

## SCAPS Version 2.9.04, November 2010

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

### Enhancements of version 2.9.04, compared to version 2.9.03

The most important new features in SCAPS 2.9.04 are in the user interface: better handling of the concept 'uniform' in graded problems, more parameters available in the recorder.

## 1 The meaning of 'uniform' in graded problems

The meaning of 'uniform' is now made more clear to avoid misunderstandings and misleading panels. The concept 'uniform composition  $y$ ' is handled differently from the concept 'uniform parameter  $p(y)$ ', where  $p$  is a parameter such as  $E_g$ ,  $\chi$ ,  $N_A$ , ...

### 1.1 Uniform composition $y$

This comes now with three options:

- 'uniform pure A ( $y = 0$ )'. The composition in this layer is  $y = 0$  for all positions  $x$ . You see only the column of the materials properties of the pure material A ( $y = 0$ ), with no button available to set a grading of these parameters. All parameters  $p$  get the value  $p(y = 0)$ . Position grading of the doping and defect density is possible, e.g.  $N_A(x)$ ,...
- 'uniform pure B ( $y = 1$ )'. The composition in this layer is  $y = 1$  for all positions  $x$ . You see only the column of the materials properties of the pure material B ( $y = 1$ ), with no button available to set a grading of these parameters. All parameters  $p$  get the value  $p(y = 1)$ . Position grading of the doping and defect density is possible, e.g.  $N_A(x)$ ,...
- 'uniform  $y$ ,  $0 < y < 1$ '. The composition in this layer is  $y = \text{constant}$  for all positions  $x$ , and you can set this constant composition in the grading panel. You see both columns of the materials properties of the pure material A ( $y = 0$ ) and B ( $y = 1$ ), and you can set a grading of each of these parameters, to give them the uniform value  $p(y)$ .

### 1.2 Uniform parameter value

You can give a parameter only a uniform value  $p$  for  $0 \leq y \leq 1$  when grading is allowed (thus when the composition grading has been set to 'uniform  $y$ ,  $0 < y < 1$ ' or any of the real grading laws (linear, ...)), and when the value of this parameter for the pure A and the pure B material has been set to the same value in the layer panel, thus when  $p(\text{pure A: } y = 0) = p(\text{pure B: } y = 1)$  was set. This is to avoid ambiguity: when  $p(0) \neq p(1)$ , it is not possible that  $p(y) = \text{constant}$  in the whole composition interval  $0 \leq y \leq 1$ , including the end points.

### 1.3 Batch parameters; compatibility

The labeling and availability of the batch parameters has been adapted to this new interpretation of the various 'uniform' cases. Definition files made with SCAPS  $\leq 2.9.03$  will run, but a uniform composition

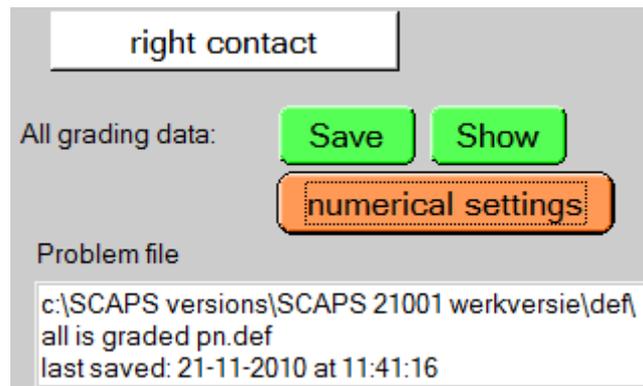
will be interpreted as 'uniform pure A'. Definition files made with SCAPS  $\geq 2.9.04$  will run in earlier versions.

## 2 Output of the graded parameters

The value of all parameters that can be graded, as they are used in the calculations, is available by clicking the green button in the Layer Properties Panel. These parameters now are:

$y, E_g, \chi, \varepsilon, v_{thn}, v_{thp}, \mu_n, \mu_p, N_A, N_D, N_{t1}, N_{t3}, N_{i3}, C_{radiative}, C_{Auger,n}, C_{Auger,n}$  and  $\alpha(\lambda, x)$ .

There are now two such green buttons instead of one, labeled Save and Show:



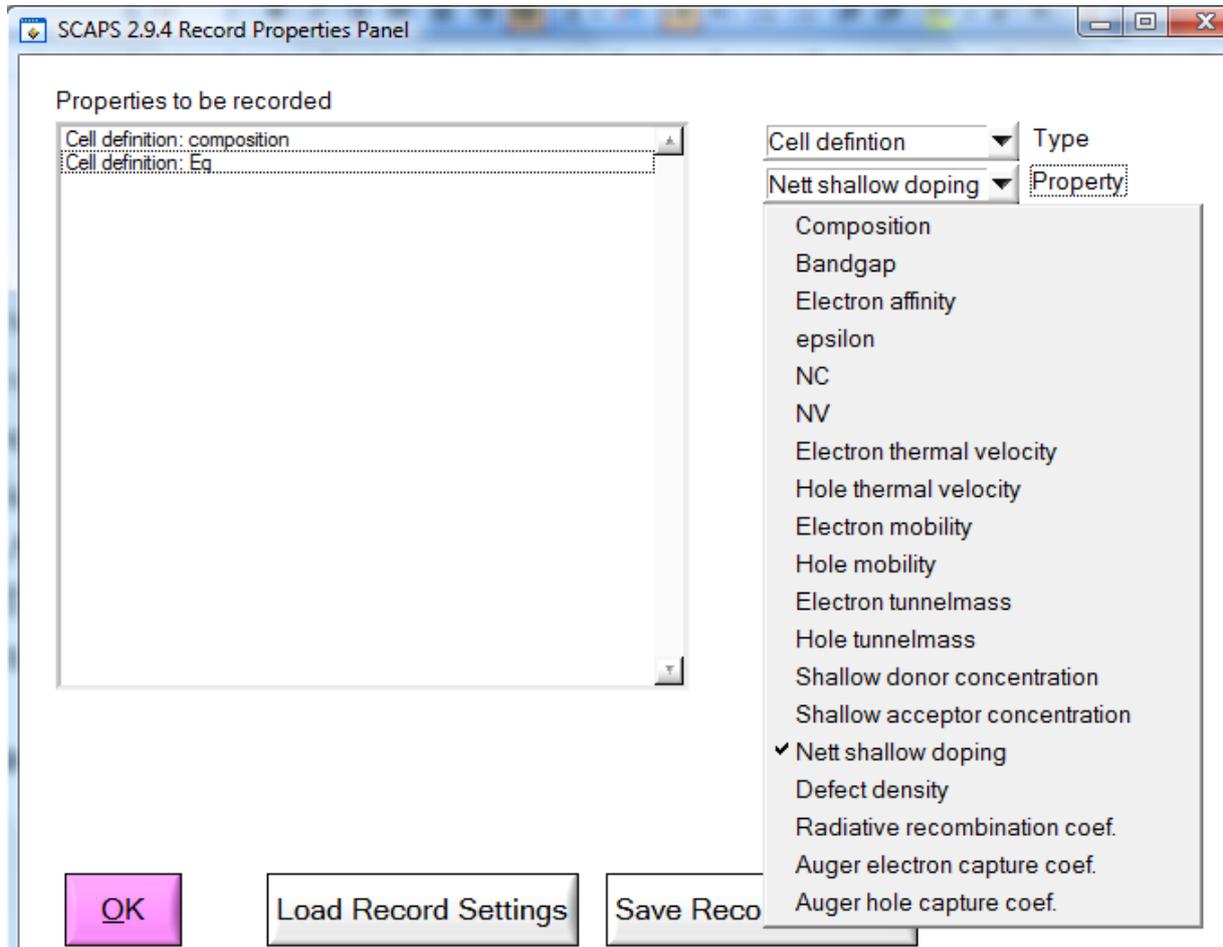
With Show, you get all data but  $\alpha(\lambda, x)$  in a window on the screen, as it was in SCAPS  $\leq 2.9.03$ . With Save, you must give a filename, and all data, inclusive  $\alpha(\lambda, x)$ , are written in a text file, that can be opened directly with Excel. Beware, a typical spectrum has 100 wavelengths  $\lambda$ , and a typical problem maybe 500 mesh points  $x$ , thus  $\alpha(\lambda, x)$  can fill a huge table! With the edition 2 AM-spectra, that have 2000 wavelength values, both Notepad and Excel 2003 will not be sufficient, but Excel 2007 should be (not tested). A future development will be to add a third green button for direct visualisation (in graphs) of the graded properties.

## 3 Recording of the graded parameters

In the Record Setting Panel, you can now also order to record the graded parameters  $y(x), E_g(x), \dots$  during a batch calculation. It is true that SCAPS now can set-up and handle quite complicated parameter profiles, and it can be difficult to keep track of what and how the parameters in fact have been changed during a batch calculation. See the screen shot below: select Cell definition as Type, and one (up to now one by one ☹) parameter as Property. Do not forget to include the selected parameter in your recorder list (insert above, insert below or replace ).

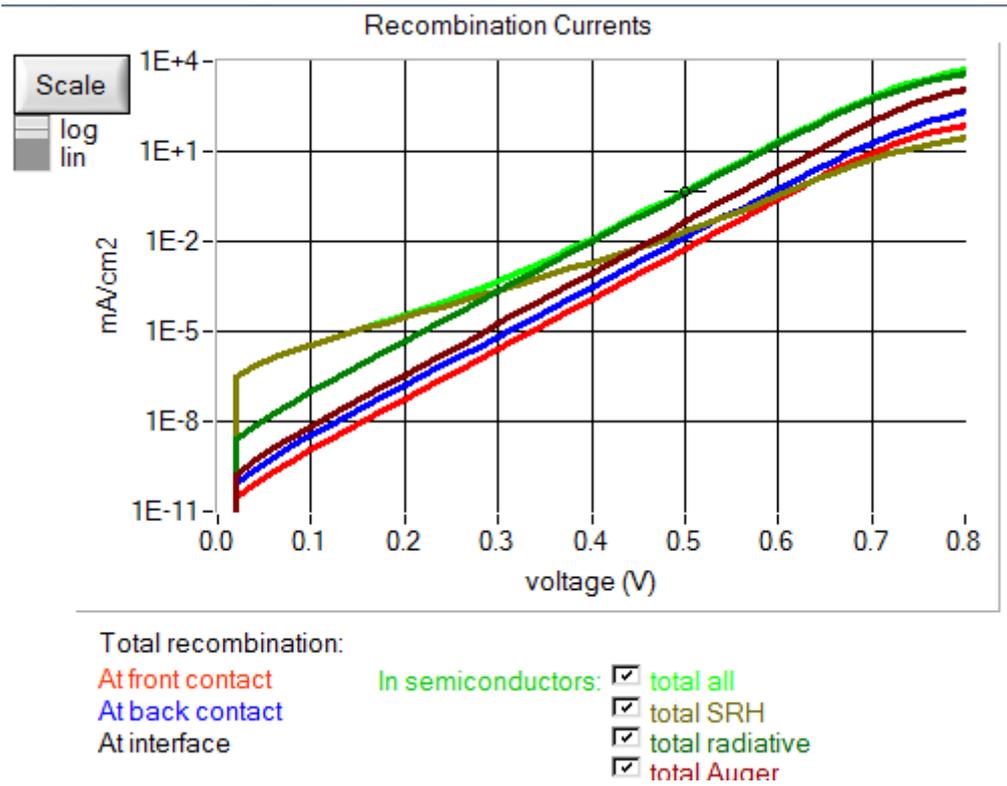
This is a good place to remind you the SCAPS policy of a recorder job: it overrules all what you have specified in the action list, and calculates precisely (and not more) what is needed to record the properties you want to record. Thus, when you asked e.g. to record  $V_{oc}, J_{sc}$  and  $\eta$ , SCAPS will do an illuminated  $I-V$  calculation with the option 'stop after  $V_{oc}$ ' checked (and extending the  $V$ -range to what is necessary), even if you have set 'dark', or even no  $I-V$  measurement at all. Also, when you asked (in the action panel) e.g. for a  $C-f$  and a  $QE$

calculation, these will not be carried out when Do Recording is checked, as these calculations are not necessary to record  $V_{oc}$ ,  $J_{sc}$  and  $\eta$ !



#### 4 Radiative recombination (and Auger, and SRH) – electroluminescence

On demand, we have enabled separate plots of the different recombination mechanisms: radiative (or direct band-to-band), Auger, Shockley-Read-Hall: see figure below. You can click and unclick the total bulk recombination and any of its constituent parts as you like. Also four output columns in the  $I$ - $V$  show or save have been added: for  $J_{SRH}$ ,  $J_{radiative}$ ,  $J_{Auger, n}$  and  $J_{Auger, p}$ . When you are sure that all direct band-to-band recombination is radiative, and that all emitted photons can get out of the cell to your measurement set-up, you can interpret  $J_{radiative}$  as the electroluminescence signal. However it is not labeled as such in SCAPS.



Marc B. 24-11-2010