# 3.003 Lab 4 – Simulation of Solar Cells

# **Objective:**

To design a silicon solar cell by simulation. The design parameters to be varied in this lab are doping levels of the substrate and the refractive index/thickness of antireflection coating. We will also explore I-V curves under different excitation intensities.

## Simulation Software: PC1D. Note that this software runs on Windows systems.

### **Procedure:**



### Fig. 1 Simulation software interface

- 1. Download and Unzip the folder "PC1D5"
- 2. Open the folder, and double-click on "PC1D"
- 3. You should be able to see the interface of the simulation program as shown in Fig. 1. Now you are in the "parameter" view. In this window, you can double click on any line and a window will pop out for you to modify the parameters
- 4. Now let us change a few parameters to set up a silicon solar cell.
  - (a) Under <u>"Device"</u>: Double-click "Device Area" and change it to 100 cm<sup>2</sup>. Double-click

<u>"No Exterior Front Reflectance"</u>. In the window that pops out, click on "coated", and input "1000" (nm) into the outer layer thickness with index=1 (refractive index of air). This way we are setting up a silicon solar cell without antireflection coating.

- (b) Under <u>"Region 1"</u>: Double-click "Thickness" and set it to 300 μm, the typical thickness of a silicon wafer; double-click "Material from program defaults" and chose the file "Si". Click on "p-type background doping" and change the P-type doping concentration level to "5e16" (cm<sup>-3</sup>). This way we are defining a lightly doped p-Si substrate. To form a P-N junction, click on "No front diffusion", check "enable" and "n-type", Peak Doping=1e19 (cm<sup>-3</sup>), depth factor "2 um", and profile "uniform" for simplicity. This way we are setting up an n-type region near the surface of the Si wafer. Click on "Bulk Recombination" and input tau-n and tau-p=10 (us) for typical solar cells. These are the carrier lifetime before electron and holes recombine.
- (c) **Excitation:** Let us launch optical excitation, or solar illumination. Click on the Excitation button shown in Fig. 1 (next to " $S_R$ ) and choose "one-sun" from the file. This way we are launching a standard AM1.5 solar radiation. Click on "Excitation mode" and change the number of time steps to 100. Click on "Base Circuit" and set the all resistances to 0; put voltage to -0.2V under transient, and initial voltage to -0. 7 V and final voltage to 0.7 V under "transient". This will enable us to see the I-V curve under illumination.

# **Exercises:**

### **1. I-V curves under different excitation intensities**

Take a look at the excitation intensity ("Constant Intensity" under "Excitation"). The number you see now is 0.1 W/cm<sup>2</sup>, which is the standard excitation power for AM1.5 solar illumination.

To obtain the I-V curve under this condition, click on the "Run" button or choose "Compute"  $\rightarrow$  "Run". Then choose "Graph"  $\rightarrow$  "Temporal"  $\rightarrow$  "Base I-V". Now you have the I-V curve under illumination. Go to "Graph"  $\rightarrow$  "Copy Graph Data" and copy the I-V data to an Excel sheet or any software you like for figure plotting. You can return to the parameter sheet by choosing "View"  $\rightarrow$  "parameter".

**Task 1.1:** Plot the I-V curve. Find the maximum output power from the I-V curve, and mark the current and voltage corresponding to maximum power output on the plot. Explain how you find this maximum output power. Compare your calculation to "Max Base Power Out" under "Results". Are they consistent? Also calculate the energy conversion efficiency and the corresponding load resistance of the solar cell under maximum power output.

Now let us turn off the light. Ideally, we would like to input "0" for "Constant Intensity" under "Excitation". However, this induces some problems in the numerical simulation of the software. So we input a very small number of 1e-9 (W/cm<sup>2</sup>) instead into the Steady State, Transient Initial and Transient Final power. Click "Run".

**Task 1.2:** Obtain I-V data under this negligible illumination condition. Show I-V curves with 1e-9  $(W/cm^2)$  and 0.1  $(W/cm^2)$  excitations in the same plot. What are the major differences? Explain the changes in I-V curves with and without illumination using the diode model you learnt in class.

**Task 1.3:** Choose a few more excitation power and plot the short circuit current  $I_{sc}$  (labeled Ib) and the open circuit voltage  $V_{oc}$  (labeled Vb) as a function of excitation power. **Can you find a model to fit these data? (Extra credit)** 

### 2. Effect of substrate doping on output voltage

You have learnt in class that the output voltage of a solar cell is related to the chemical potential difference across the P-N junction. Now let us explore it through simulation.

**Task 2.1**: Change the excitation intensity back to  $0.1 \text{ W/cm}^2$ . Vary the P-type background (substrate) doping level between 1e14 and 1e17/cm<sup>3</sup> (you can choose a few data points), and record the corresponding open circuit voltage (V<sub>oc</sub>), short circuit current (I<sub>sc</sub>), and the max output power (V<sub>max</sub>) in a data sheet. Make a plot of these parameters vs. P-type substrate doping. You can use a log scale for the doping level in x-axis. Explain the results according to what you learnt about the effect of doping on chemical potential of electrons in class.

### **3. Finding the Band Gap of Silicon**

You have learnt in class that a semiconductor material like Si has a "band gap". Photons below this band gap energy cannot excite an electron from the ground state (valence band) to the excited state (conduction band), so it cannot be absorbed by the material and generate electricity. On the other hand, photons above this band gap energy can be absorbed by the material and generate free carriers. In this section we will find out the band gap of Si by looking its absorption spectrum.

Change the background doping density back to 5e16/cm<sup>3</sup>. Click on "Excitation modified from one-Sun", and choose the file "SCAN-QE". This will enable you to check out internal quantum efficiency (IQE), external quantum efficiency (EQE), and reflectance as a function of wavelength (RFL). EQE and IQE are defined as

$$EQE = \frac{Number of carrier pairs generated}{Number of incident photos} \times 100\%$$

$$IQE = \frac{Number of carrier pairs generated}{Number of photos absorbed by the material} \times 100\%$$

"Carrier pair" refers to "electron-hole pairs" here. Note IQE and EQE are different from the power conversion efficiency. Click "Excitation mode: transient" and increase the number of steps to 200. Click on "Monochorome, wavelength from..." and change the spectrum range from 300 nm to 1250 nm.

Run the program, and find the IQE, EQE and RFL spectra by going to "Graph"  $\rightarrow$  "Temporal"  $\rightarrow$  "Quantum Efficiency". The red, green and yellow lines correspond to IQE, EQE and RFL, respectively. You can copy the data to an Excel sheet for more detailed analysis.

Task 3.1 Find out the band gap of Si in unit of eV. Note the horizontal axis is wavelength in unit of

(nm) and you will need some conversion to calculate the band gap.

**Task 3.2** Derive the refractive index of silicon as a function of wavelength from the reflectance (RFL) spectrum using the equation:

$$RFL = \left(\frac{n_1 - n_2}{n_1 + n_2}\right)^2$$

**Task 3.3** From these spectra, can you also find out a simple equation describing the relationship among EQE, IQE and RFL for photon energy much larger than the band gap?

**Task 3.4 (Extra credit)**: Can you describe how to derive the short circuit current  $I_{sc}$  using EQE spectrum and solar spectrum? Can you further derive the power conversion efficiency using an ideal diode model?

### 4. Design an antireflection coating

You have noticed that a significant portion of optical power is reflected at the air/silicon interface, which reduces the external quantum efficiency. As we discussed in class, an adequate layer of antireflection (AR) coating can be used to match the optical impedance and reduce the reflection. Now you can try different AR coating designs and check out the result.

You can add an AR coating by double-clicking "Front surface optically coated", and input the film thickness and refractive index.

**Task 4.1** Design your own single-layer AR coating using the simple approach explained by Prof. Kimerling in class. Input an index of  $n_{AR} = \sqrt{n_{air} * n_{Si}(\lambda_0)}$  and a thickness of  $\lambda_0/(4*n_{AR})$  for the AR coating. This will minimize the reflection at  $\lambda_0$ . Now you can look at the solar spectrum in the lecture notes and decide which wavelength  $\lambda_0$  could give you the optimal solar cell performance. Plug in the corresponding refractive index and thickness. Obtain the IQE, EQE and RFL spectra for this case and compare it to the data obtained in Section 3. Do you see a significant decrease in RFL? From the RFL spectrum, can you determine what color is the surface of the solar cell with AR coating?

Change the excitation file back to "ONE-SUN" again and find out the cell efficiency. Is it improved from the bare Si cell data you obtained in Section 1?

**Task 4.2.** Choose a few wavelengths shorter or longer than  $\lambda_0$  to optimize your single-layer AR coating design for maximum solar cell efficiency. You can switch the excitation files back and forth between "ONE-SUN" and "SCAN-QE" to obtain the overall cell efficiency and the IQE/EQE/RFL spectra for comparison.

**Task 4.3 (Extra credit).** Try some double or triple layer design and see if you can further reduce reflection and increase cell efficiency

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