

SCAPS Version 3.0, March 2011

This is not a stand-alone manual of SCAPS. It only describes the novelties in SCAPS 3.0 compared to SCAPS 2.9.04 and earlier. A (kind of) manual of the SCAPS programme is contained in another document. This is complemented with (so far) four add-on manuals, for SCAPS 2.8 ('grading'), for SCAPS 2.9.02 ('multivalent defects'), for 2.9.03 ('script') and for 2.9.04 (better handling of 'uniform'). Also, there is a short and recommendable document `Getting Started.pdf`, which does exactly what it promises.

Enhancements of version 3.0, compared to version 2.9.04

The most important new features in version 3.0 are in the facilities for tunneling, in the script and in the user interface.

1 Additional tunnel paths

With respect to SCAPS version 2.9.02 and earlier only two extra tunnel paths have been added: tunneling to contacts and intraband tunneling between two bulk states. In SCAPS version 2.9 tunnelling to interface defects and intraband tunnelling were already possible. But intraband tunnelling was limited with the restriction that one of the states needed to be located at an interface. However as the tunnel mechanisms have never been explained in one of the (add-on) manuals, this might be the place to do it.

The algorithms used by SCAPS to calculate tunnel currents have been published in:

- [1] J. Verschraegen and M. Burgelman (2007). "Numerical modeling of intra-band tunneling for heterojunction solar cells in SCAPS." *Thin Solid Films* 515(15): 6276-6279.

This article only describes intraband tunnelling, but the algorithms for tunnelling to contacts and to interface defects are very similar. A more elaborate description is only available in Dutch:

- [2] J. Verschraegen, "Karakterisering en modellering met SCAPS van de CISCuT dunne-filmzonnecel", Ph.D. Thesis, Gent 2007 (in Dutch).

1.1 Intraband tunnelling

Intraband tunnelling is the tunnelling between states both in the conduction/valence band. Tunnelling between conduction and valence band states (interband tunnelling) is not (yet) available in SCAPS. The valence and conduction band consists in (almost) every structure out of bulk layers and interfaces. For each layer/interface you can indicate whether a tunnel process with a state in this layer/at this interface is allowed and you can define the tunnel masses for these processes. These settings are available on the layer and interface panels.

effective mass of electrons	1.000E+0	1.000E+0	uniform ▼
effective mass of holes	1.000E+0	1.000E+0	uniform ▼

ND grading dependent on composition y: ND (y) ▼ Allow Tunneling

Figure 1: Setting of the layer tunnel properties.

1.2 Tunnelling to interface defects and contacts

Next to tunnelling in the conduction and valence band, also tunnelling between the bands and an interface defect, or the bands and a metal contact is possible. These processes can be set for each defect separately on the interface defect properties panel and for each contact on the contact definition panel.

1.3 Tunnelling and the numerical panel

The tunnel probability is determined by the effective mass of the two states which are involved in the process. These masses can be different, and can be set differently in SCAPS. You can select which of the two masses to use on the numerical panel. The default choice is to use the minimum effective mass.

SCAPS uses the WKB-approximation in order to calculate tunnel probabilities. This approximation is only strictly valid for large enough barriers. When no precautions are taken, the tunnel rate for very thin and shallow barriers is hugely overestimated. In order to avoid this you can set a minimum height of the tunnel barrier (default = $2kT$), for such small barriers the current is determined by drift and diffusion rather than tunnelling anyway.

Minimum height of bulk tunnel barrier (kT)	2.00
Choice of Tunnelmass	Minimum ▼

Figure 2: Numerical settings for tunnelling

1.4 Displaying tunnel currents

When at least one tunnel mechanism is active the total electron and hole tunnel currents are displayed in the Energy Band panel, next to the drift-diffusion electron/hole current and the total current. As tunnelling often only occurs over a small distance, you will usually have to rescale the graph to get a good view on the behaviour of the tunnel currents.

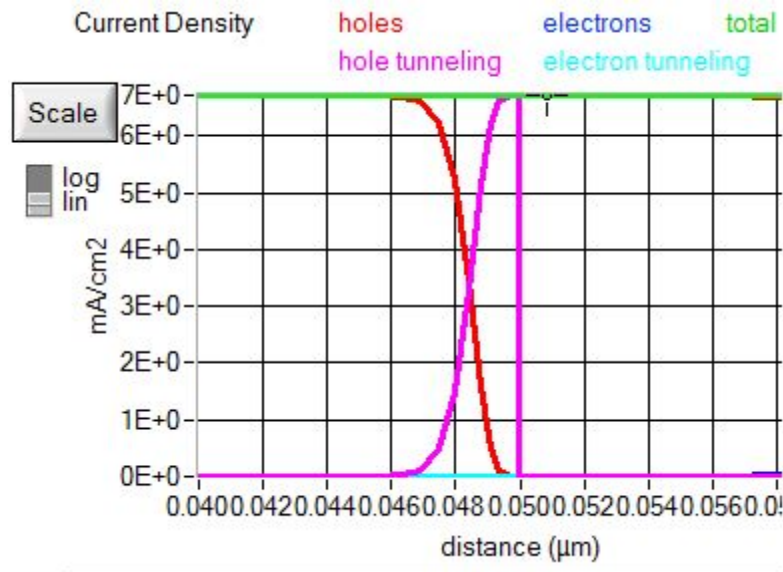


Figure 3: Visualization of tunnel currents.

2 Updated action panel

It is now possible to run SCAPS script files from within the user interface. This might seem contradictory at first, but it allows you to automate commonly performed operations and to make custom designed plots of all available SCAPS variables.

As a consequence the action panel has been redesigned. The former *calculate* button has been split in four new buttons:

- *calculate single shot*
- *calculate batch*
- *calculate recorder*
- *calculate script*

The former checkboxes '*do batch calculation*' and '*do recording*' have been removed.

All graph panels can now easily be accessed from the action panel without having to go around the energy band panel.

3 New script commands

With respect to SCAPS version 2.9.03, where the script was introduced, several new options have been added. In this manual we will shortly discuss the new options with respect to the previous version, but will not go into detail about its use. An entire description of the script language is contained in a separate document called the *SCAPS script manual*. Moreover an overview of all available script commands can interactively be accessed using the *set script* button.

3.1 New script variables + set commands

The number of available vectors have been extended from two (`xvector` and `yvector`) to six (`xvector`, `yvector`, `zvector`, `uvector`, `vvector` and `wvector`), which are generally referred to as `{m}vector`. As a consequence also the variable `nx` and `ny` have been extended in a similar way.

Additionally six extra variables have been added called `{m}name`, and consisting out of character strings with a maximum size of 256 bytes. As a consequence a new set command has been added: `set scriptvariable. {m}name`.

In set commands the indexing of vectors was only possible with constant integers. This has been extended so that the expressions below are also allowed:

- `set argument {w}vector[loopcounter]`
- `set argument {w}vector[xvalue]`
- `set argument {w}vector[{w}vector[...]]`
- ...

3.2 New get + load commands

The `get` command does no longer result in a default storing of variables in the vectors `x` and `y`. In stead the vectors should be passed by the user.

Some extra commands are available:

- `get recombination.tot`
- `get recombination.SRH`
- `get recombination.rad`
- `get recombination.aug`

Almost all variables present in SCAPS are accessible in the script via `get recorder`. This involves a recorder calculation. A recorder calculation with a batch settings with only one calculation at the working point is possible through `load singleshotbatch`.

3.3 New save command

The command `show scriptvariables` results in showing all script variables. However only the beginning and the end of large vectors is displayed. In order to access the entire vectors you can use `save scriptvariables filename`.

3.4 New calculate commands

The reshaping of the action panel results in an update of the script commands as well. The commands `action batch.checkaction` and `action recording.checkaction` are no longer in use. They have been replaced by extra calculate commands:

- `calculate singleshot`
- `calculate batch`
- `calculate recorder`

The command `calculate` still works however and is equivalent to `calculate singleshot`.

3.5 New commands `math` + `plot`

A new command `math` has been introduced to allow (mathematical) manipulation of script variables, and thus (via `get recorder`) of all SCAPS variables. Together with the `plot` command this allows you to make your own self made SCAPS graphs, next to the standard graphs available in SCAPS.

A list of the `math` commands is given below:

<code>add</code>	<code>multiply</code>	<code>subtract</code>	<code>divide</code>
<code>exp</code>	<code>log</code>	<code>power</code>	<code>push</code>
<code>constant</code>	<code>linear</code>	<code>rangeLin</code>	<code>rangeLog</code>

There are only two `plot` commands:

- `plot draw`
- `plot clear`

The graphs get plotted on the script results panel. On this panel a list of all plotted graphs is shown. You can check the graphs you want to display and press the *refresh* button in order to update the graph.

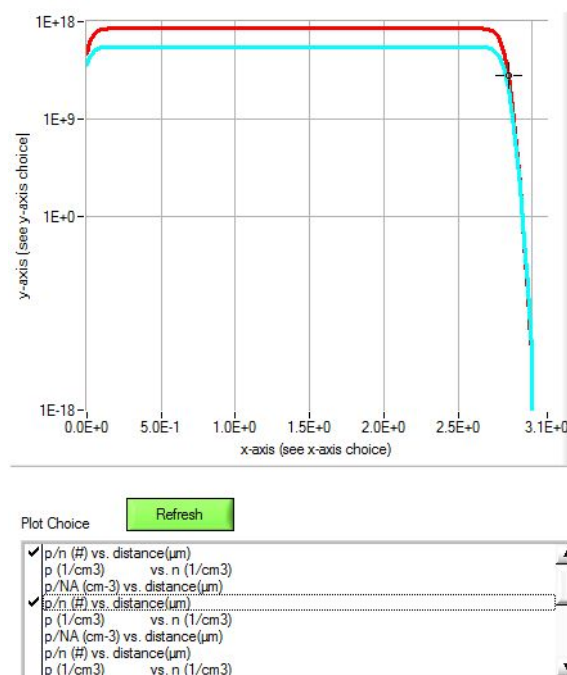


Figure 4: The script result panel

3.6 New dll

As there are extra script variables the prototype of the dll-function has been extended to:

```
int DLLEXPORT SCAPSUserFunction (int mode, double *xvalue,
double *yvalue, double *svector[6], int sn[6], double
*looperror, char *filename);
```

In the new version of the dll-code accompanying the SCAPS installation, it is shown how you can easily adapt a former dll to this new prototype.

3.7 An example exploring new script properties

An example script `PersonalisedSCAPSgraph.script` which illustrates some of the new options is distributed along with the program. It makes use of `Numos CIGS baseline.def` and `PersonalisedSCAPSgraph.srf`, which are both distributed as well.

This script records the free carrier densities and the shallow acceptor density for different temperatures. The free hole density is then compared with the free electron density and the shallow acceptor density. The results are plotted.

The different steps in the script are commented out intensively. Please pay attention to:

- How to fill a vector with temperatures.
- The use of `load singleshotbatch`.
- The use of `get recorder`.
- The declaration of the vector variables in `get - math - plot`.