

EBIC simulations in SCAPS

Marc Burgelman

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Correspondence address: Dept. of Electronics and Information Technology (ELIS),

University of Gent, 'Belgium'.

E-mail: Marc.Burgelman@ugent.be

1. Introduction

The SCAPS application discussed in this document uses:

- SCAPS version 3.3.07 of February 2019, or more recent.
- The following files that are not included in the standard SCAPS installation:
 - Definition files and all-SCAPS files that must be present in the folder [your SCAPS]\def:
 - ✓ the all SCAPS file `(quasi)EBIC with batch+recorder.scaps`
 - Files that must be present in the folder [your SCAPS]\generation:
 - ✓ A file that contains a list of generation file names: `list of generation file names.txt`
 - ✓ The generation files listed in the above file:
 - `G(x) e-beam at 0.05 μm.gen`
 - `G(x) e-beam at 0.10 μm.gen`
 - ...
 - `G(x) e-beam at 3.05 μm.gen`
 - File that must be present in your folder [your SCAPS]\script:
 - ✓ `calculate QE(x) from list of generation files.script`

2. EBIC simulation in SCAPS: options

In EBIC or LBIC measurements, an electron beam or optical laser beam provoke intense generation in a small sheet of the cell. The position of this zone of intense generation is then swept over the cross section of the cell (e.g. from the front surface to the rear surface), and simultaneously the current response is recorded. Scanning the position over the thickness can be done directly if the beam is incident on a cross section of the cell. And indirectly (and approximately) with an e-beam incident on the 'normal' surface of the cell, by varying the e-beam energy or acceleration voltage (and hence the penetration depth and generation profile).

In all cases, the experiment is simulated in SCAPS (or other programs) by specifying a generation profile $G(x)$ along the cell's thickness axis. Typically, that would be a 'rather peaked' $G(x)$ profile. In SCAPS, there are two options:

2.1 Direct EBIC simulation in SCAPS (batch and recorder): fast

Since December 2016, one can set-up a $G(x)$ profile in SCAPS by a variety of analytical models. This is treated in detail in the SCAPS application note *SCAPS Application Note Generation and Spectrum Models.pdf*, downloadable from the SCAPS installation site. We advise to read the relevant sections of this document first.

Several $G(x)$ models can generate more or less sharply peaked $G(x)$ profiles: rectangular, exponential, Gaussian, rectangular with exponential tails, rectangular with Gaussian tails. We here show the results with a Gaussian profile $G(x)$, containing a total number of eh pairs corresponding to $J_{ideal} = 1 \text{ mA/cm}^2$, and having a beam width with standard deviation $0.05 \text{ }\mu\text{m} = 50 \text{ nm}$ (if that narrow, it would be an e -beam, not an optical beam). The central position of the beam is scanned over the cell thickness with the SCAPS batch setting as $x = 0.05, 0.10, 0.15, \dots 3.00, 3.05 \text{ }\mu\text{m}$ (in our example; the cell thickness of NUMOS GIGS baseline.def is $3.10 \text{ }\mu\text{m}$). The recorder setting is set to record the cell characteristics η , J_{sc} , V_{oc} , FF . Clicking ‘calculate recorder’ and then looking to the recorder results quickly leads to the result of Fig. 1.

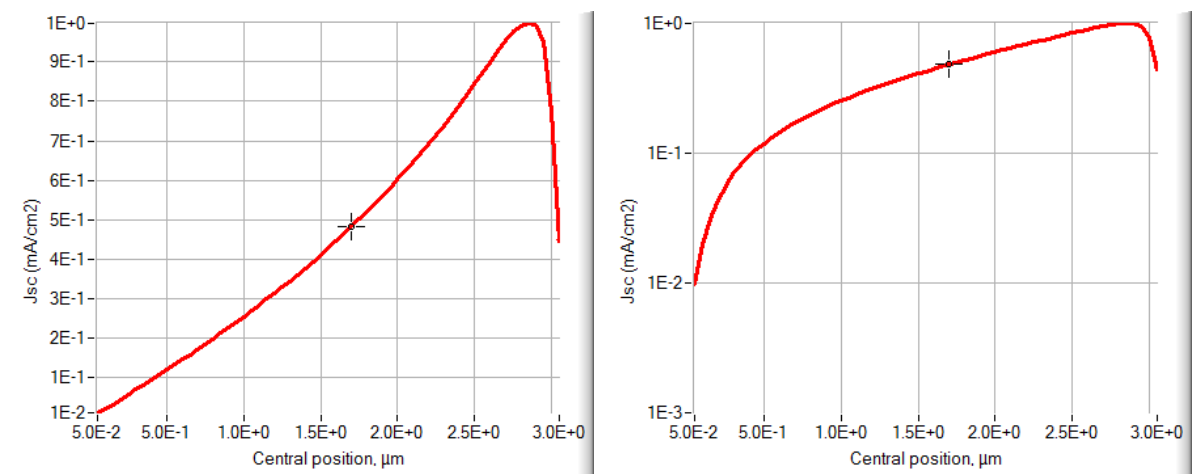


Fig. 1 Result of the EBIC simulation for the Numos CIGS baseline cell: the short circuit current *versus* the central position $x_{central}$ of the beam. $x_{central}$ was varied in the Batch set-up, and J_{sc} was recorded with... the Record set-up. Left in a linear view of J_{sc} , right in a logarithmic view.

One can nicely see the space charge layer SCL (roughly at $2.7 \text{ }\mu\text{m} < x < 3 \text{ }\mu\text{m}$) where the collection efficiency is almost equal to unity ($J_{sc} \approx J_{ideal} = 1 \text{ mA/cm}^2$, meaning that $QE \approx 1$). At the left side ($x < 2.7 \text{ }\mu\text{m}$) we see that QE is decreasing when going to $x \rightarrow 0$, thus away from the junction and the SCL. In a logarithmic plot, one could in theory deduce the minority carrier diffusion length L_n in CIGS from the slope, if the $\log(J_{sc})$ - x plot were a straight line. The deviation from the straight line near the left contact can be attributed to minority carrier contact recombination.

All settings (cell definition, batch setting and recorder setting) are saved in the all-scaps file (quasi)EBIC with batch+recorder.scaps, that goes together with this application note.

This method is a straightforward and fast way of simulating EBIC with SCAPS. But real EBIC profiles do not behave as simple as the SCAPS analytical generation models. If the precise shape of the EBIC $G(x)$ profile is important or under investigation, the user should consider the next option.

2.2 Indirect EBIC simulation (defining own $G(x)$ profiles): more accurate

2.2.1 Introduction

In the past, number of users have applied SCAPS with a file input for $G(x)$ to simulate electron beam induced current (EBIC) measurements. Typically, they would calculate intense generation in a small sheet of the cell by own models or programmes, and then calculate the current response when the central position of the beam (the position of the ‘intense generation’) is swept or scanned over the cell thickness. For each position of the e -beam, a separate generation file should be made, and this was at the time a complicated and time consuming procedure. There was an improvement when script commands were introduced that called one file from a list of file names (july 2015), but still it is a labour intensive work, and the accuracy was not always convincing. This was due to problems with the numerical mesh, thus the set of x values. SCAPS has an internal mesh generator that defines the positions x where the semiconductor equations are solved. But a user often has his own mesh generator for his own optical model. When the two meshes do not coincide, interpolation is used by SCAPS, but that can be a cause of numerical inaccuracy. In a worst case, a narrow EBIC profile $G(x)$ specified by a user could fall completely between two adjacent SCAPS mesh points in the middle of a thick layer, so that SCAPS wouldn’t even ‘see’ the e -beam...

This was remedied SCAPS 3.3.05 of December 2016 (analytical models for $G(x)$ and for the spectrum): an option was introduced in the numerical panel to merge the internal SCAPS x -mesh and the x -mesh that is used in the $G(x)$ file.

In the most recent SCAPS version 3.3.07 of february 2019, one can set or un-set this ‘merge x -meshes’ option also in the SCAPS script. Also more complicated file names, containing multiple dots and spaces, or that are very long names, are treated correctly now (before, a file path like $G(x)$ e-beam at 0.05 μm .gen was interpreted as filename= $G(x)$ e-beam at 0 and file extension = 05, of course leading to errors (the problem was not the dot in 0.05, but the space after 0.05)). A word of caution for users (in East Asia?): some computers do not accept Greek letters in filenames, so please first replace μ with m or micro or whatever.

2.2.2 EBIC - SCAPS strategy: application example

So the way to go is clear now:

1. Do your own calculations/simulations... to obtain the eh generation profiles, and assemble them in files: one file per beam center position x . The files should have the format of a SCAPS generation file (see also SCAPS Manual). This means that you can write whatever file header (a header line should not begin with two numbers); and then a list of x , $G(x)$ value pairs; SCAPS expects you to express x in μm (micrometer) and $G(x)$ in $\#/m^3s^{-1}$ (not $\#/cm^{-3}s^{-1}$!), and separated by white space (spaces or tabs).

In the example here, these are 32 files named $G(x)$ e-beam at 0.05 μm .gen... and so on. These files do not contain realistic EBIC profiles, but were just calculated by SCAPS by taking the generation $G(x)$ from the analytical Gauss model, with the same parameters as in section 2.1.

2. Make a text file that contains a list of the above file names (one file name per line). You can place this list file and the (e.g.) 32 .gen files in whatever directory/folder; the suggested place is [your SCAPS]generation.
3. Make a list of the beam positions belonging to the $G(x)$ profiles, in the same order as the $G(x)$ file names are listed in your list file. In the example here, this file is `list of generation file names.txt`.
4. In the example here, we made a SCAPS script that is abundantly commented: `calculate QE(x) from list of generation files.script`
5. In this SCAPS script, load successively each of the $G(x)$ files and the accompanying beam position, and do (=simulate) what you want to be done.
6. This script performs the following actions, that you might include in your script or not:
 - ✓ It starts from clean conditions: the `clear` and `action` commands. You can also do this in the interactive (=normal) SCAPS mode before running your script.
 - ✓ Load the SCAPS cell definition file that should be used for simulation. You can do also this interactively on forehand.
 - ✓ Prepare the script vectors to contain input and results. In the example this is done with `math fill...` commands. Remark the ‘semi-manual’ way that we used to set the x -positions 0.05, 0.10... in the scriptvariable `xvector`. If your position sequence has not much regularity, you should do it almost completely manually (with `set scriptvariable.xvector[...]` commands ☹, there is not (yet) a more elegant script command to read a vector from a file ☹). The scriptvectors `yvector`, `zvector` and `uvector` will contain calculated results. We reserve space (the vectors have the same size as `xvector`, thus `size = nx`). We also give appropriate titles to these vectors, so that the results are readable.
 - ✓ Now we start a loop (here there is only one). The variable `loopcounter` will take the values 0, 1... `maxiteration-1=31`.
 - ✓ In each pass of the loop (thus for each value of `loopcounter`), we pick the $G(x)$ file name from the list file, and load it as `generation file`. Check if the files exist, can be found and read before you go further!
 - ✓ Then we do a single shot simulation, we get the results we are interested in (here $J_{sc}(x)$ and $J_{ideal}(x)$), and we place the results in the appropriate vectors (`zvector` and `uvector`).
 - ✓ Do the data processing needed. Here it is just taking the ratio J_{sc}/J_{ideal} and place it in `yvector`.
 - ✓ After completion of the loop (`loop stop`), do whatever needed/wanted with the result vectors. Here we make 3 plots (`plot draw`). One could also save results to file(s), launch external programs that do further processing, ...

2.2.3 Further remarks

- Replace my SCAPS path `c:\SCAPS versions\Scaps 3.3.00\` with your path.
- Verify that the file `list of generation file names.txt` exists and is found in that folder
- Stick to the advices given in our SCAPS Manual:

- Frequently insert `show scriptvariable` commands, to check the proper working of your script (you can stop the script when something is not as expected). When all is running well, you can outcomment these `show` commands.
- Do not define directly a loop with 32 steps in your first tryout. Instead, do a try with a more modest number (2 is enough to learn already something...), and go for the full simulation marathon when you are rather sure that everything goes well.
- There is a small sophistication over the simple batch + recorder strategy of Section 2.1:

We notice that only part of the e-beam is incident on the cell when the beam centre is close to the edges (the fraction on the cell would be 0.5 for central position 0.00 μm or 3.10 μm). Hence we also accessed the ‘ideal current’ J_{ideal} incident on the cell for each position, and divided the short circuit current by this to obtain $QE = J_{sc}/J_{\text{ideal}}$. The result is shown in Fig. 2.

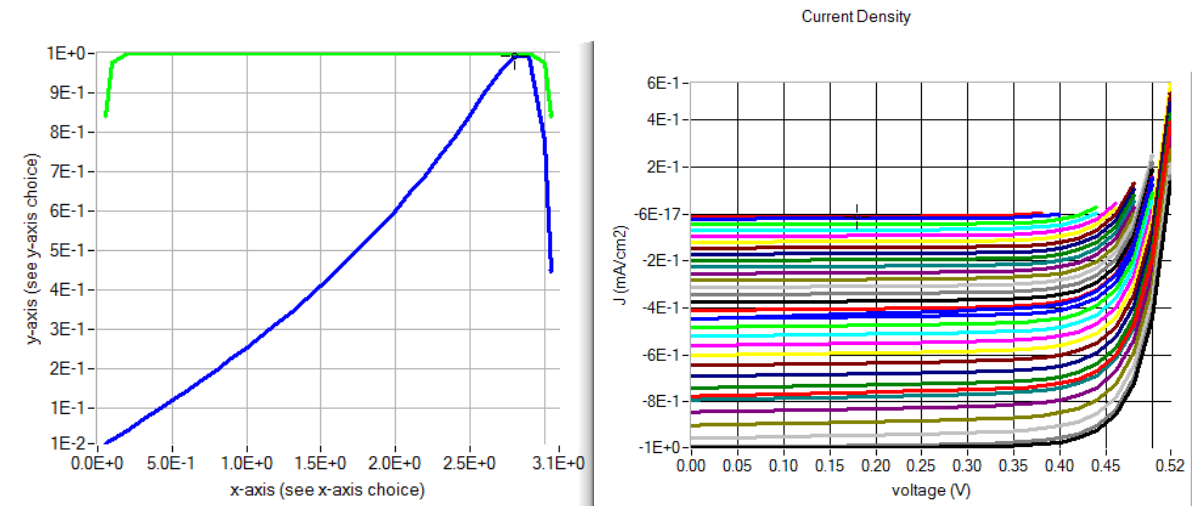


Fig. 2 Result of the EBIC simulation with the script `calculate QE(x)` from list of generation files `.script`, based on the definition file `NUMOS CIGS baseline.def`. Left: the light current J_{sc} (green), and the J_{ideal} in the cell (blue). Right: The corresponding IV curves.

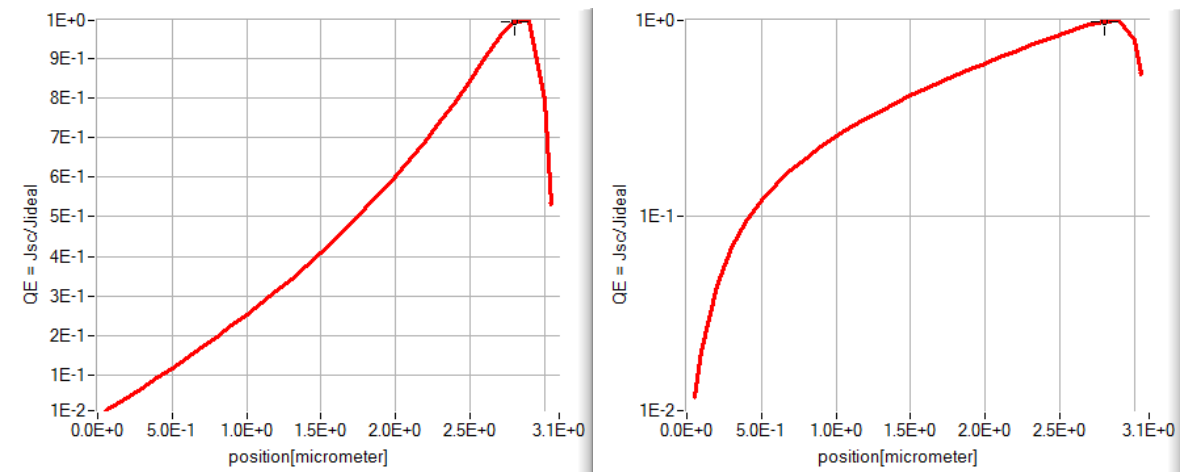


Fig. 3 The EBIC simulation, where the blue curve of Fig. 2 is divided by the red curve. Left: on a linear scale. Right on a logarithmic scale.

2.3 Which option to choose?

The *batch + recorder* option of Section 2.1 is more straightforward, faster, but can handle a limited variety of $G(x)$ shapes.

The *script + $G(x)$ files* option of Section 2.2 is much more elaborate, but it gives you all freedom to define your own $G(x)$ profiles. It should also be said that developing a SCAPS script is not always as fast and straight forward as could be desired. Having the Manual on the table, and some experience and practice however do help.

I would advise to check the difference in the final result with both methods, and see if there is an appreciable difference. If this is not the case, one could do the fast *batch + recorder* simulation for the bulk of the work, and the more elaborate but more accurate *script + $G(x)$ files* simulation to make the final illustrations for publications or reports.