

SOLUTION SERIES 9

The purpose of this series of exercise is to become familiar with the simulation software PC1D. In order to start, you will have to download the folder PC1D from the Moodle and save it on your computer. Then, open the application "pc1d.exe" in the "PC1D58" folder, and open the file *Exercise07_ex01.prm*, which contains a model of a typical device (p-n junction) with a p-doped base and an n-doped emitter at the front.

The file automatically opens in the tab "parameter view" (look at the small icons in the top of the window). Here, you can find the simulation settings on the left, devided in 3 parts:

- "Device" where you can set the device parameters
- "Region 1" where you can set the parameters of the base and emitters regions of the solar cell
- "Excitation" where you can set the incident light properties. The incident light comes from the top of the device

On the right, you have a scheme of the device modeled.

The emitter at the front side (red part on the scheme, "1st front diff" on the settings part) has a thickness of $d_e = 1 \mu\text{m}$ and is highly doped $N_D = 10^{20} \text{ cm}^{-3}$. The base (blue part) is $d_b = 180 \mu\text{m}$ thick and has a doping concentration of $N_A = 1.513 \times 10^{16} \text{ cm}^{-3}$. The initial values for the surface recombination velocities are $S_n = S_p = 10^4 \text{ cm s}^{-1}$ for the front side (emitter) and $S_n = S_p = 10^3 \text{ cm s}^{-1}$ for the back side (base). The bulk lifetime is set to the same value in both regions $\tau = 30 \mu\text{s}$.

In the following we will try to improve the efficiency of the solar cell in a first step by enhancing the electrical properties and in a second step by reducing the optical losses.

Please note:

- bulk refers to the base, i.e. the $180 \mu\text{m}$ thick piece of p-doped crystalline silicon
- In the bulk lifetime tab (icon with τ) the first two fields show the Shockley-Read-Hall (SRH) lifetime of electrons (τ_n) and holes (τ_p) in the base. these are called τ or SRH lifetime. The field below called *NET LLI tau* refers to the total lifetime in the base. The diffusion length is also displayed.
- *Front* refers to the front surface (emitter) and *Rear* refers to the back surface (base). The front and rear recombination velocities are respectively displayed in the Front and Rear surface tabs.
- The Front and Rear Surface tabs give also access to the saturation current, which is function of the surface recombination. It is called *Equivalent J_0* and can be divided into 3 contributions: J_{0e} (emitter), J_{0b} (base) and bulk recombinations.
- There are two different pre-sets for the excitation file, the *one-sun.exc* file is for the calculation of the current-voltage curve and the *scan-qe.exc* is for the calculation of the quantum efficiency.

Introduction

This short introduction will help you to find the most important parameters in PC1D.

- Double clicking on the different layers in the scheme of the device or on the different parameters on the left, give you access to the main electrical parameters, i.e. doping type, doping level, resistivity, mobility and diffusion coefficient (diffusivity). For the diffused emitter you have also control over the peak doping, doping depth (depth factor) and peak position. Note that it is also possible to set the resistivity value instead of the doping value. For example concerning the Base the target resistivity of $\rho = 0.9997 \Omega \text{ cm}^{-1}$ gives $p = 1.513 \times 10^{16} \text{ cm}^{-3}$ (according to the formula $\rho = (e n \mu)^{-1}$).
- Click on the "Four graphs view" tab (just beside the "Parameter view" tab). Here, you can display 4 different parameters (like e.g. the dopant densities, the carrier (holes and electrons) densities, the internal electric field, etc.) that you can choose in Graph –> Spatial or Temporal. Run the simulation clicking on the "Run" tab (the small guy running), display the electric field and explain its profile. Note: to go back to the 4 graph view, you can use Esc.

Solution:

As seen during the course the field is localized at the junction. This is the reason why we call this type of solar cell a "diffusion device". The collection of the carriers happens due to the diffusion of the minority carriers. In contrast, a thin film silicon solar cell is a "drift devices" where an electrical field is necessary across the active region to collect the carriers.

- Go back to the "Parameter view" and find the bulk lifetime in the base, as well as the front and back surface recombination velocities. Is it a good base? Are the surfaces well passivated?

Solution:

The base lifetime $\tau_b = 30 \mu\text{s}$ is a pretty low value for the carrier lifetime. Nevertheless, the diffusion length of the minority carriers is equal to $283.3 \mu\text{m}$ which is bigger than the base width of $180 \mu\text{m}$. Thus electrons can reach the junction easily by diffusion. The values for the surface recombination velocities of electrons and holes at the front and back surface, are much higher than the ones that can obtain for good surface passivation, e.g. $<10 \text{ cm s}^{-1}$ but still lower than for really bad passivation quality $<1 \times 10^7 \text{ cm s}^{-1}$.

Exercise 1: Influence of surface recombination on efficiency

- Load the excitation file "one-sun.exc". For this, double click on "Excitation from..." and find the right file. Then run the simulation to obtain the V_b , I_b and the max. power. What is the cell efficiency and its FF?

Solution:

Parameter	Value
Short-circuit I_b	-2.839 A
Max base power out	1.378 W
Open-circuit V_b	0.615 V

The cell efficiency is 13.78% and the FF is 78.9%

b) To model a very bad surface passivation, set S_n and S_p equal to 10^7 cm s^{-1} for both emitter and base regions. What do you expect? What are V_b , I_b and the cell efficiency obtained by simulation?

Solution: With a higher surface recombination velocity, we decrease the excess electrical carrier density and then the V_b . If these carriers recombine before they reach the contact, the short circuit current is also decreased. Finally, if both V_b and I_b decrease, the cell efficiency is also lower.

Parameter	Value
Short-circuit I_b	-2.575 A
Max base power out	1.224 W
Open-circuit V_b	0.602 V

c) Simulate a good surface passivation by setting S_n and S_p equal to 1 cm s^{-1} for both surface. What do you expect? What are the V_b , I_b and the cell efficiency that you obtain? What is the diffusion length?

Solution:

For the same reason than the previous question, we expect to reach higher V_b and I_b . The diffusion length $L_T = 283.3 \mu\text{m}$

Parameter	Value
Short-circuit I_b	-2.953 A
Max base power out	1.458 W
Open-circuit V_b	0.625 V

d) Do the same simulations as in part b) and c) with $\tau = 3 \mu\text{s}$. What do you expect? What do you obtain for V_b , I_b and the cell efficiency?

Solution:

With $\tau = 3 \mu\text{s}$, the diffusion length is lowered to $90.1 \mu\text{m}$. Hence, the surface has less influence because electrical carriers can less easily reach it. Hence, we expect to have a lower variation for the V_b and for the I_b than in the previous case with $\tau = 30 \mu\text{s}$.

Parameter	$S_{n,p} = 10^7 \text{ cm s}^{-1}$	$S_{n,p} = 1 \text{ cm s}^{-1}$
Short-circuit I_b	-2.443 A	-2.601 A
Max base power out	1.127 W	1.207 W
Open-circuit V_b	0.588 V	0.591 V

e) Set $S_{n,p} = 10^4 \text{ cm s}^{-1}$ for the emitter (front), $S_{n,p} = 10^7 \text{ cm s}^{-1}$ for the base (rear) and $\tau = 30 \mu\text{s}$. To limit the surface recombination at the back surface, it is possible to create a Back Surface Field (BSF) by introducing Al atoms in the bulk during the firing. Model this BSF by adding a rear diffusion with a peak doping of 10^{19} cm^{-3} and a doping depth of $10 \mu\text{m}$ with

an uniform profile. Run the model with and without the BSF. How does the BSF work and which parameters does it influence?

Solution: The BSF repels the minority carriers (electrons) from the back surface. Since the minority carriers control the recombination, less surface recombination will occur and the V_b and the I_b will be increased.

Parameter	With BSF	Without BSF
Short-circuit I_b	-2.885 A	-2.657 A
Max base power out	1.421 W	1.262 W
Open-circuit V_b	0.623 V	0.603 V

f) Nevertheless, a very well passivated wafer is better than a BSF without passivation. Run the model again with $S_{n,p} = 1 \text{ cm s}^{-1}$ for both surfaces. What do you obtain?

Solution: Note: The open circuit voltage improvement will be more important with a better carrier lifetime. Indeed, by improving τ , the cell becomes more sensitive to the surface passivation.

Parameter	Value
Short-circuit I_b	-2.901 A
Max base power out	1.430 W
Open-circuit V_b	0.624 V

Exercise 2: Influence of base and emitter lifetime on efficiency

a) Set $S_n = S_p = 1 \text{ cm s}^{-1}$ at the front and rear surfaces and the bulk lifetime in the base to $\tau_{bulk} = 30 \mu\text{s}$ and run the simulation to obtain the values for the current, the voltage and the power.

Solution:

Parameter	Value
Short-circuit I_b	-2.901 A
Max base power out	1.430 W
Open-circuit V_b	0.624 V

b) Change τ_b to 5 ms (good base material quality). What value do you expect for the V_{oc} ? Higher or lower? Run the simulation to check.

Solution:

Parameter	Value
Short-circuit I_b	-2.978 A
Max base power out	1.511 W
Open-circuit V_b	0.639 V

The efficiency does not change a lot as both the voltage and the current only change by about 3 % increase. Due to the high emitter doping (10^{20} cm^{-3}) the total lifetime is strongly limited by Auger recombination. Thus even increasing the SRH lifetime won't help much, as it is dominated by the Auger lifetime. Although the base material is good and the passivation is ok, the low total lifetime in the emitter leads to a high J_{0e} which limits the V_{oc} . The current increases due to the improvement of the SRH lifetime as more electrons can reach the junction.

c) Load the *scan-qe* excitation file, set $S_n = S_p = 10^7 \text{ cm s}^{-1}$ for the top and rear surfaces and compute the spectral response by running the simulation. On the graphs, determine the IQE value (you can click on the graphs to display (in the very bottom left of the window) the desired value) at 300 nm and 400 nm. Change the surface recombination velocities at the front to $S_n = S_p = 1 \text{ cm s}^{-1}$. Run the simulation again and note the IQE values for the same wavelengths. Change the emitter thickness to 50 nm and determine the IQE values for the two different recombination velocities above. Explain the result.

Solution:

Results for $S_n = S_p = 10^7 \text{ cm s}^{-1}$:

Parameter	Value
IQE(300 nm)	0.43 %
IQE(400 nm)	5.43 %

Results for $S_n = S_p = 1 \text{ cm s}^{-1}$:

Parameter	Value
IQE(300 nm)	17.64 %
IQE(400 nm)	19.23 %

Results for an emitter thickness of 50 nm and (1) $S_n = S_p = 1 \text{ cm s}^{-1}$ and (2) $S_n = S_p = 10^7 \text{ cm s}^{-1}$:

Parameter	Values	
	(1)	(2)
IQE(300 nm)	99.4 %	19.52 %
IQE(400 nm)	99.84 %	81.90 %

There are mainly the following four points to understand here:

- For a 1 μm emitter and any surface recombination, the IQE is lower than for the emitter thickness of 50 nm. This can be explained by the fact that, for the thick emitter, less carriers are collected. Indeed only carriers that are created further than 500 nm from the front surface are collected, as the junction is deeper within the material (compare the carrier densities). The *real* collection starts only at wavelengths of around 400 nm as these photons can travel further without being absorbed. Photons of 300 nm wavelength get absorbed over a very short distance, thus the IQE at 300 nm is even lower.
- For high surface recombination (10^7 cm s^{-1}) the IQE is extremely low as even the carriers created at 500 nm inside the material will have a high probability to recombine at the surface.

- For an emitter thickness of 50 nm the junction is moved closer to the front surface and thus carriers created by high energy photons near the surface will be collected. Besides, the carrier diffusion length is longer than the emitter thickness, which enables good carrier collection. On the other hand, the device is more sensitive to surface passivation, as high surface recombination velocities will drastically reduce the number of collected carriers, i.e. the IQE is lower.
- As the device is much more sensitive to the surface recombination with a 50 nm thick emitter, the carriers created by high energy photons, e.g. 300 nm, that are created near the surface will almost all recombine. The carriers created by photons with lower energy, e.g. 400 nm, on the other hand will be created deeper within the material and have therefore a higher chance of being collected.

d) Change back to $S_n = S_p = 1 \text{ cm s}^{-1}$ at the back surface and front surface, $\tau = 5000 \mu\text{s}$ and an emitter thickness of 1 μm . Load the *one-sun* excitation file. What will happen if you now change the emitter doping to 10^{19} cm^{-3} ? Run the simulation and see if you were right.

Solution:

For an emitter doping of 10^{19} cm^{-3} and 10^{20} cm^{-3} :

Parameter	Values	
	10^{19}	10^{20}
Short-circuit I_b	-3.681 A	-2.978 A
Max base power out	2.001 W	1.511 W
Open-circuit V_b	0.684 V	0.639 V

It is clear that for lower doping, the Auger recombination is lower as well and thus the lifetime is higher. Therefore, more of the created carriers can be collected before they recombine. This leads to both an increase in current I_b and voltage V_b . As the latter is given by $V_{oc} \propto \ln(J_{ill}/J_0)$ it increases due to two effects:

- (1) the increase of the current and
- (2) the reduction of J_0

Exercise 3: Emitter thickness and doping optimization

In this section, the goal is to establish the optimized thickness and doping concentration for the emitter.

Set $S_n = S_p = 1.1 \times 10^4 \text{ cm s}^{-1}$ in the emitter (a standard value). Check that you have $S_n = S_p = 1 \text{ cm s}^{-1}$ in the Base and that $\tau_n = \tau_p = 5 \text{ ms}$.

To optimize two parameters at the same time, PC1D offers the possibility to compute sets of values automatically and thus, you do not need to enter and compute each set of values individually. To set a batch, go to the *Compute* menu, select *Batch*, *Quick batch* and set the following parameters:

- (1) Doping ranges from $1.1 \times 10^{17} \text{ cm}^{-3}$ to $1.1 \times 10^{20} \text{ cm}^{-3}$ in 10 steps:
Select "FrDoppeak1" parameter (1st Front Doping Peak) from 1×10^{17} to 1×10^{20} and *No of Steps* 10. Choose also a log spacing.

- (2) Thickness values vary from 50 nm to 2 μm in 10 steps:
Select "FrDopDpth1" parameter (1st Front Doping Peak) from 0.05 to 2, mark the *Permute* box and *No of Steps* 10.
- (3) Choose the ouptut paramters:
BaseVoc, BaseIsc, BasePmax

Close clicking "Ok" and run the simulation. You have 100 lines and different efficiencies (BasePmax).

- a) What is the best set of values of doping versus thickness?

Solution:

Table 1: $4.64 \times 10^{19} \text{ cm}^{-3}$, 50 nm in the emitter

	Values
Base I_{sc}	-3.703 A
Base V_{oc}	0.674 V
Max base power out	1.974 W

- b) Explain why there is an efficiency maximum

Solution:

For a given doping, I_{sc} and the efficiency decrease as the doping depth increases. This is mainly due to free carrier absorption (FCA) in the emitter. FCA is proportional to the carrier concentration and thus to the emitter depth. For a given thickness, a maximum for the V_{oc} and the efficiency is observed. Two competing effects are present: On one hand, increasing the doping concentration enhances the built-in voltage, i.e. the V_{oc} . On the other, a highly doped region will have increased recombination mechanisms (Auger, radiative and non-radiative) and, as a consequence a lower lifetime. Thus, charges created in the emitter will recombine more likely than if they were created in the base.

At relatively low doping concentration, the latter effect will be dominant whereas at high doping, Auger recombination will dominate. Moreover, at high doping concentration, heavy doping effects, such as bandgap narrowing, occur leading to a further decrease in the V_{oc} .

- c) Disable the batch mode and choose a 50 nm emitter, a doping of $4.64 \times 10^{19} \text{ cm}^{-3}$ and $S_n = S_p = 1 \text{ cm s}^{-1}$ in the emitter and in the base, keeping $\tau_n = \tau_p = 5000 \mu\text{s}$. How do you expect the efficiency to evolve? What is the obtained efficiency ?

Solution:

Table 2: $4.64 \times 10^{19} \text{ cm}^{-3}$, 50 nm with $S_n = S_p = 1 \text{ cm s}^{-1}$ in the emitter

	Values
Base I_{sc}	-3.704 A
Base V_{oc}	0.688 V
Max base power out	2.026 W

Exercise 4: Optical improvement

To obtain highly efficient solar cells, light needs to be effectively coupled into the wafer to be able to contribute to the photo-current. In this section, we will try to understand how to optimize this coupling. The optical characteristics are best observed in the EQE. To plot the EQE in PC1D, you need first to have a scanning wavelength and not a one-sun excitation. Click on the tab with the pink arrow just beside the "Run" tab, and choose the "scan-qe.exc" file. Run the simulation and look at the EQE in the graph view.

a) Plot the EQE with a bulk lifetime of 5 ms and then of 7 μ s (careful of units!). Comment on the effect of this electrical change on the EQE.

Solution:

The EQE is reduced for every wavelength but the main losses take place in the red region where the absorption coefficient is the lowest. You can observe a similar behavior in the IQE, pointing to a carrier collection problem.

Explanation: the blue light has a much larger absorption coefficient in silicon, compared to lower wavelengths. Thus, the energetic light is absorbed near the surface, so, close to the pn junction, and carriers generated by blue light don't have to cross a big distance to be separated thanks to the p-n junction. On the contrary, less energetic light (= higher wavelength light) will be absorbed within the entire 180 μ m of the solar cell, and carriers will have to cross large distances in silicon before being collected near the p-n junction. Red light generated carriers are generated at distances (from collection, so from p-n junction) which could be bigger than the diffusion length if the bulk lifetime is not high enough, but blue light generated carriers are anyway generated at distances (from the p-n junction) that are very low compared to diffusion length, even for low lifetimes. Red light generated carriers are then much more sensitive to the diffusion length, and thus the bulk lifetime, than blue light ones.

In this exercise, we will keep good electronic properties in order to observe more clearly the effect of the optical properties on the solar cell's performance.

b) Set the bulk lifetime back to 5 ms. The optical properties can be changed by clicking on the "Reflectance" tab, to the right of the print tab. For the front external reflection a common choice is to put an anti-reflective coating (ARC) of 70 nm with an index of refraction (n) of 2.2, as already set in the model. This layer is responsible for the low reflection in the 600 nm. If you change the anti-reflective layer thickness (bigger or smaller), what do you expect to happen to the reflection? Check this in PC1D. Why, in a standard cell, is the anti-reflective layer designed to be the most efficient at 600 nm? What is the gain in efficiency compared to the same cell without an ARC?

Solution:

Changing the thickness changes the wavelength of the reflection minimum, due to constructive interference of the light.

$$\text{ARC thickness} = \frac{\text{wavelength}}{4n} \quad (1)$$

600 nm corresponds approximately to the peak of the terrestrial solar spectrum, i.e. the energy for which the photon flux is maximum. Thus, the ARC is optimized for this wavelength.

Setting the ARC thickness to 0 nm, decreases the power output from 2.026 W to 1.446 W

c) Keep the ARC (70 nm with $n = 2.2$) and set the excitation back to one sun. One can improve the front and back surfaces of a solar cell so that more light is trapped in it (this light is called internal diffuse reflected light). How can you do that in practice?

In PC1D, this trapped light is modeled by the "Internal diffuse reflectance" parameter. To control this, go to the "Reflectance" tab – > "Internal reflectance", and set 90% for the first bounce and 95% for the subsequent bounces (front and rear). Run the simulation to see how the efficiency has changed and comment on the result.

Solution:

In practice, you can improve the light absorption both by introducing a surface texture (causes light trapping for any internal reflected light) and by replacing the back side aluminium with high quality silver to improve the back reflection. In that way, you increase the light coupling inside the cell as mentioned above, due to the double rebound effect.

Table 3: Effect of changing the internal reflectance and light trapping of a cell

Parameter	Original Refl.	90-95% Refl.
Base I_{sc}	-3.704 A	-3.786 A
Base V_{oc}	0.688 V	0.688 V
Max base power out	2.026 W	2.059 W

d) Silicon wafers can be easily textured as seen in the lecture. Here is a way to simulate textured surfaces in PC1D.

On a flat surface of silicon, about 30% of the incoming light is reflected, whereas on textured silicon it is only 10% (double rebound). Therefore, to simulate a flat solar cell in PC1D, one can add in the reflectance properties a broadband reflectance of 30% and decrease it to 10% to simulate a textured surface. Additionally for textured surfaces, you can simulate the physical texturing in PC1D going to the *Device* menu, click on *Texture* and add a front texture.

Set back the "internal diffused reflectance" at their initial values (75, 92, 80 and 80 % respectively) and simulate a flat solar cell with real broadband reflection, a flat solar cell with a broadband reflection of a textured cell and a real textured solar cell (broadband reflection properties and physical texturization). Compare and comment the results.

Solution:

The flat solar cell with the broadband reflection of a textured cell (10 %) might give the best V_{oc} . Indeed, texturing will increase the surface area and thus the J_0 , so slightly decrease the

V_{oc} . However, the physical texturing will also increase J_{sc} , and then will give the cell with the best efficiency. Note that if you have a high surface recombination velocity, the increase in current by adding a texture can be overcome by the loss in V_{oc} . Results are shown in Table 4 (always with an ARC).

Table 4: a) Broadband reflection 30% b) Broadband reflection 10% c) Broadband reflection 10% and textured surface

Parameter	Values		
	a)	b)	c)
Base I_{sc}	-2.479 A	-3.296 A	-3.314 A
Base V_{oc}	0.677 V	0.685 V	0.682 V
Max base power out	1.358 W	1.804 W	1.805 W

e) How could you further increase the light coupled in the cell?

Solution: Several paths can still be followed: e.g. adding a second anti-reflective coating, design all the contacts at the back of the cell (avoiding front shadowing), etc. The light coupling could then be simulated by a fixed reflectance of 2% (see Table 5).

Table 5: Cell with very good optical properties, good surface passivation, and with BSF

Parameter	
Base I_{sc}	-4.106 A
Base V_{oc}	0.688 V
Max base power out	2.31 W

NOTE: Moreover, we would like to point out that, with such low surface recombination velocity ($S_n = S_p = 1 \text{ cm s}^{-1}$), a BSF is not necessary current-wise and induces more losses due to Auger recombination than the reckoned improvement. According to this, the table below (Table 6) summarized this change. Note that removing the BSF in PC1D doesn't influence the contact resistance, whereas in a real cell it would!

Table 6: Cell with very good optical properties, good surface passivation, and without BSF

Parameter	
Base I_{sc}	-4.212 A
Base V_{oc}	0.722 V
Max base power out	2.425 W

To conclude, by changing the optical properties of a solar cell, the efficiency can be dramatically improved. With all the changes we have made with electrical material parameters and with the optical parameter, we have still not reached the world record of 25.1% for crystalline silicon solar cells.

Exercise 5: Towards a 30% solar cell...

a) Which parameter have we still not improved?

Solution:

Resistances (series resistance, contact resistance, shunt resistance, etc.). Some of them cannot be modeled in PC1D.

b) What happens if you change the base contact resistance (in parameters, part "Device" – > "Base contact") from 0.01 to 0.001, or 10^{-6} Ohm? Comment on the FF (you can have a look at the IV curves).

Solution:

The FF slightly decreases when contact resistance is higher.

c) We are going to simulate the cell under a concentrator. Set back the base contact resistance to 0.1 Ohm. In the parameters, in "Excitation part, double click on "Primary light source" (or in the Menu "Excitation" – > "Photogeneration" – > "Primary"). Change all the intensities for the steady state and transient cases from 0.1 (corresponding to an intensity one sun) to 1 (10 suns) W/cm^2 . Run the simulation. What happens if you change again the base contact resistance from 0.01 to 0.001, or 10^{-6} Ohm? Compare with the normal case (1 sun). *HINT:* If you have a problem, simulating the cell, check the IV curve. You can change the applied voltage by going to the *Excitation* menu and selecting *circuit*. Why would this be necessary?

Solution:

Under concentration, a very high change in the FF occurs when changing the base contact. This is due to Joule losses within the contact when a high current is collected throughout the contact. You can see this by going back to no concentration light, and noticing that the effect on the IV curve when changing the base contact is not as big.

d) Design a cell with an efficiency of more than 30% under 1 sun.

Solution: Please refer to the PC1D model given in the moodle.

Table 7: Near perfect cell

Parameter	
Base I_{sc}	-4.491 A
Base V_{oc}	0.765 V
Max base power out	3.039 W