Getting started with SCAPS

SCAPS (a <u>Solar Cell Capacitance Simulator</u>) is a simulation program developed at ELIS, University of Gent. The presentation here is based on version 3.0, March 2010.

0. The basics

SCAPS is a Windows-oriented program, developed with LabWindows/CVI of National Instruments. We use here the LW/CVI terminology of a 'Panel' (names used in other softwares are: a window, a page, a pop-up...). SCAPS opens with the 'Action Panel'.

	SCAPS 3.0.0 Action Panel	
	Working point Temperature (K) \$300.00	Action list —— All SCAPS settings
	Voltage (V) 0.0000 no no	Load Action List Load all settings
	Frequency (Hz) 1.000E+6 Rs Ohm.cm ² 2 Rsh 1.00E+3	Save Action List Save all settings
	Number of points \$5 S / cm ² Gsh 1.00E-3	
3.	Illumination: Dark Light G(x): From internal SCAPS calculation	Read from file
	Light source for internal G(x) calculation Spectrum file: Illuminatedside: from right (n-side) light power (Wim2)	External file to read G(x) from Generation file:
	Select Scaps\SCAPS 3.0 werkversie\spectrum\AM1_5G 1 sun.spe sun or lamp 0.00	Select *.gen
	Spectrum cut off? yes Short wavel. (nm) 0.0 after cut-off 0.00	Ideal Light Current in file (mA/cm2) 20.0000
	Long wavel. (nm)	Attenuation (%)
	Neutral Dens. 0.0000 Transmission (%) 100.000 after ND 0.00	Ideal Light Current in cell (mA/cm2) 0.0000
	Action Pause at each step	number
	□ Current voltage V1 (V) \$0.0000 V2 (V) \$0.8000	
Λ	□ Capacitance voltage V1 (V) \$-0.8000 V2 (V) \$0.8000	⇒81 = 0.0200 increment (V)
4.	Capacitance frequency f1 (Hz)	
	☐ Spectral response WL1 (nm) ♣300 WL2 (nm) ♣900	€1 €10 increment (nm)
2	Set problem loaded definition file:	Problem file: Set Problem
	Calculate: single shot Continue Stop Results of c	Calculations Save all simulations
_	Calculate: batch Batch set-up _ EB G,R AC I-	V C-V C-F QE Clear all simulations
5.	Calculate: recorder Record setup	r results SCAPS info
	Execute script Script set-up Script c	graphs Quit

There are dedicated panels for the basic actions:

- 1. Run SCAPS.
- 2. Define the problem, thus the geometry, the materials, all properties of your solar cell
- 3. Indicate the circumstances in which you want to do the simulation, i.e. specify the working point
- 4. Indicate what you will calculate, i.e. which measurement you will simulate.
- 5. Start the calculation(s)
- 6. Display the simulated curves, ... (see section 6)

This is further explained below.



Click the above pictogram on the Desktop, or double-click the file $c:\SCAPS210\scaps3000.exe$ in the file manager. SCAPS opens with the Action Panel.

2. Define the problem:

Set problem

Click the button set problem in the action panel, and chose load in the lower right

corner of the panel that opens. Select and open e.g. the file NUMOS CIGS baseline.def: that is the example problem file of the practicum session at the NUMOS workshop, Gent, 30 march 2007. This file is supposed to be in the folder /scaps30/def. If



necessary, browse to find this file. In a later stage, you can alter all properties of the cell by clicking set problem in the action panel.

3. Define the working point

The working point specifies the parameters which are not varied in a measurement simulation, and which are relevant to that measurement. Thus:

- the temperature T: relevant for all measurements. Note: in SCAPS, only $N_C(T)$, $N_V(T)$, the
- thermal velocities, the thermal voltage kT and all their derivatives are the only variables which have an explicit temperature dependence; you must input for each T the corresponding materials parameters yourself.
- the voltage V: is discarded in *I*-V and *C*-V simulation. It is the dc-bias voltage in *C*-f simulation and in $QE(\lambda)$ simulation. SCAPS always starts at 0 V, and proceeds at the working point voltage in a number of stars that you also should appear



voltage in a number of steps that you also should specify.

- the frequency *f*: is discarded in *I-V*, $QE(\lambda)$ and *C-f* simulation. It is the frequency at which the *C-V* measurement is simulated.
- the illumination: is used for all measurements. For the $QE(\lambda)$ measurement, it determines the bias light conditions. The basis settings are: dark or light, choice of the illuminated side, choice of the spectrum. A one sun (= 1000 W/m²) illumination with the 'air mass 1.5, global' spectrum is the default, but you have a large choice of monochromatic light and spectra for your specialized simulations. If you have an optical simulator at your disposal you can immediately load a generation profile as well in stead of using a spectrum.

4. Select the measurement(s) to simulate

In the action-part of the Action Panel, you can select one or more of the following measurements to simulate: *I-V*, *C-V*, *C-f* and $QE(\lambda)$. Adjust if necessary the start and end values of the argument, and the number of steps. Initially, do one simulation at a time, and use

rather coarse steps: your computer and/or the SCAPS program might be less fast than you hope, or your problem could be really tough... A hint: in a C-V simulation, the I-V curve is calculated as well, no need then to specify it separately.

5. Start the calculation(s): Calculate: single shot

Click the button calculate: single shot in the action panel. The Energy Bands

Panel opens, and the calculations start. At the bottom of the Panel, you see a status line, e.g. "iv from 0.000 to 0.800 Volt: V = 0.550 Volt", showing you how the simulation proceeds. Meanwhile, SCAPS stands you a free movie how the conduction and valence bands, the Fermi levels and the whole caboodle are evolving. When you see the hated divergence message, you're



entitled to get into a bad mood, but don't exaggerate. Anyway, you did not loose the *I-V* points already calculated.

6. Display the simulated curves, ...

After the calculation(s), SCAPS switches to the Energy band panel (or the AC-band panel). You can now look at your ease to the band diagrams, carrier densities, current densities,... at the last bias point calculated (stop your calculations earlier, or use the pause button on the Action Panel if you want to look at an intermediate state at ease). You can output the results (buttons print, save graphs, show (then the numbers are shown



on screen; cut & paste to e.g. Excel is possible), or save (then the numbers are saved to a file). You can switch to one of the specialized output Panels (if you have already simulated at least one corresponding measurement). We only show the example of the IV Panel.

7. ...e.g. the *I*-*V* curves

The meaning of the plot, show or save buttons is as for the Energy Bands Panel. Again, you can switch to the other output panels (energy bands, ac, *C-V*, *C-f* and *QE*, if already calculated), and to the Action Panel to do a new calculation, or to stop (important: you can only leave SCAPS from the Action panel!). Several small remarks:

- 1. The color of the last calculated curve is indicated (tip: when the graph gets too crowded, go to the Action Panel and click clear all simulations to clear all graphs). The recombination curves are only shown for the last simulation. The color of the legend corresponds to the color of the curve (indicated as 1bis).
- 2. If Curve Info is switched ON and you click the cursor on a curve in a graph, a pop-up panel will appear which gives information about the graph, curve and the point which you clicked.

- 3. Here you can display a measurement file (only one measurement at a time!). Select e.g. the file Numos Ex 1 light.iv or Numos Ex 1 dark.iv which you should find under /scaps210/measurements.
- 4. Hint: when you are doing many simulations, be friendly and helpful write yourself, and some to comments in the comment box before printing the Panel: you'll be glad to have done so when the time writing (an article, of your doctorate) comes...
- 5. You can change the range and scaling of the axes with the Scale button. If you press the CTRL-button and select a rectangular area in a graph, the graph will zoom-in to the selected area. Pressing the CTRL-button and clicking the right mouse button results in zooming out.



8. Editing the problem

Go to the Action Panel, click set problem. You are now in the Solar Cell Definition Panel. Click on a layer name, and you enter the Layer Properties Panel where you can change all parameters of that layer. Use your intuition and/or read the manual., or just raise your hand (the last possibility is only in Gent, Friday 30 march 2007, from 15h to 17h...).

9. Speeding up: Batch calculations

Calculate: batch

Batch set-up

When you want to explore the influence of one or a few parameters to the solar cell characteristics, you can take profit of the batch option. When you click Batch set-up, a panel opens where you can choose which parameter to vary, over which range, and in which mode (Lin, Log or custom). You can also define more than one parameter, and vary all of them (in a nested way or 'simultaneous'), but be modest to start. A batch calculation is launched when calculate: batch is clicked.



In a regular single shot or batch calculation, the detailed panels are only available for the last measurement point. To be able to see them as a function of the batch parameters you can launch a record calculation. You should first select the properties which you want to keep track of by clicking Record set-up. Browse through the property-lists, and don't forget to press one of the insert buttons to add a property to the recorder list. By clicking calculate: recorder, a recorder calculation is launched. Cell parameters are varied according to the Batch set-up, and all simulations are performed which are needed to



The manual of SCAPS consists out of a (messy B) collection of Add-on manuals. However, most features of SCAPS are described there in a detailed way. It is strongly recommended to collect them in one folder and keep them close at hand whilst exploring the SCAPS. Most algorithms which are implemented have been reported in literature. An overview is given when clicking the SCAPS info button.

Good luck !

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