SCAPS Version 2.8.02, May 2009

Add-on manual

This is <u>not</u> a stand-alone manual of SCAPS. It only describes the novelties in SCAPS 2.8 compared to SCAPS 2.7 and earlier. A (kind of) manual of the SCAPS programme is contained in another document. Also, there is a short and recommendable document `Getting Started.pdf`, which does exactly what it promises.

Enhancements of version 2.8.02, compared to version 2.7.03

Version 2.8.02 (may 2009) is the first to be distributed externally after version 2.7.03 of november 2007: the intermediate versions were internal test versions. The most important new feature is the implementation of solar cell structures with graded properties.

1. Grading

1.1 Principles

The principles of numerical simulation of solar cells with graded properties are presented in:

[1]   M. Burgelman and J. Marlein, "Analysis of graded band gap solar cells with scaps", Proc. 23rd European Photovoltaic Solar Energy Conference, Valencia, Spain, 1-5 september 2008.

To give a suitable and materials oriented description of the grading of the various materials parameters, we have chosen to derive all parameters consistently from the composition grading of a layer. Each layer is assumed to have composition $A_{1-y}B_y$. The user defines the properties of the pure compounds A (e.g. A = $CuInSe_2$) and B (e.g. B = $CuInS_2$), and the composition grading $y(x)$ over the thickness of the layer: thus defining the composition values y at the left and right side of the layer, and by specifying some grading law in between. All materials properties P are then derived from the local composition parameter $y(x)$, that is, $P[y(x)]$ is evaluated. Several grading laws are implemented in SCAPS and offered by the user interface: linear, logarithmic, parabolic (two laws), power law, exponential, effective medium and a Beta function. These grading laws can be used to set the composition grading $y(x)$ over a layer, as well as to set the composition dependence $P(y)$ of a property. The following properties can be graded in SCAPS: E_g, χ, ε, N_C, N_V, μ_n, μ_p, v_{thn}, v_{thp}, N_D, N_A, N_t (all defects) and $\alpha(\lambda)$.

In this SCAPS version, these facilities have been extended with the option to define a direct position dependence of the shallow doping densities and the defect densities, thus $N_D(x)$, $N_A(x)$, $N_t(x)$. This is to allow for the possibility that N_D, N_A, N_t are not always pure materials properties and as such defined by the materials composition y, but they can also be determined by external influence, e.g. in- or out-diffusion of impurities.

It is clear that grading considerably complicates the numerical simulation tool, not only by adding extra terms to the equations (see [1]), but also the management of all variables and properties in the user interface and internally in the programme. We have put a large effort in the design of the user interface, to allow the user to keep a good view on the problem she or he is actually setting up.

1.2 Compatibility with earlier SCAPS versions

To save all new features of a problem in a `.def` file, the format of this file has changed substantially. As a result, this SCAPS 2.8 definition files become rather complicated and look rather chaotic. It is strongly unadvised to edit them directly. Instead, manipulate them only from within SCAPS. The good news is that the new format is both upward and downward compatible with the former format: versions 2.7 and earlier of SCAPS will correctly read the SCAPS 2.8 definition files, and SCAPS 2.8 will correctly read definition files generated by SCAPS 2.7 and earlier. Of course, the earlier SCAPS versions cannot handle all options present in the new problem definitions, but when such options are defined, they do something sensible with it. This will be detailed at the end of this add-on manual.

1.3 To start setting up a graded problem: define the composition grading $y(x)$

The first thing to do is to set the composition grading $y(x)$, see Fig. 1.

Fig. 1   Setting the composition grading $y(x)$. Select a grading law for the composition (here graded linear is selected). The values $y_{left} = 0.200$ and $y_{right} = 0.800$ are just indications here. You can vary them only in the Grading Panel, which is accessed by selecting a grading law.

When "uniform" is selected, the composition and all composition dependent properties are uniform, thus not graded. The grading facilities of these parameters is not shown. This is e.g. what you will see when you are loading a definition file made by SCAPS < 2.7(see Fig. 2).
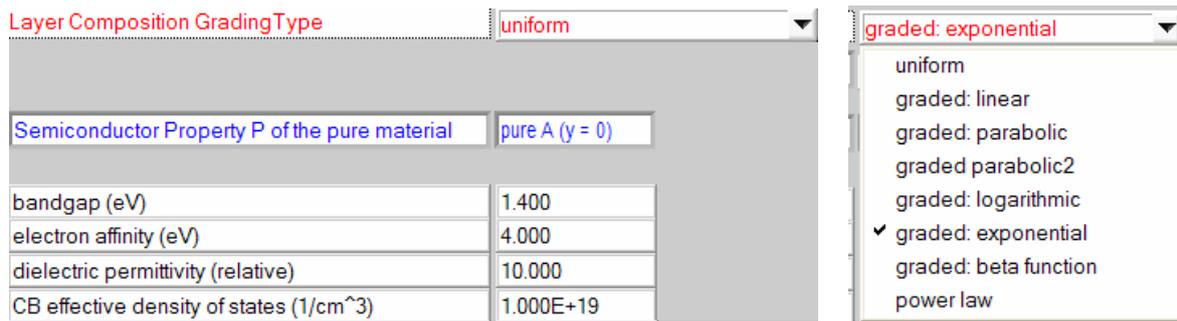
Fig. 2   [Left] When no composition grading is set (uniform is selected), all composition dependent properties are uniform and cannot be given a grading. The panel looks like the SCAPS<2.7 panel. [Right] A variety of grading laws can be selected; upon selecting one of them, the Grading Panel is opened (Fig. 3).

When any other grading law is selected (Fig. 2 right), the Grading Panel opens (see Fig. 3) to set further properties of this selection, and, above all, to visualise the grading being set up. Upon returning to the Layer Properties Panel (click OK or CANCEL in the Grading Panel) the composition dependence $P(y)$ can be set. In Fig. 1, a parabolic law is set for $E_g(y)$, a linear law for $\chi(y)$, and no grading for ε and N_C. To assist the user, a colour code is used consistently in SCAPS 2.8: red is for position dependent grading, e.g. $y(x)$, and blue is for composition dependent grading, e.g. $E_g(y)$ (Fig. 1).

1.4 To continue: define the composition grading of the properties $P(y)$

The same grading laws are used for position and for composition grading. An example for an exponential composition grading $N_D(y)$ is given in Fig. 3.
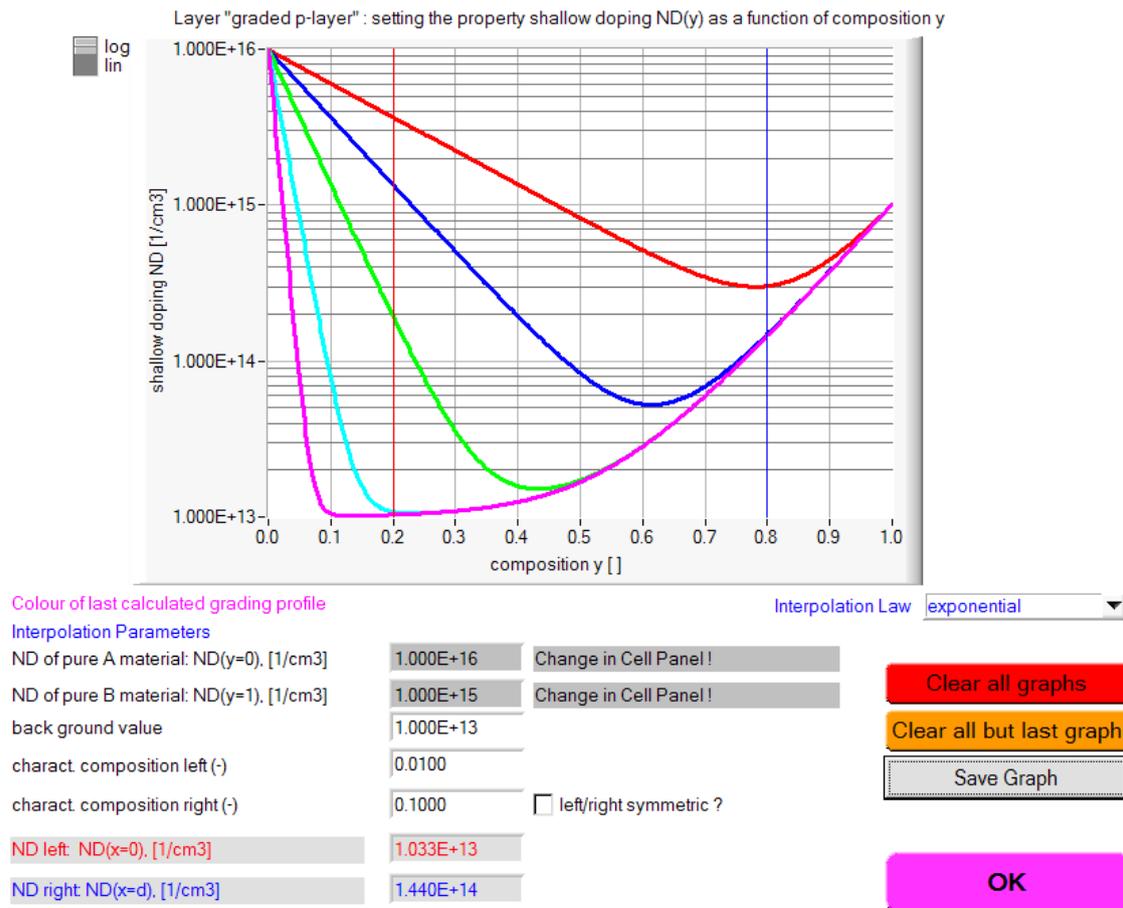
Fig. 3   View of the SCAPS Grading Panel. An example of an exponential composition grading of the shallow donor density N_D (y). The values N_D (y=0) (this is called `"pure A") and $N_D$ ($y$=1) (this is called `"pure B") cannot be set in this panel, but should be set in the Layer Properties Panel of Fig. 1. Three more parameters can be set here: a background value, and two 'characteristic compositions'. In the graph, $N_D(y)$ is plotted for 5 values of $L_{char, left}$: 0.2 (red), 0.1 (blue), 0.05 (green), 0.02 (cyan) and 0.01 (magenta). The composition at the left side of the layer (here y=0.2) and at the right side (here y=0.8) is also displayed. For the mathematics of this grading law, see [1].

1.5 Some variables can be graded as a function of position or composition

As announced, materials physics impose that we should implement position dependent grading (and not only composition dependent grading) as an option for the shallow doping densities N_D and N_A, and for the defect densities N_t.

ND grading dependent on composition y: ND (y)	▼		
shallow donor density ND(y) (1/cm3)	1.000E+16	1.000E+15	exponential ▼
NA grading dependent on position x: NA (x)	▼		
shallow acceptor density NA(x) (1/cm3)	1.000E+14	1.000E+15	exponential ▼

Fig. 4   Here, the shallow donor density is given a grading as a function of composition y: N_D (y). The two values displayed are the values of the pure A material (10^{16} cm^{-3}) and the pure B material (10^{15} cm^{-3}). The shallow acceptor density $N_A(x)$ is given a grading as a function of position x: $N_A(x)$. The two values displayed are the values at the left side (10^{14} cm^{-3}) and at the right side (10^{15} cm^{-3}). Notice the use of the colour code (red for position, blue for composition grading).

1.6 The grading of the optical absorption constant $\alpha(\lambda)$

A dedicated interpolation scheme was proposed [1] to estimate the optical absorption constant $\alpha(\lambda)$ of a compound $A_{1-y}B_y$ when the absorption constants α_A and α_B of the pure materials A and B are known. The SCAPS Grading Panel visualises this by plotting $\alpha_A(\lambda)$ and $\alpha_B(\lambda)$ of the pure materials, and also $\alpha_y(\lambda)$ corresponding to the compositions $y = 0.1, 0.2, \ldots, 0.9$. An example is given in Fig. 5.
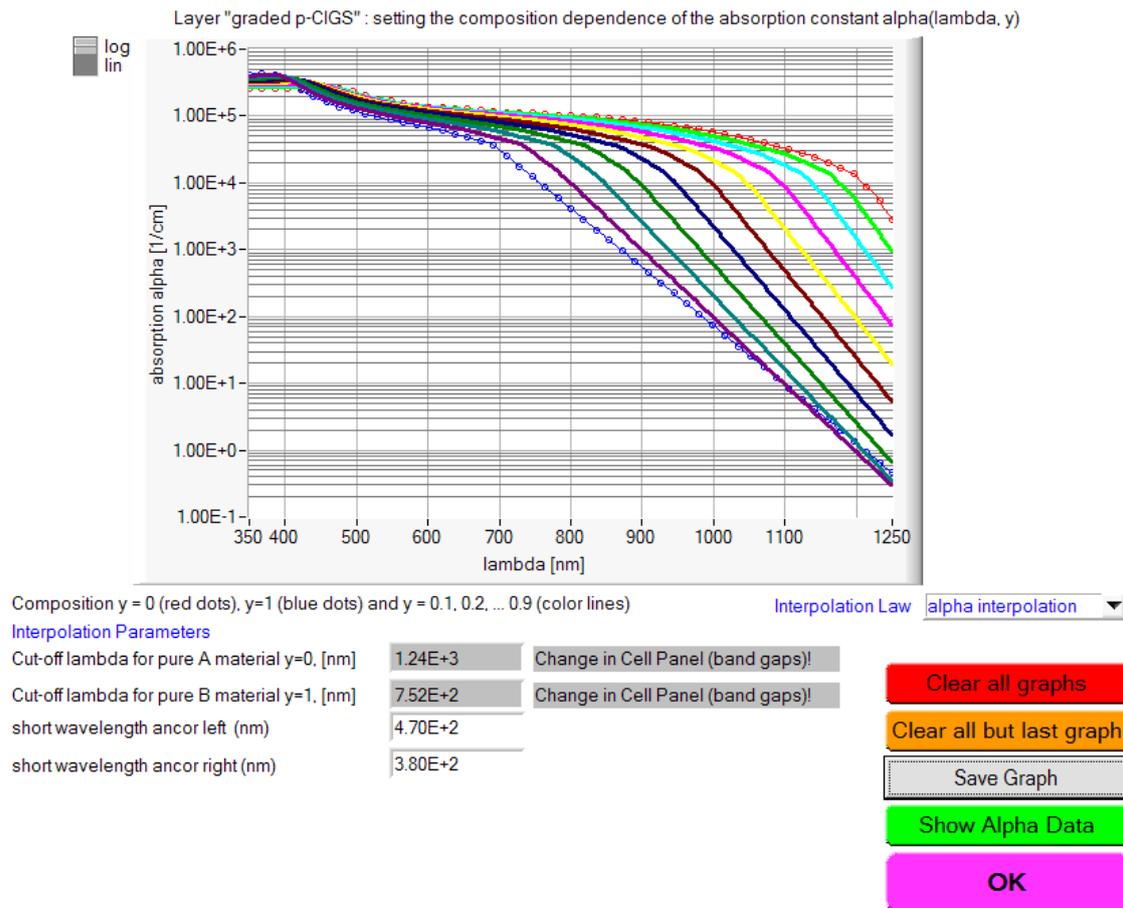
Fig. 5   The optical absorption constant $\alpha(\lambda, y)$ of a compound material with composition y, thus $A_{1-y}B_y$, calculated by SCAPS with a dedicated interpolation algorithm. Here, the pure A material is CuInSe$_2$, and the pure B material CuGaSe$_2$. The data can be obtained in tabular form by clicking Show Alpha Data (the green button).

1.7 The actual, position dependent properties

The graded properties get their position dependence directly ($N_D(x)$, $N_A(x)$, $N_t(x)$ when these options are selected), or indirectly via the x-dependence of the composition y: $P[y(x)]$, all other cases. The x-dependent values that are finally used in the calculations can be obtained from the Cell Definition Panel, but only after at least a calculation is done (a work point calculation is dark is sufficient, unclick I-V, C-V, C-f, and QE). Click the green button in Fig. 6.
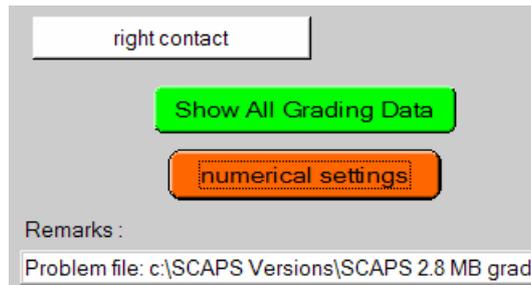
Fig. 6   When at least one calculation is done, the green button in the Cell Definition Panel becomes active. By clicking, one gets all position dependencies in a tabular form: $y(x)$, $E_g(x)$, …, $N_D(x)$, $N_A(x)$, $N_{t1}(x)$, $N_{t2}(x)$, and $N_{t3}(x)$.

2. Further extensions in SCAPS 2.8

2.1 A reference level for defect energies can be defined

In SCAPS2.7 and earlier, bulk defect energy were always defined with respect to the valence band edge E_V. This is no longer satisfying when the energy bands are graded, and thus SCAPS 2.8 offers new options, see Fig. 7.
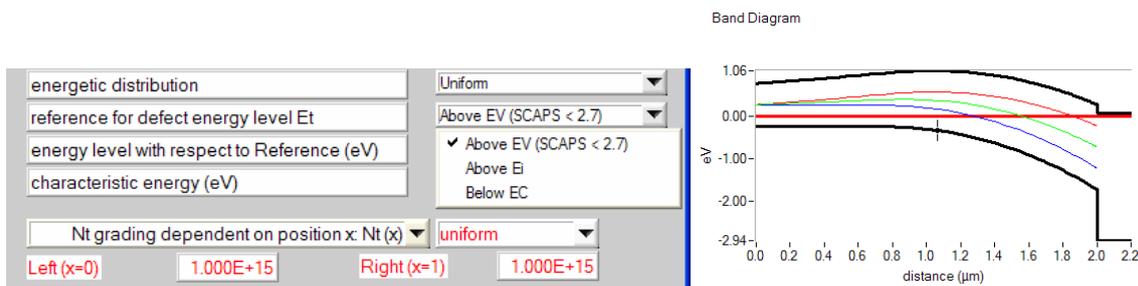
Fig. 7   Left: Detail of the SCAPS2.8 Defect Properties Panel. Three reference levels can be selected to define the defect level E_t: 'above E_V', 'above E_i' or 'above E_i'. Right: energy band diagram of a pn^+ junction with a strongly graded p layer. Three bulk defects have been defined: at $E_V + 0.5$ eV (blue), at $E_i + 0$ eV (green) and at $E_C - 0.5$ eV (red). At the left side, these three levels coincide, at the junction, they differ appreciably.

Perhaps, one could select 'above E_V' for a rather shallow acceptor level (e.g. In in Si), 'below E_C' for a rather shallow donor level (Ti in Si ?), and 'above E_i' for a deep level. Of course, a detailed knowledge of the materials defect physics and chemistry will assist to make a suitable selection.

Though it is not relevant in the context of grading, also a choice of energy reference levels is offered for interface states. In SCAPS 2.7 and earlier, E_t at an interface always was referred with respect to E_V of the material at the left. Sometimes it required some puzzling to point out the precise energy position of an interface defect. The new possibilities are illustrated in Fig. 8.
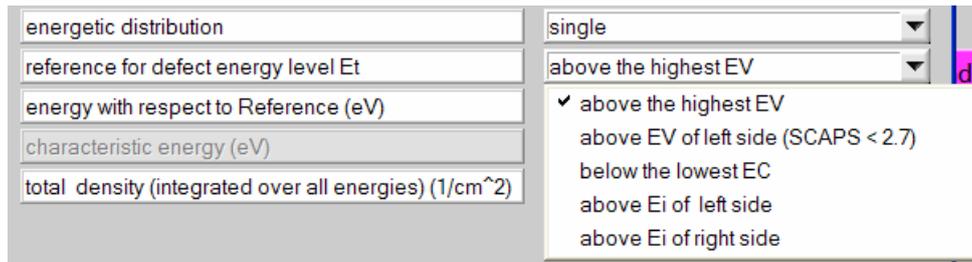
Fig. 8   Detail of the SCAPS 2.8 Interface Defect properties panel. Five possible choices are offered to refer the energy E_t of an interface defect.

The choice of E_{ref} of all defects (bulk and interface) is saved in the problem definition file (the .def file). When such file is read by SCAPS 2.7 and earlier, the E_{ref} lines are not read, and all E_t values are referred to E_V (bulk) of $E_{V, \text{left}}$ (interface), which might lead of course to an erroneous interpretation of the .def file. Beware of this when you save a problem that might need to be opened in earlier versions of SCAPS later on!

2.2 Defect densities N_t are given in cm^{-3} <u>and</u> in cm^{-3}eV^{-1}

In SCAPS 2.7 and earlier there was some ambiguity in the definition of the defect density N_t. When there was no energy distribution (thus 'single level'), N_t was interpreted as total density in cm^{-3}. But when an energy distribution was defined (thus: uniform, Gauß, CB tail or VB tail), N_t was interpreted at the density per energy at the peak energy of the distribution, and thus was expressed in cm^{-3}eV^{-1}. It was left to the user to figure out the total density in cm^{-3} in these cases: straight forward for a uniform distribution, a little bit less for a Gaussian distribution.

In the SCAPS 2.8 user interface, the total N_t in cm^{-3} and the energy density $N_t(E_{\text{peak}})$ in cm^{-3}eV^{-1} are always treated together: you see both, you can alter one of them, and the other will be adapted automatically and immediately. This also applies to interface defects (then the units are cm^{-2} and cm^{-2}eV^{-1}). This new facility is illustrated in Fig. 9.

Internally, SCAPS 2.8 treats the total density as the primary variable. Thus, when you vary the characteristic energy width E_{char} of a defect distribution, SCAPS will keep N_t(total) constant, and vary $N_t(E_{\text{peak}})$ for each E_{char} value. This strategy differs from earlier SCAPS versions, where $N_t(E_{\text{peak}})$ was kept constant, and N_t(total) varied for each E_{char} value. Beware of this when comparing SCAPS 2.8 with SCAPS 2.7 results !
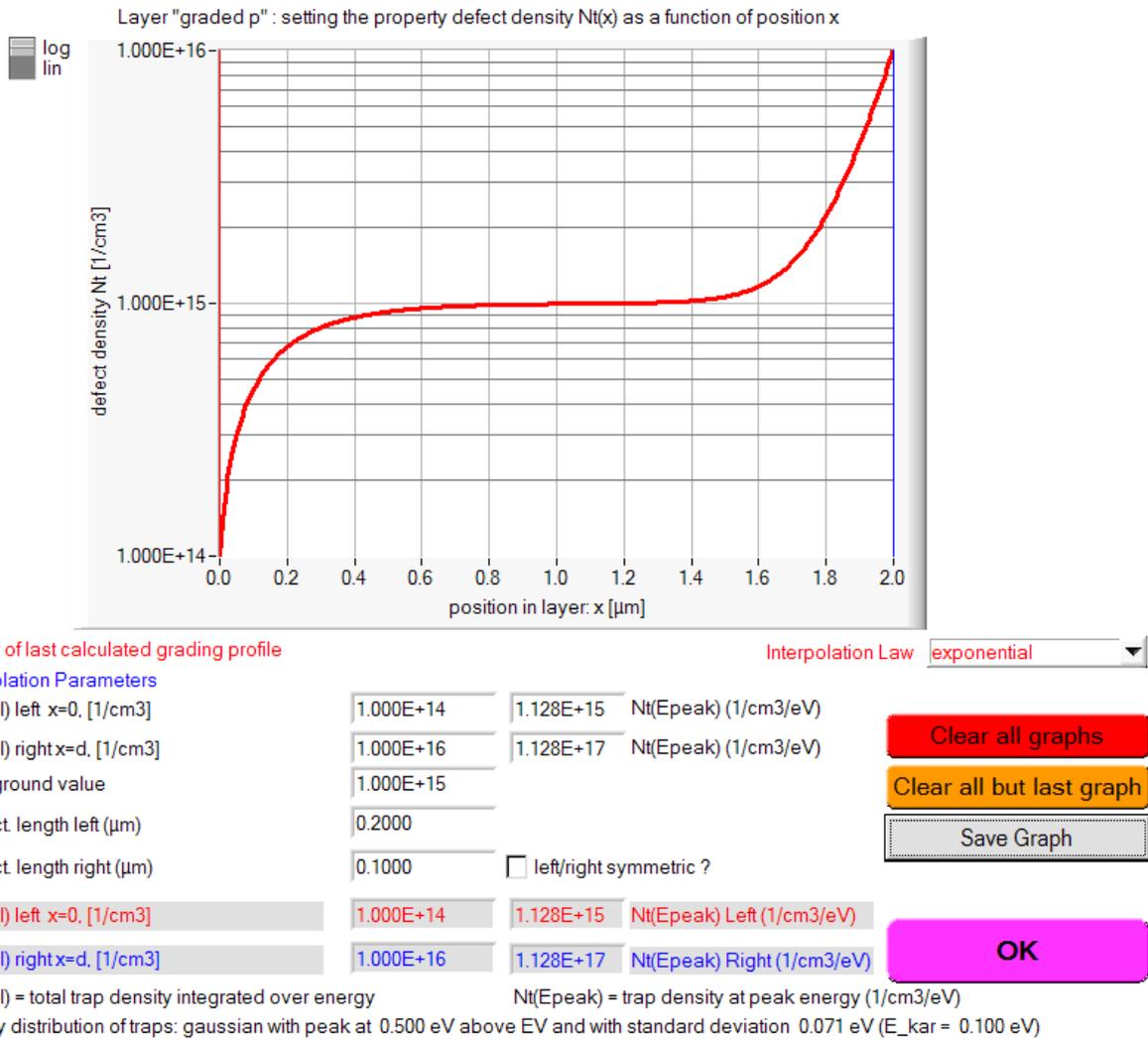
Fig. 9 Top: When defining the grading of a defect with an energy distribution, the Grading Panel allows to set both $N_{t, total}$ (in cm^{-3}) and $N_t(E_{peak})$ (in cm^{-3}eV^{-1}). Also, a summary of the defect distribution is given at the bottom of this panel. Bottom: in the Interface defect properties Panel, one can set both $N_{i, total}$ (in cm^{-2}) and $N_i(E_{peak})$ (in cm^{-2}eV^{-1}).

2.3 An external shunt conductance can be included

On request from many users, SCAPS 2.8 can handle an external shunt resistance (an external series resistance was already there). For your convenience, you can define either $R_{sh}.A$ or G_{sh}/A. Also, the option 'shunt' can be switched on or off (Fig. 10 left). This option affects the *I-V*, *C-V* and *C-f* calculations. The voltage range you set in the *I-V* and *C-V* action set up is the internal voltage. The voltage shown in the graphs and output tables will be the external voltage, which can differ form the set voltages if series resistance is present. The same applies to the working point voltage, when calculating *QE* with bias voltage. The series and shunt

settings are written in the .def file. SCAPS 2.7 will disregard the shunt information in this file, and assume $G_{sh} = 0$ (no shunt, the only thing it can handle).
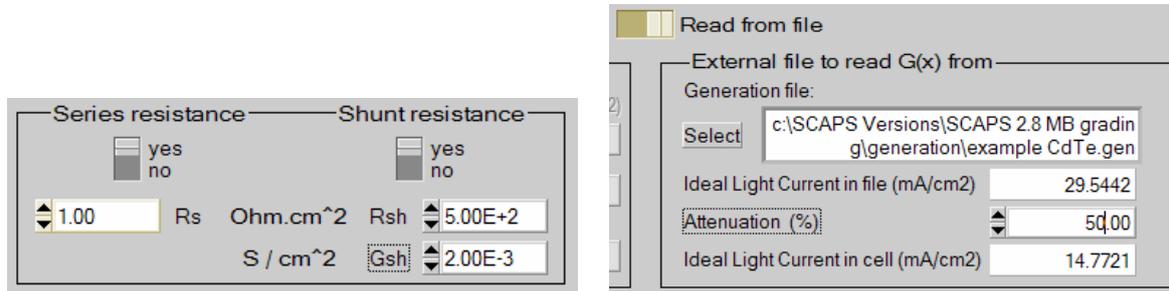
Fig. 10   Left: The series and shunt setting facility in the upper right part of the SCAPS 2.8 action panel. Right: The $G(x)$ from file facility is restored in the action Panel.

2.4 The facility '$G(x)$ input from file' is restored

This facility, present in early SCAPS versions, had unfortunately been disabled in SCAPS 2.7 when the impurity photovoltaic effect (IPV) was implemented. Indeed, when IPV is present, the local absorption constant $\alpha(\lambda, x)$ becomes dependent on the local carrier densities $n(x)$ and $p(x)$, and hence a preset $G(x)$ input table becomes meaningless. However, not too many SCAPS users need the IPV facility, and there were several requests to restore the '$G(x)$ input from file' facility: this is done now. Care is taken in the Action Panel and in the Defect Properties Panel that IPV and $G(x)$ input from file will not coexist. As an extra, you get the ideal light current contained in the generation file, before and after applying a possible attenuation (neutral density filter) (Fig. 10 right).

2.5 Error messages can be captured in a log-file

Nasty error messages ("convergence failure…") can now and then pop up, and they require an acknowledgment (clicking 'OK' or enter) to proceed. This was inconvenient in long batch jobs, over lunch time or even over night. Therefore we have implemented an option to catch these messages in an error log file, see Fig. 11. The log file always has the same name: SCAPSErrorLogFile.log, and it resides in the directory where your scaps2802.exe file is. It is a normal text file. These error options are not saved. When starting up SCAPS, this option is always set to 'inform on screen and wait for acknowledgment'. It needs a deliberate action to alter this option before e.g. launching a large batch task.
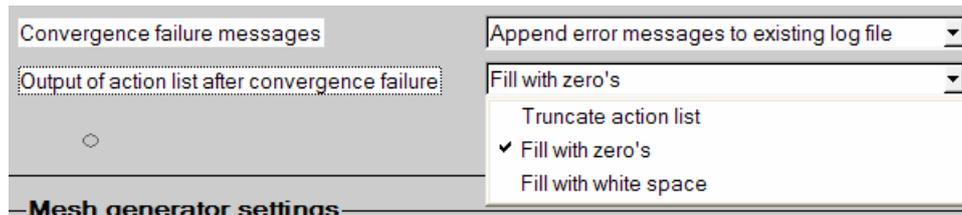
Fig. 11　　In the Numerical Panel of SCAPS 2.8 you can define your strategy of handling error messages. The options for convergence failure messages are: 'inform on screen and wait for acknowledgment', 'append error messages to existing log file' (shown here), and 'overwrite existing log file with error messages'. The options for the results (e.g. *I-V* tables) are show in the Figure.

2.6 The quantum efficiency can be shown against λ or against *h*ν

The quantum efficiency QE now can be shown as a function of wavelength λ (in nm), or as a function of photon energy *h*ν (in eV), to serve all tastes (Fig. 12). Both are given in the output tables.
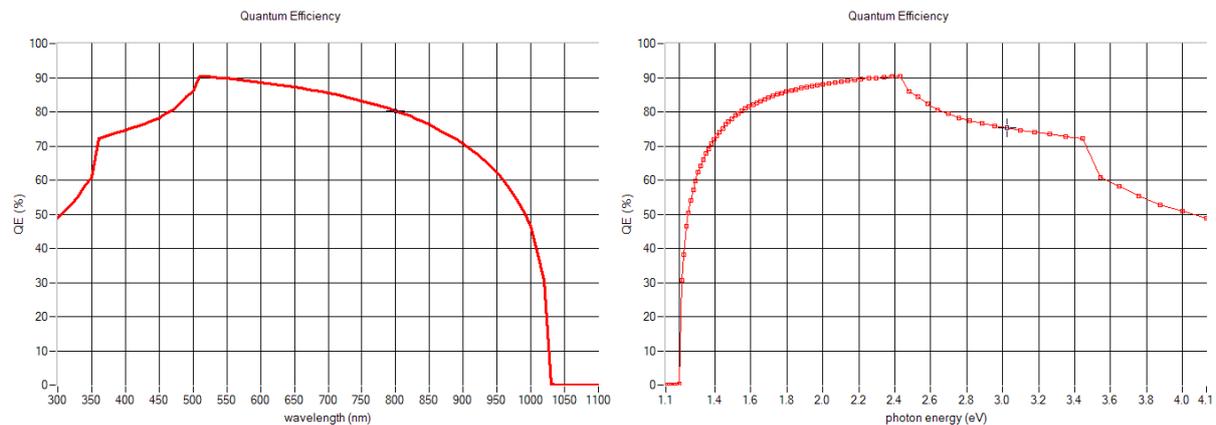
Fig. 12　　The quantum efficiency can now be shown as a function of wavelength $QE(\lambda)$, left, or as a function of phonon energy $QE(h\nu)$, right. In this graph the calculated points are shown, because they are not equidistant on the *h*ν axis.

2.7 Panels and graphs can be saved in a graphical format

All panels containing one or more graphs, and all graphs can be saved in a graphical format, see Fig. 13. This feature is ideal for quickly preparing presentations (or user manuals…) with SCAPS illustrations. These graphical formats supported by National Instruments LabWindows however are not of a sufficient quality to use them in e.g. a publication.
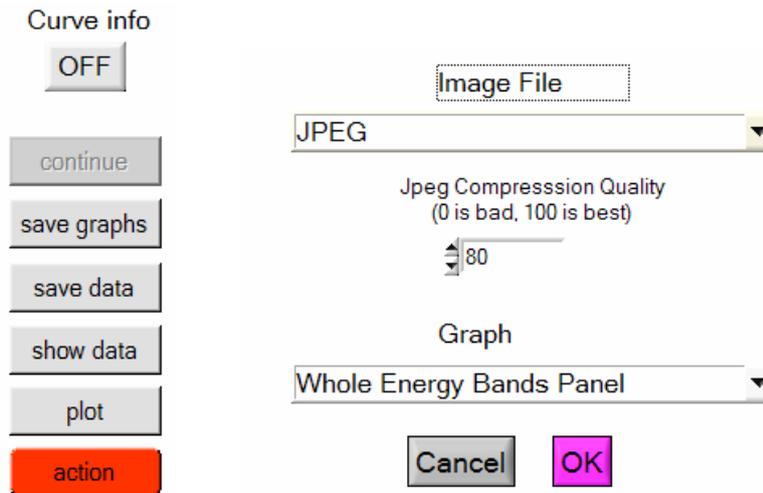
Fig. 13   Left: All panels containing one or more graphs can now be saved in a graphical format; use the grey 'save graphs' button. Right: One can select the .png, .jpeg or .bmp format; the .png format gives the best results. One can save the whole panel, or select one graph in it.

2.8 The new Air Mass 1.5 spectra 'edition 2'

Recently, almost all cell record efficiencies were boosted a little bit by the introduction of a new standard ('edition 2') for the solar spectra. The SCAPS format of these new spectra is distributed with SCAPS 2.8. These 'edition 2' spectra contain 2002 wavelengths – power density lines, compared to only 60 for the spectra hitherto. Thus, some calculations (e.g. *QE* under bias light) will be somewhat slower.

Also, some spectra have been renamed: e.g. 'AM1_5 G.spe' and 'new AM1_5 G.spe' in SCAPS 2.7 are renamed to 'old AM1_5 G.spe' and 'AM1_5 G.spe' in SCAPS 2.8.

We also want to draw your attention to a variety of monochromatic spectra which have been available for a while. They come in two versions. They either contain a total illumination power of 1000 W/m^2 (1 sun) in the wavelength band (e.g. '600 nm .spe'), or they contain a number of photons that would yield a light current J_L = 20 mA/cm^2 if *QE* were unity (e.g. '600nm fixed JL.spe').

3. Problem definition files distributed with SCAPS 2.8

The new facilities implemented in SCAPS 2.8 have made this programme more powerful, but also more complicated. We therefore offer more problem definition files to illustrate the new features, and run quickly though them here.

These problem definition files are:

- `Example CIGS SCAPS28.def` and `Example CdTe SCAPS28.def`: the same files as distributed with all earlier versions, but now saved in SCAPS 2.8 format.

- `CdTe-base.def`, based on the work of Gloeckler and Sites, Osaka World PV Conference 2003.

- `Numos Exercise 1.def`, `Numos Exercise 2.def` and `Numos GIGS baseline.def`: These files were distributed after the NUMOS Workshop, Gent, march 2007.

- `linear single layer N(x).def`, `linear single layer N(y).def`, `linear two layers.def`: New files, that illustrate three ways to implement a linearly graded diode. There is ample of information in the comment section of these .def files.

- `single layer N(x).def` and `single layer N(y).def`: New files, that represent two ways to implement an exponentially graded front region in a uniform base layer. There is ample of information in the comment section of these .def files.

- `Symmetric graded.def` and `graded pseudo CIGS-ZnOS.def`: These files illustrate several grading features of SCAPS 2.8. There is ample of information in the comment section of these .def files.

- `IPV.def`: This problem does not simulate any real or realistic solar cell, it is just set up to illustrate the Impirity Photovoltaic Effect (IPV) in SCAPS. There is ample of information in the comment section of this .def file. A result obtained with this file is shown in Fig. 14 left.

- `Intraband tunnelling.def`: This problem does not simulate any real or realistic solar cell, it is just set up to illustrate the facility of intra-band tunneling in SCAPS. There is ample of information in the comment section of this .def file. A result obtained with this file is shown in Fig. 14 right.
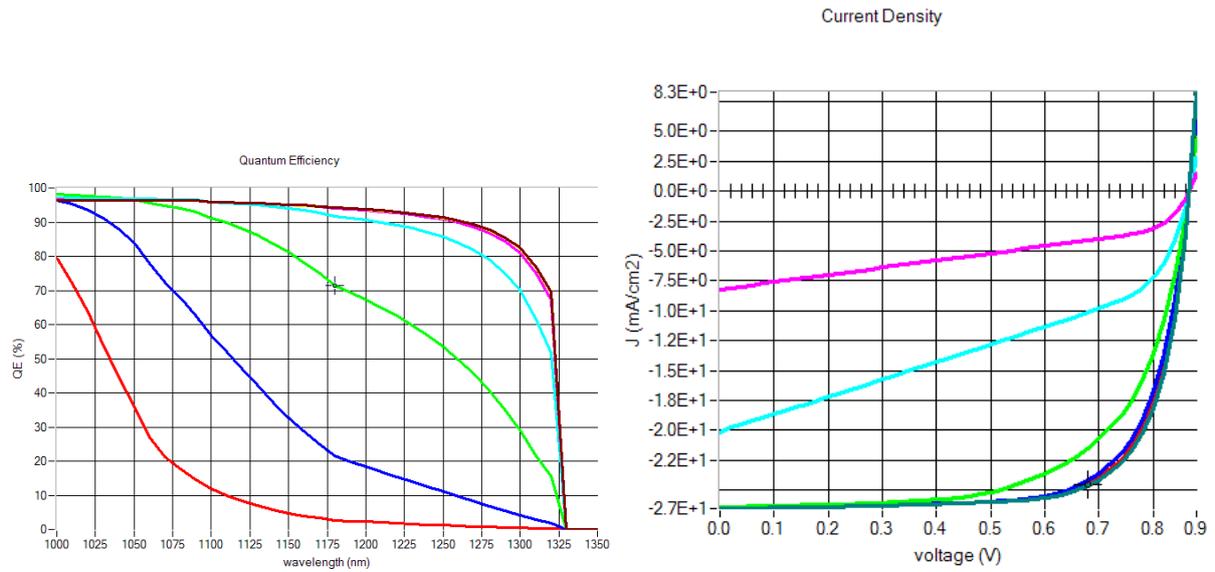
Fig. 14   Left: Result obtained with `IPV.def`. The option IPV is enabled. The batch parameter is the internal transmission *T* at the front contact; it varies from 0.1 (upper right) to 10^{-6} (lower left, red) (logarithmically, 1 step/decade). Right: Result obtained with `intraband tunneling.def`. The batch parameter 1 is tunneling off/on (at the first interface), and batch parameter 2 is the electron affinity of the window, which takes the values χ = 4.100, 4.125, 4.150, 4.175 and 4.200 eV (leading to an increase of the VB spike). The curves with tunneling are insensitive to the spike height (all curves crowded in the lower right part of the graph). The *I-V* curves without tunneling rapidly degrade with spike height (in this χ range; e.g. green, cyan and magenta are for χ = 4.15 eV, 4.175 eV and 4.2 eV, no tunneling).

4. SCAPS compatibility issues

As stated above, there is upward and downward compatibility of the SCAPS definition files: the new SCAPS version 2.8 will correctly read old .def files, and the old SCAPS versions ≤2.7 will read correctly new .def files, inasmuch they do not contain any information on phenomena not implemented in these earlier SCAPS versions (e.g. grading, shunt,…). The *caveats* mentioned above are summarised here:

1. SCAPS 2.7 and earlier ignores all information on grading. It assumes that all layers are uniform; that all parameters take the value defined in the new def file as the value for the 'pure A material' (thus for *y* = 0) (notice: it does <u>not</u> take the value 'at the left side', thus for *x* = 0). When there is a $N_t(x)$ grading defined in the new .def file, it will be recognised when it the grading law is 'uniform', 'linear' or 'exponential'; all other grading laws ('logarithmic', …) are not recognised and replaced with 'uniform'. There are slight differences between the mathematical equations used in SCAPS 2.7 and SCAPS 2.8 to calculate exponential grading. This is in part because SCAPS 2.7 did not recognise a 'background concentration'. The equations internally used are (in the symmetrical case $L_{char,\,left} = L_{char,\,right} = L$):

$$N(x) = N_{right} + \left(N_{left} - N_{right}\right) \cdot \exp\left(-\frac{x}{L}\right) \quad , \quad N_{left} > N_{right}$$

(SCAPS 2.7)

$$= N_{left} + \left(N_{right} - N_{left}\right) \cdot \exp\left(-\frac{d-x}{L}\right) \quad , \quad N_{right} > N_{left}$$

$$N(x) - N_0 = \frac{1}{\sinh(d/L)} \cdot \left[\left(N_{left} - N_0\right)\sinh\left(\frac{d-x}{L}\right) + \left(N_{right} - N_0\right)\sinh\left(\frac{x}{L}\right)\right] \quad \text{(SCAPS 2.8)}$$

where the layer extends from $x = 0$ to $x = d$, and where N_0 is the background density. (Of course with due numerical precautions for very small or very large values of d or L).

2. SCAPS 2.7 and earlier ignores the information about the reference energy level of defects. It will assume that the defect energy E_t of all bulk defects is referred 'above E_V", and that E_t of all interface defects is referred 'above E_V left".

3. The difference in the interpretation of the defect density N_t has been explained above (section 2.2).

4. SCAPS 2.7 ignores all information about shunt, and assumes $G_{sh} = 0$.

… and now: on your marks, ready, go!

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