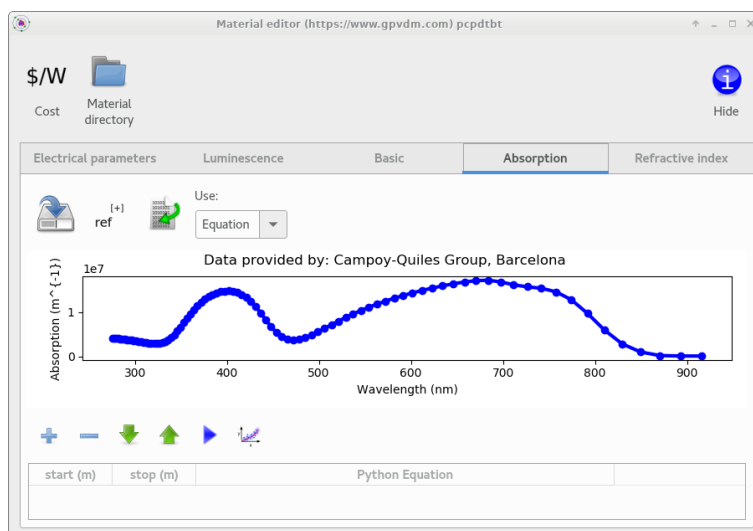

Figure 10: The materials database

Figure 11: Optical absorption of the light.

Question 5: What color of light does the polymer *p3ht* absorb best? Which material in the *polymers* directory do you think will absorb the suns light best?

Now, set the active layer thickness back 50 *nm* and go to the optical *Simulations* tab in the device simulator window. Click the *Opticalsimulation* button. This will bring up the optical simulation window. Click the run button (blue arrow), then select the tab named *Photonsabsorbed*. This plot will show where the photons have been absorbed within the device. Go back to the output window, and open up *sim_info.dat* again, there should be a value in there telling you how many photons have been absorbed in the active layer of the solar cell.

Question 6: By running 5 or 6 with different active layer thicknesses, plot a graph of active layer thickness, v.s. the number of photons absorbed in the device. At what thickness do almost all photons get absorbed in the device? [Hint: I would run the simulations from $40nm$ to $200nm$]

2.6 Understanding recombination in solar cells

When the device is very thin, it can't absorb very many photons, hence the efficiency will be low. When the device is very thick the device can absorb all the photons incident on it from the sun and the efficiency will higher. You should have found this out above. However, the thicker the device becomes, the further the electrons and holes will have to travel, from where they are generated to the contacts, where they eventually exit the device and perform useful work in the external circuit.

The further the electrons/holes have to travel, the longer they stay in the device after photogeneration, and thus the more probable it is that an electron will meet a hole, or a hole will meet an electron. When an electron and hole meet, because one is positive and one negative, they annihilate each other and are both instantaneously destroyed, this is called *recombination*. Recombination lowers the efficiency of a solar cell because, it means an electron/hole which were generated by a photon have been wasted.

Question 7: In no more than two sentences describe what an electron and hole are.

The rate (R) at which free electrons and holes meet each other and recombine in a device is given by the equation:

$$R(x) = kn(x)p(x) \tag{1}$$

When n(x), is the density of electrons at any given point in the device, and p(x) is the density of holes at any given point in the device. The constant k is called the recombination constant, and determines how efficient the electron/hole recombination process is. If $k = 0$, then clearly no electrons or holes will recombine. Conversely, if k is very large, electron and hole recombination will be very probable. You can set the value of for k, in the model by, going to the $main simulation window$ (see figure 4), clicking on the $electrical parameters$, button, this should open a new window. Click on the $Electrical parametes tab$, then scroll down until you find the value "n_{free} to p_{free} Recombination constant" scrolling down to the very bottom and finding the value 'n_{free} to p_{free} recombination rate constant', this should be set to a value of 1×10^{-20}. Try changing this value 1×10^{-15}. And rerun the simulation a for five or so different thicknesses of active layer between 50nm and 300 nm.

Question 8: Plot a new graph of active layer thickness v.s. device efficiency. By looking at your graph, what is the optimum device thickness for a device with a recombination constant of $k = 1 \times 10^{-15}$?

2.7 Charge carrier mobility and it's impact on solar cell efficiency

Key to a solar cell being efficient is having as many photogenerated carriers from the active layer reaching the contacts as possible. One way to achieve this is to have a low recombination rate, as discussed in the previous section. Another way to make the device more efficient, is to make the electrons and holes (otherwise known as charge carriers) spend as little time in the device as possible. If we can get the charge carriers out of the device as quickly as possible after they are generated, then the chance of an electron meeting a hole will be reduced. The speed at which electrons and holes move within a device is determined by the electron and hole charge carrier mobility. You can find the values of electron and hole mobility in the 'Electrical Parameters' window, under the 'Electrical parameters' tab, under the section 'Electron/Hole mobility'.

Put the recombination constant back up to 1×10^{-20} and then reduce the values of both electron and hole mobility to 2.48×10^{-8}, then rerun the simulation. Run 4-5 simulations with different thicknesses of active layer, to find the optimum thickness for the device with the lower mobility.

> Question 9: What is the optimum active layer thickness with the lower mobility value? If you wanted a really efficient solar cell what values of mobility and recombination rate would you use?

2.8 The mu-tau product

The symbol for mobility is μ, one can define an average mobility for the device by taking the electron mobility, adding it to the hole mobility and dividing by two. You can find the values of mobility in the Electrical parameters window. Now calculate the average mobility by using the equation.

$$\mu_{avg} = \frac{\mu_e + \mu_h}{2} \tag{2}$$

Recombination in a device, can be thought of the average time a charge carrier will survive in a device without recombining. This time is often given the symbol tau or τ. This value can be found by looking in the file $sim\_info.dat$, you will find the value under the heading $Recombination time constant$

The value of μ dictates how long it will take a charge carrier to exit the device after being generated. The value of τ will describe how likely it will be for a charge carrier to recombine in the device. Thus we can use the value of $\tau * \mu$, as a measure of how good/efficient the solar cell is. A large $\tau * \mu$ means charge carriers exit the device quickly and take a long time to recombine, a low $\tau * \mu$, means charge carriers exit the device slowly and and have a high chance of recombining.
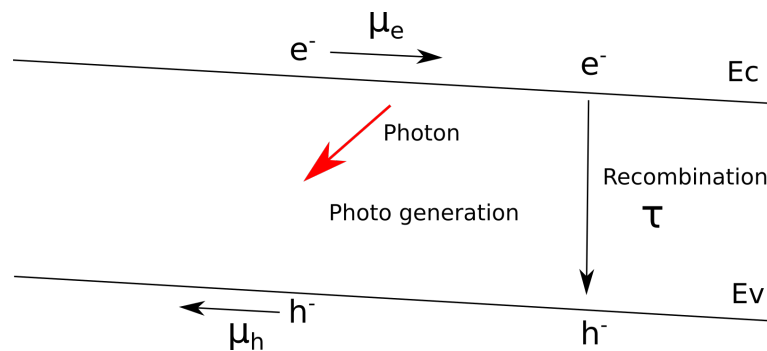

Figure 12: The physical processes governing the operation of a solar cell. The photon is shown, generating an electron and a hole. These then, these charge carriers move to the contacts governed by the mobility (μ). There is also a finite probability of them combining at rate τ

Question 10: Make a fresh simulation. Set both the electron mobility to $1x10^{-6} m^2/(Vs)$ and the hole mobility to $1x10^{-5} m^2/(Vs)$. Then calculate the value of $\tau * \mu$, for your device. Show your working in your report.

2.9 Parasitic components

A solar cell is just a diode like any other diode, gpvdm is really just a complex diode simulation program. Unfortunately, solar cells are never perfect diodes and in reality they have both series (R_s) and shunt resistance (R_{shunt}) (see figure 13). Also due to the flat broad contacts on a solar cell, there is often a capacitance associated with the device, although we won't discuss this further now. The series resistance accounts for things such as the resistance of the contacts (The Al and ITO), while the shunt resistance accounts for impurities in the active layer forming short circuits between the ITO top contact and Al bottom contact. Clearly if R_{shunt} were zero (i.e. a full short circuit), the solar cell would not work at all, and if R_{shunt} were very big say $1M\Omega$, the solar cell would work a lot better.
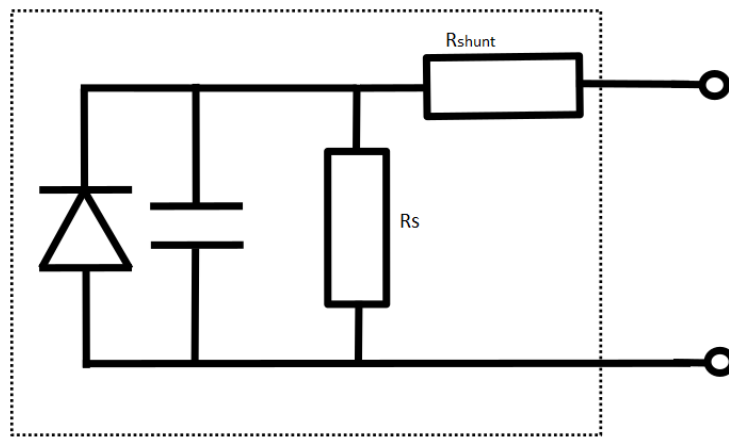

Figure 13: Circuit model of a solar cell.

You can change the values of series and shunt resistance in gpvdm, by going to the 'Device structure' tab and then clicking on the 'Parasitic components' button.

> Question 11: Make a fresh simulation, then run two JV curve simulations with a shut resistance of $1x10^6\Omega$ (a very high value) one with a resistance of 100Ω. What happens to the solar cell efficiency as the shunt resistance is reduced? Plot a graph with shunt resistance on one axis, and device efficiency on the other (a minimum of four points) showing this effect. What is the reason for the trend on the graph?

2.10 Solar cells in the dark

So far, all the simulations we have run have been performed in the light. This is a logical, as usually we are interested in solar cell performance only in the light. However, a lot of interesting information can be gained about solar cells by studying their performance in the dark. We are now going to turn off the light in the simulation. From the 'Home' tab set the light intensity to 0.0 Suns. The photons in the 3D image should disappear as seen in figure 14.
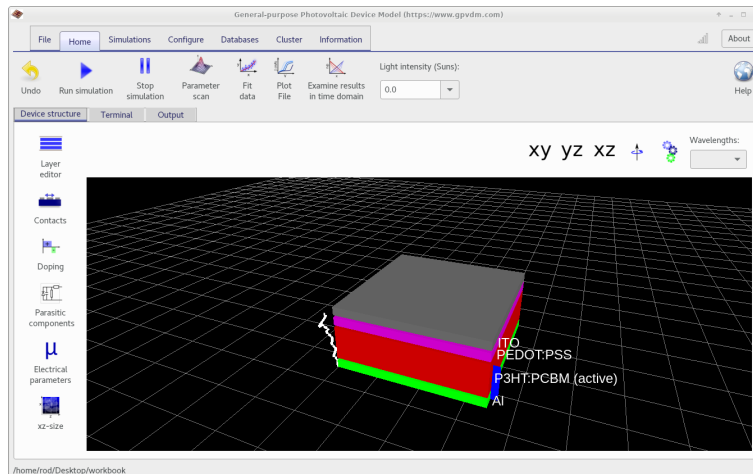
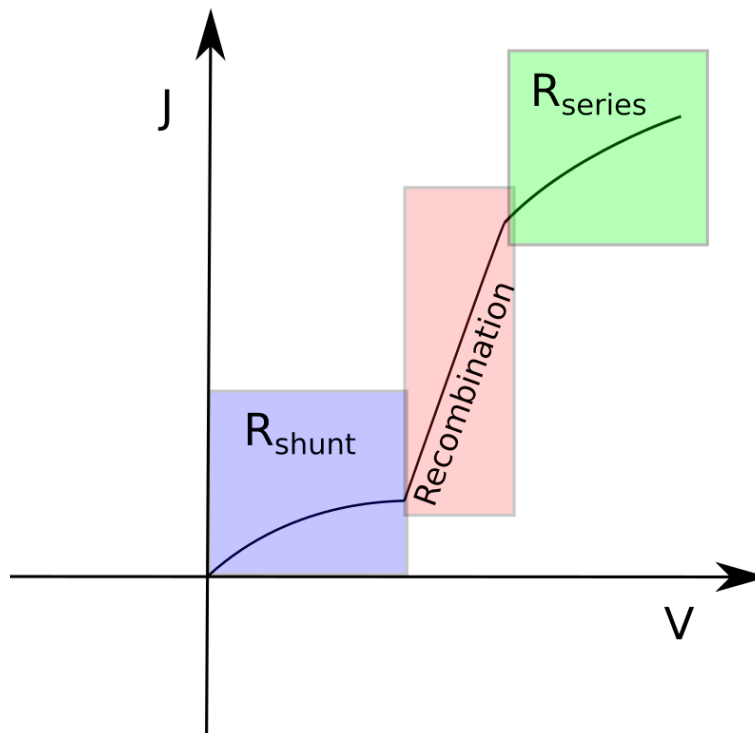

Figure 14: Running gpvdm in the dark.

Figure 15: A sketch of a typical dark JV curve.

Now set the shunt resistance to $1M\Omega$, and run a simulation. Plot the jv curve. It is customary to plot jv curves on a x-linear y-log scale. To do this in the plot window, hit the 'l' key to do this. The shape should resemble, the JV curve in figure 15. Certain solar cell parameters affect different parts of the dark JV curve

differently, the lower region is affected very strongly by shunt resistance, the middle part is affected strongly by recombination, and the upper part is strongly affected by the series resistance.

> Question 12: What values of series and shunt resistance, would produce the best possible solar cell? Enter these values into the device simulator and copy and paste the dark JV curve into your report.

2.11   Trap states in solar cells

The material from which solar cells are made often have impurities in them. These impurities can be made of anything, ranging from oxygen being trapped in the material during manufacture, to a spec of carbon. In traditional, semiconductor materials such as silicon, the number of impurity sites are quite low because a lot of effort is put into remove these defects through purification. However, extensive purification of these semiconductors requires significant amounts of energy and makes the solace cells expensive. Currently, there is significant world wide effort to produce new semiconductors which require less purification, the down side to this is that these more novel semiconductors have more defect states in them.

The problem with having defects in semiconductors is that electrons, or holes get trapped on these sites, where they stay. When a passing charge carrier of the opposite polarity gets close to the trapped charge carrier, it gets sucked into it's potential well and recombination happens. This is called free-to-trap recombination, or Shockley-Read-Hall recombination to give it it's full name. Let's take a look at how these trap states effect the efficiency of the solar cell. In the "electrical parameters", window where you changed the mobility and recombination rate, find the lines which say "electron trap density", and "hole trap density". Set both these values to $1x10^{10}m^{-3}$, this number might seem big but it is in fact a very small value of trap states, when you consider the number of silicon atoms per m^{-3} in a typical semiconductor is $1x10^{28}$.

> Question 13: Run a JV curve simulation in the light, with the number of trap states set to $1x10^{10}m^{-3}$, copy the resulting JV curve into your report. Then up the number of traps to $1x10^{25}m^{-3}$, and rerun the simulation, copy the result into your report. What happens to J_{sc} and V_{oc} when the number of trap states are increased?

2.12 Using time domain methods to study solar cells.

When solar cells are used, they are used in steady state. This means that there is no sudden change of voltage or light intensity. Clearly, as the sun moves though the sky, during the day there will be a change in light intensity, but this is very slow in comparison to the speed at which the processes in solar cells happen. However, in an experimental setting, changing the voltage or light intensity rapidly can be a useful thing to do. Measurements which are performed as a function of time, are called transient measurements. Transient measurements, an example of this type of measurement is called the CELIV measurement, CELIV stands for Charge Extraction via Linearly Increasing Voltage. Make a new simulation, then in this measurement a voltage ramp is applied to the solar cell as a function of time. Initially the voltage is kept constant, then it is slowly, changed from $0Volts$, to a a negative voltage, finally the voltage suddenly returned to $0V$, this is depicted in figure 18.

To perform a CELIV measurement, we need to change the mode the simulator is in. Click on the Simulation tab and then change the simulation mode to "CELIV", as shown in figure 16.
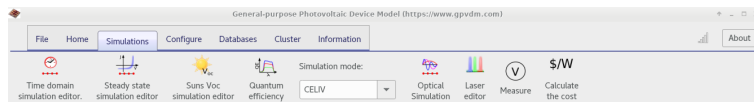

Figure 16: Set the simulation mode to CELIV.

Now, let's have a look at the voltage pulse which will be applied, click on the Simulation tab, then click on 'Time domain simulation editor', you should get a window looking like figure 17
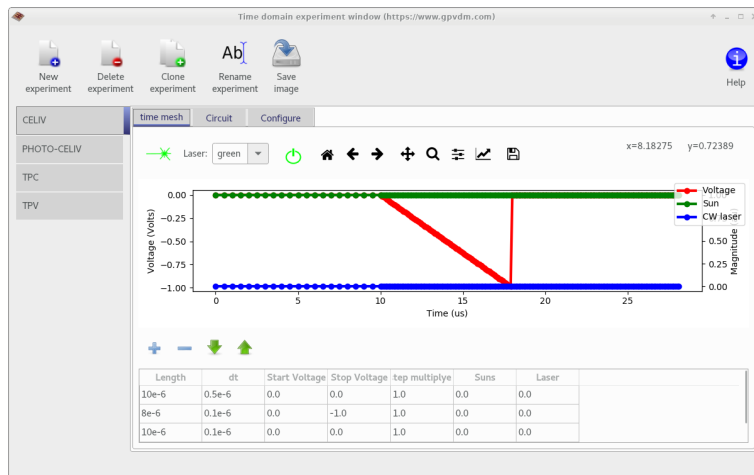

Figure 17: Set the simulation mode to CELIV.

Now, click on the run button and the simulation will run. This time, the current is stored in a file, $pulse\_j.dat$, then in the plot window select 'Math' and 'Invert y-axis', and your plot should look something like figure 18.

> Question 14: Increase the electron and hole mobility by two orders of magnitude, then copy and paste the graph into your report. What happens to the transient? Do you think the CELIV measurement could be used to detect changes of mobility in the cell? Write your answer in your report.
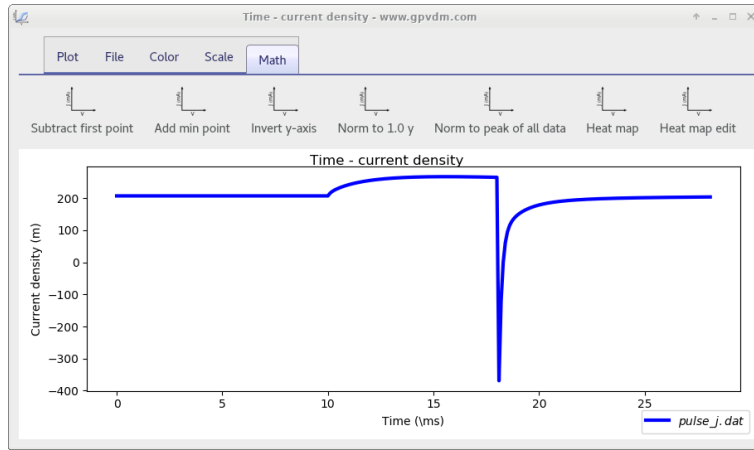
Figure 18: An example of a CELIV transient

2.13 Summary

Summarize in a few sentences what electrical and optical material properties would make a good solar cell.