

SCAPS Version 3.1.02, October 2011

This is not a stand-alone manual of SCAPS. It only describes the novelties in SCAPS 3.1.02 compared to SCAPS 3.0 and earlier. A (kind of) manual of the SCAPS programme is contained in another document. This is complemented with (so far) five add-on manuals, for SCAPS 2.8 ('grading'), for SCAPS 2.9.02 ('multivalent defects'), for 2.9.03 ('script'), for 2.9.04 (better handling of 'uniform') and for 3.0.00 (revision of 'tunnelling'). Also, there is a short and recommendable document `Getting Started.pdf`, which does exactly what it promises, and a presentation `SCAPS introduction.pdf` with more 'Getting Started' illustrations, and covering more topics than the Getting Started manual. All these documents are available on the SCAPS download site.

Enhancements of version 3.1, compared to version 3.0

There are two important new features in version 3.1. One is scientific: analysis of the C - f measurements (admittance spectroscopy). The other should contribute to the user comfort: built-in curve fitting.

1 Analysis of C - f measurements and simulations (admittance spectroscopy)

A facility is added to analyse admittance (thus $C(f)$ and/or $G(f)$) measurements and simulations, according to a method outlined by T. Walter et al., that was recently extended to cover also measurements under varying (also forward) bias voltage by K. Decock et al.

T. Walter, R. Herberholz, C. Müller, H.W. Schock, Determination of defect distributions from admittance measurements and application to Cu(In,Ga)Se₂ based heterojunctions, *Journal of Applied Physics*, **80** (1996) 4411-4420.

K. Decock, S. Khelifi, S. Buecheler, F. Pianezzi, A.N. Tiwari, M. Burgelman, Defect distributions in thin film solar cells deduced from admittance measurements under different bias voltages, *Journal of Applied Physics*, **110** (2011) 063722.

The 'AS-panel' is opened by clicking an orange button on the C - f panel, see Figure 1.

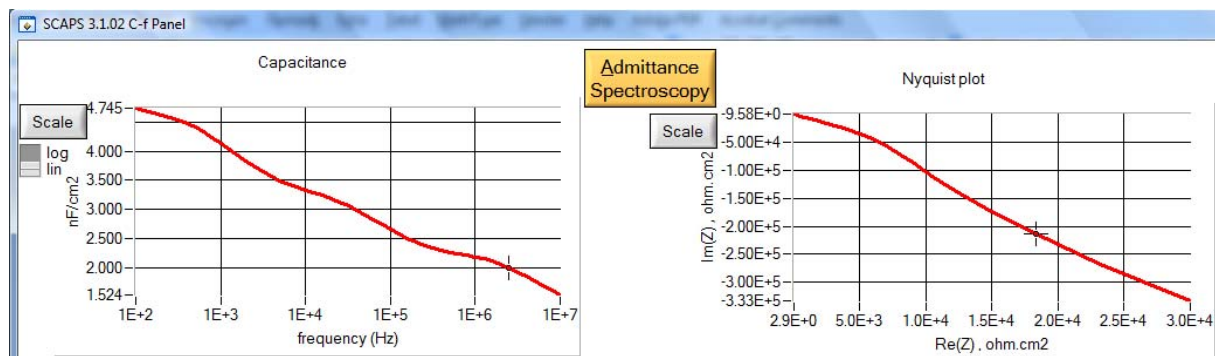


Figure 1 The orange button 'Admittance Spectroscopy' is available in the C - f panel.

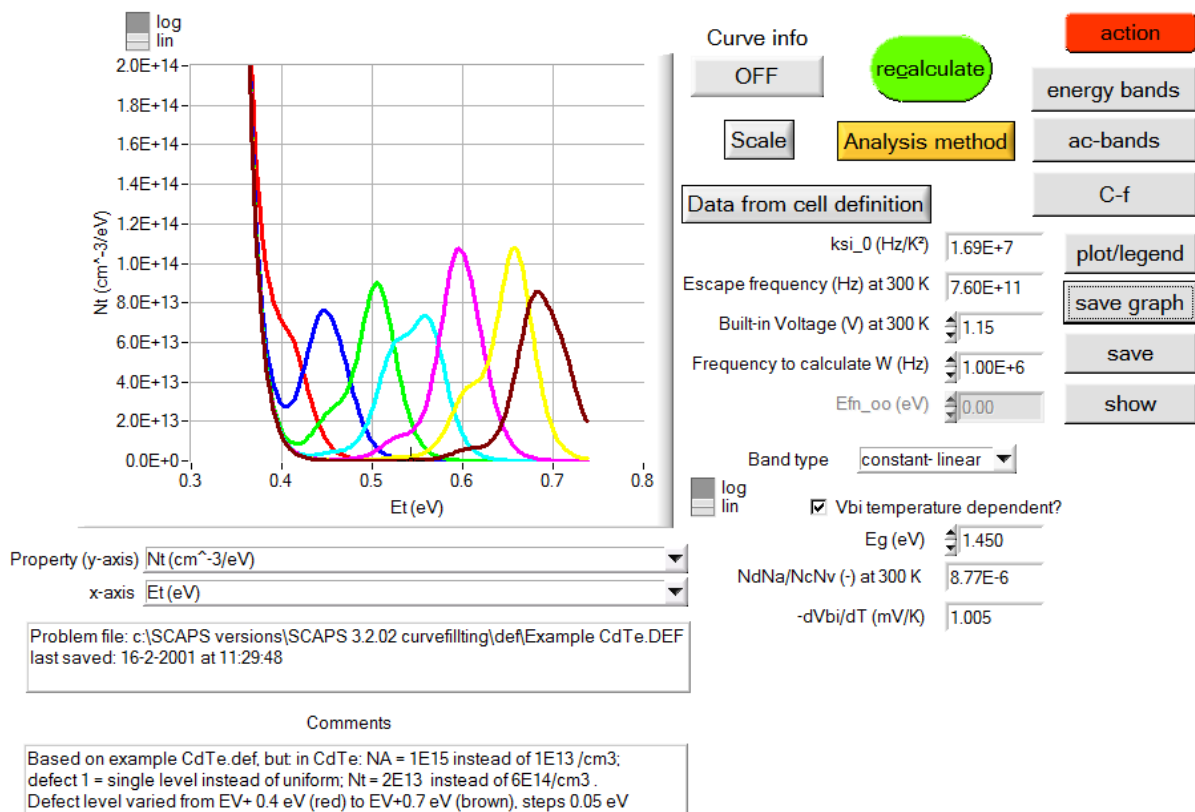


Figure 2 The admittance spectroscopy panel.

The terminology and parameters used in this panel are those defined in the work of Walter and Decock. You can select some properties as abscissa (x -axis) and some as ordinate (y -axis) to visualise the admittance analysis, see Figure 3.

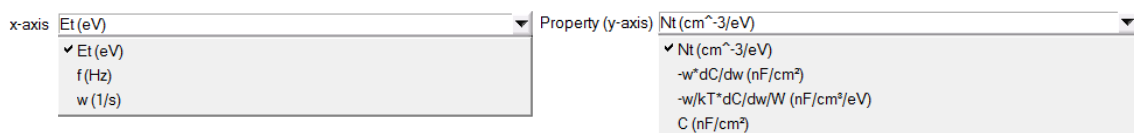


Figure 3 Choice of abscissa's (left) and of ordinates (right) in the admittance spectroscopy panel.

2 Curve fitting

2.1 General principles

The purpose of curve fitting is to vary one or more parameters in the cell definition to obtain a fit between one or more measured curves and the simulation. The numerical algorithms are taken from:

W.H. Press, S.A. Teukolsky, W.T. Vetterling, B.P. Flannery, *Numerical recipes in C*, 2nd ed., Cambridge University Press, 1992.

- If there is only one parameter to fit: the golden section search (*The recipes*, p. 401).
- When there are 2 to 9 parameters to fit: the downhill simplex method, or Nelder-Mead method (*The recipes*, p. 408).

The parameters to fit are the parameters set in the batch set-up, together with their range and linear or logarithmic character. Not all batch parameters are usable as curve fitting parameters: parameters that are file names (e.g. definition files, spectrum files, absorption files), and parameters of an on/off nature (e.g. ‘illumination on/off’, ‘tunnelling on/off’) are not usable. The curve fitter can only be set up when at least one parameter allowable for curve fitting has been defined in the batch set-up.

The measurements to fit should be selected in the curve fitting set-up. Currently, a maximum of 9 measurements is possible. A fixed parameter can be attached to each measurement. This can be useful when you want e.g. to fit 4 dark *I-V* measurements at 4 different temperatures, or 5 illuminated *I-V* curves at 5 illumination intensities. A limited selection of parameters is offered by the user interface as a fixed parameter of a measurements: only those which can be controlled in an experiment (as we think: we do e.g. not believe that one can make different samples that differ by their electron capture constant c_n of some defect...).

2.2 Setting up the curve fitter

A set of new buttons has been added to the calculation-block of the action panel, see Figure 4

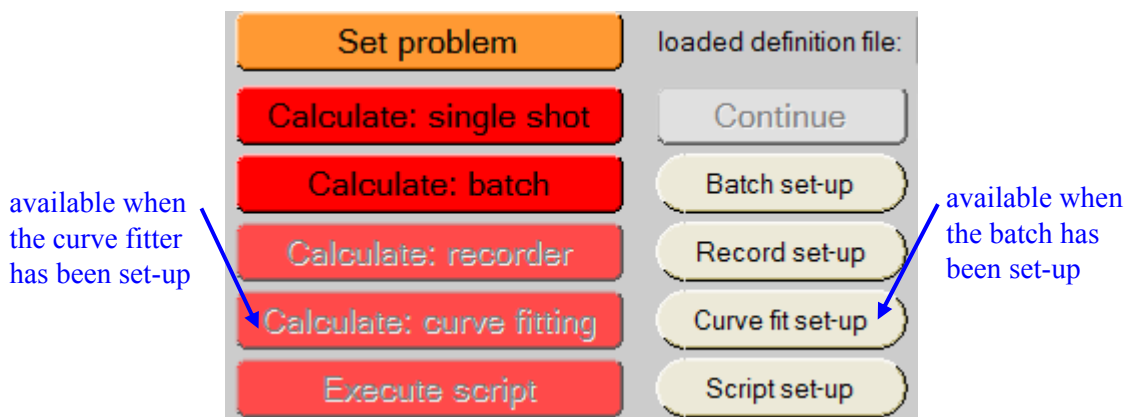


Figure 4 New buttons in the calculation block of the action panel for setting up and for executing curve fitting.

As already mentioned, the curve fitting set-up takes the allowable parameters from the batch set-up, complete with their range and linear/logarithmic nature. In the curve fitting set-up, the starting value of this parameter should be set, see Figure 5: by default it is the central value in the range (taking into account the linear or logarithmic character). You can also start from the actual value of a parameter in the present cell definition.

Parameters to be fitted to the measurements		Minimum	Maximum	Lin / Log	Start Value	Start Value = Actual Value ?
(These can only be changed in the Batch Set-up Panel !)						All None
p-CIGS (L1)	thickness[μm]	1.000E+0	5.000E+0	linear	2.350E+0	<input checked="" type="checkbox"/>
n-CdS (L2)	shallow donor density[1	1.000E+15	1.000E+18	log.	3.162E+16	<input type="checkbox"/>

Figure 5 Curve fitting parameters taken over from the batch set-up; setting the start value to the central value in the range, or to the actual value in the cell definition.

Then the measurements should be set, see Figure 6. If ‘show’ is clicked, the measurement is shown in the simulation panel (*I-V*, *C-V*, *C-f* or *QE*). At present, only one measurement can be shown in each of these panels.

Measurements to be fitted (you should define at least one measurement)							Fixed Value	
	Measurement file name	Type	Light	Show	Is there a fixed parameter for this measurement?			
Remove	Set	Numos baseline dark IV 280 K.iv	I(V)	<input type="checkbox"/>	log	<input checked="" type="checkbox"/>	T [K]	2.800E+2
Remove	Set	Numos baseline dark IV 300K.iv	I(V)	<input type="checkbox"/>	log	<input checked="" type="checkbox"/>	T [K]	3.000E+2
Remove	Set	Numos baseline dark IV 340K.iv	I(V)	<input type="checkbox"/>	log	<input checked="" type="checkbox"/>	T [K]	3.400E+2
Remove	Set	asurements\Numos Ex 1 dark.cv	C (V)	<input type="checkbox"/>	lin	<input type="checkbox"/>		

Add

Figure 6 Measurement set-up in the curve fitter: the measurement type and illumination, the linear/logarithmic character, and a possible fixed parameter.

The correspondence between a simulation and a measurement is expressed by the χ^2 sum ('Chi square'), that we define here as:

$$\chi^2 = \frac{\sum_i (y_{\text{meas}} - y_{\text{calc}})^2}{\sum_i (y_{\text{meas}})^2} \quad (\text{linear}) \quad \text{or} \quad \chi^2 = \frac{\sum_i (\log|y_{\text{meas}}| - \log|y_{\text{calc}}|)^2}{\sum_i (\log|y_{\text{meas}}|)^2} \quad (\text{logarithmic}) \quad (1)$$

where y_{calc} is the simulated property and y_{meas} the measured property (thus: I , C or QE), and only the points i are considered from the overlap in the simulation and measurement range of x (thus: V , f or λ). In these expressions, the simulations are linearly or logarithmically interpolated at the x_{meas} values. Our normalisation of χ^2 ensures that the χ^2 of all measurements are dimensionless and are scaled to 1: a fit is good if $\chi^2 \ll 1$. It also allows that the χ^2 values of the individual measurements/simulations can be compared and summed. We use χ_{tot}^2 as the figure of merit of the whole curve fitting action:

$$\chi_{\text{tot}}^2 = \frac{1}{n} \sum_i \chi_i^2 \quad (2)$$

where χ_i^2 are the χ^2 values of the individual measurements, and n is the number of measurements.

Some numerical parameters should also be set in the curve fitting set-up, see .

max #steps initial step minimal step size (stop criterion) minimal Chi-square (stop criterion)

 write the fitted parameters in the cell definition?

Figure 7 Numerical parameters in the curve fitting set-up

The step size of a parameter variation is relative to the range of this parameter (taking into account the linear or logarithmic nature of this parameter). Do not expect a perfect curve fitting after 25 steps only: 100 steps or so is more realistic, ... but takes more time. The curve fitter walks around though the parameter space, and stops when any of the stop criteria is met (maximum number of iterations exceeded, or step size small enough, or total χ_{tot}^2 low enough). The parameter set then obtained is only written in the cell definition when the button at the bottom right is clicked. When you visualise the results of the curve fitting (see next section), you will be able to judge the quality of the curve fitting, and you will get another

chance to write the ‘fitted’ parameters in the cell definition. The curve fitting settings can be saved and loaded, and are also included in the ‘save/load all SCAPS settings’ actions. At this moment, curve fitting is not supported by the script.

2.3 Visualisation of the curve fitting results

The curve fitting results can be visualised by clicking the a yellow button in the action panel, Figure 8.



Figure 8 The yellow button to visualise the curve fitting results is active once a curve fitting calculation has been executed.

You then see the curve fitting results panel, that allows you to select a variety of graphs to visualise and evaluate the whole curve fitting, Figure 9.

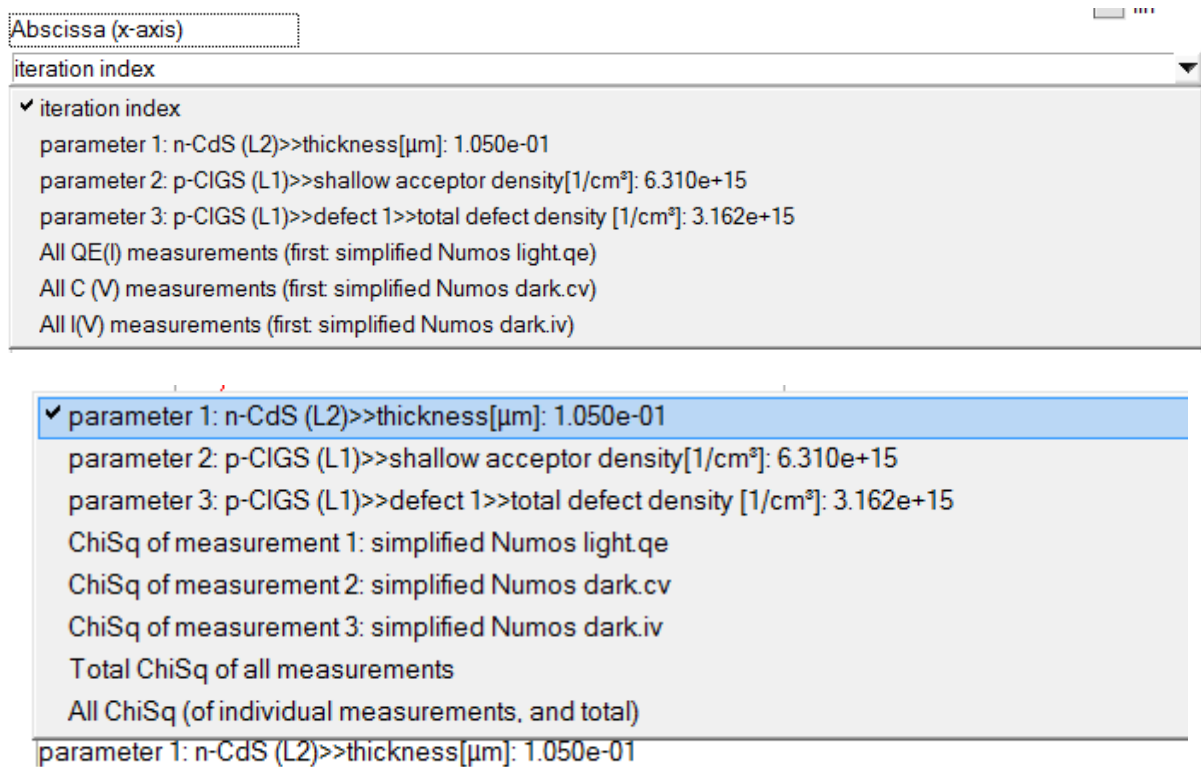


Figure 9 Choices of abscissa (x-axis, top) and ordinate (y-axis, bottom) to visualise the curve fitting results.

The examples shown in Figure 10 to Figure 13 illustrate the Numos exercise 1 example. The file Numos CIGS baseline.def first has been simplified to simplified Numos CIGS baseline.def, by taking a single energy defect level wherever a band of defects was presents: this is speeding up the calculations substantially. All settings, including the batch settings and the curve fitting settings, are saved in ‘simplified Numos curvefitting.scaps’. This calculation took 24 minutes on my computer... The iteration was stopped after 73 steps because the required accuracy ($\chi_{tot}^2 < 10^{-7}$) was met. Please note:

- do not expect a decent curve fit after e.g. 10 iteration steps only! In the example here, 50 – 60 steps seem to be necessary (Figure 10, Figure 11).
- do not expect such a very nice fit in a real situation! Here, the measurements were ‘constructed’, that is, calculated with SCAPS. Thus, an exact fit is possible. With real measurements, it can very well be that χ^2 never gets below 10^{-2} or 10^{-3} , meaning that your measurements can not be fitted very well with the present cell definition.
- it is also clear that you should not exaggerate with the number of parameters and the number of measurements. Though 9 is (now) the allowed maximum for both, I would recommend to use much more modest numbers, e.g. ≤ 3 , certainly to start with.
- *The recipes* state that it is a good idea to start a curve fitting over again starting with the parameters obtained from a previous curve fitting calculation. You can do so by saving the fitted parameter values in the cell definition, and running the curve fitting calculation again starting from the ‘actual values’, possibly with a smaller initial step, and/or with a narrower range for the parameters.

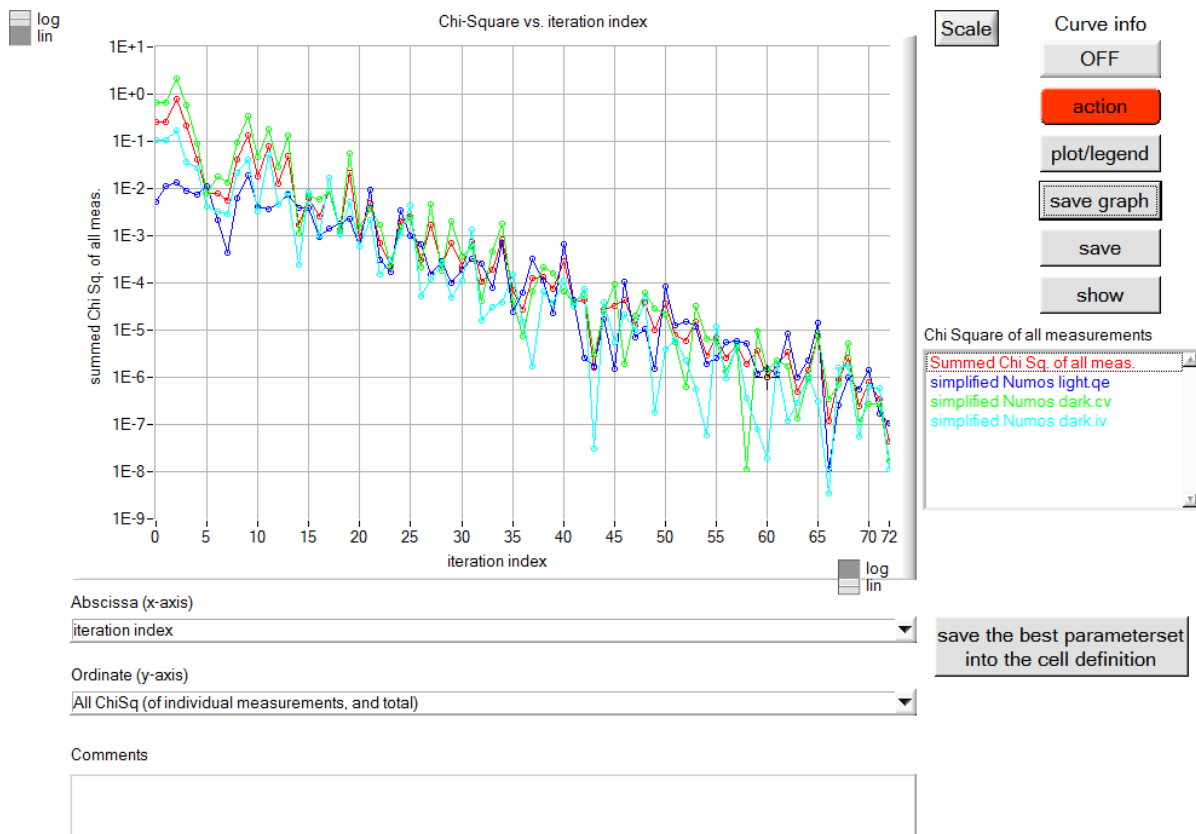


Figure 10 Some examples of curve fitting results: Numos exercise 1, with a simplified problem file. The evolution of all χ^2 values with iteration index. When you are satisfied with the results, you can insert the fitted parameter values in the cell definition by clicking the grey button.

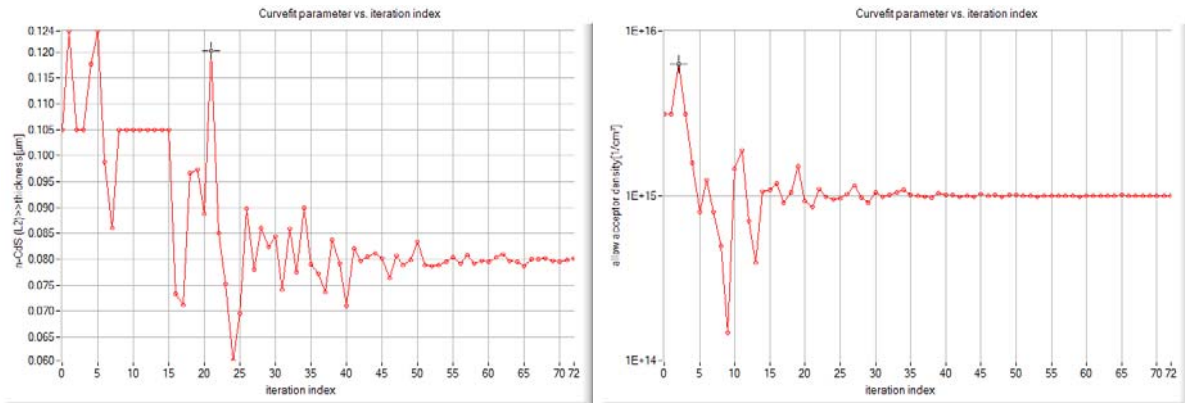


Figure 11 Some examples of curve fitting results: Numos exercise 1, with a simplified problem file. The evolution of the parameters d_{CdS} and $N_{\text{A, CIGS}}$ with the iteration index

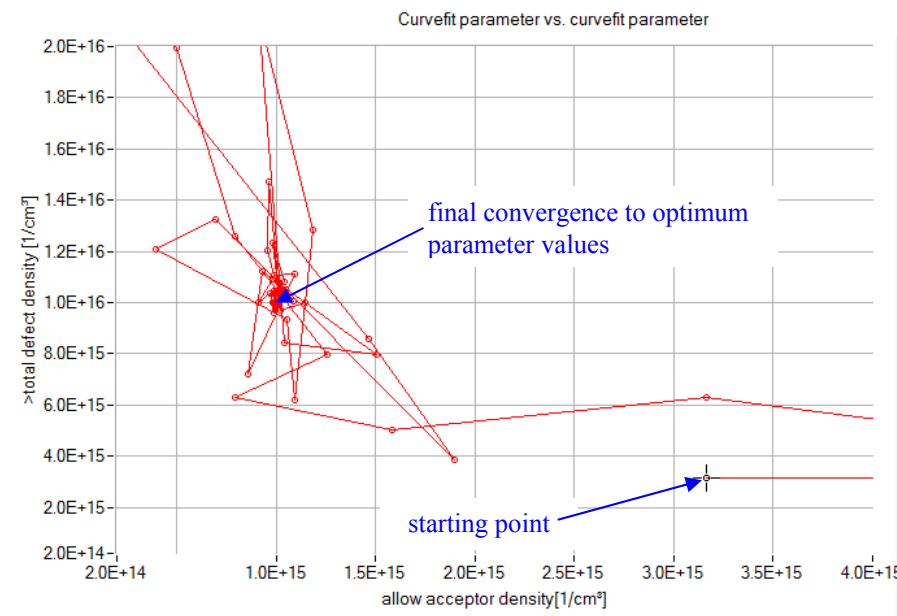


Figure 12 Some examples of curve fitting results: Numos exercise 1, with a simplified problem file. Walking in the parameter space to find optimum values for $N_{\text{A, CIGS}}$ and $N_{\text{t, CIGS}}$.

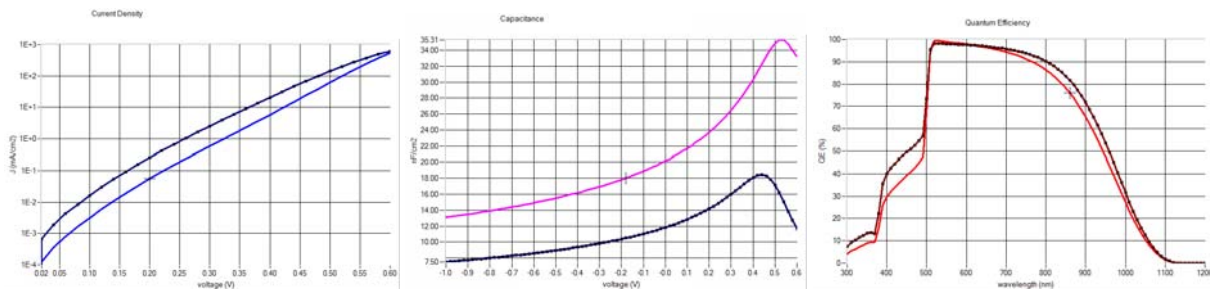


Figure 13 Some examples of curve fitting results: Numos exercise 1, with a simplified problem file. The measurements (dots), the initial calculation (simplified Numos CIGS baseline.def) and the calculation after 73 curve fitting iterations: I - V (left), C - V (middle) and QE (right).

2.4 Curve fitting résumé

1. Set up a rough SCAPS model for your cell

2. Verify that SCAPS is reading your measurements correctly (units, normalisation per area,...): display your measurements and check if all is OK.
3. Refine the model, by hand. As there are probably > 100 parameters to input in your model, you can't leave this to the computer, you should do it yourself. Consider the SCAPS curve fitting facility only as a fine-tuning.
4. Define the parameters you want to fit in the batch set-up, together with their range and linear/logarithmic nature. Do a quick batch calculation (only very few steps per parameter) to check if your measurement indeed could be fitted by the parameters you have selected
5. Set-up the curve fitter: the parameters were already set in the batch set-up; now only specify the starting value (mid-range or actual value). You have already checked that the measurements are available and readable by SCAPS. Now select the measurements to curve-fit, set their linear/logarithmic nature, and set one fixed parameter for a measurement if necessary.
6. First use a modest number of iteration steps, e.g. <10 , and run the curve fitting calculations, to see if everything is going as expected.
7. If it looks promising, set a higher number of steps, run the curve fitter, be patient and wait, and hope that the computer will have solved your problem. Do not be too disappointed when the result is less than you hoped for...

3 Other extensions since SCAPS 3.0.0

3.1 Composition grading

The composition grading profile can be loaded from a file since version 3.0.1. The files containing these profiles should be saved in the folder 'grading', and the default extension is .grd. The file which contains the grading profile should consist of two columns of numerical data, the first number representing the position in the layer in μm , the second representing the composition (usually a number between 0 and 1). All lines which cannot be interpreted as two numerical data are treated as comment.

3.2 Width of energy distribution of defects

Up to version 3.0.0 the width of the energetic defect distributions was fixed: $7 \times E_{char}$ for a tail-like distribution, and $6 \times E_{char}$ for a Gaussian distribution ($3 \times E_{char}$ to the left and $3 \times E_{char}$ to the right of the central level). Since SCAPS 3.0.2 these values can be set on the numerical panel.

3.3 A curve legend and selection facility

A legend facility has been added to most plots, see Figure 14. It allows to display the individual curves in a graph or not, and gives a short legend, with a colour label in each legend line corresponding with the colour of the curve in the graph.

Also, scale settings can now be saved and loaded to and from a file. The default extension of scaling settings files is .scl, and their default place is ... scaps/scaling.

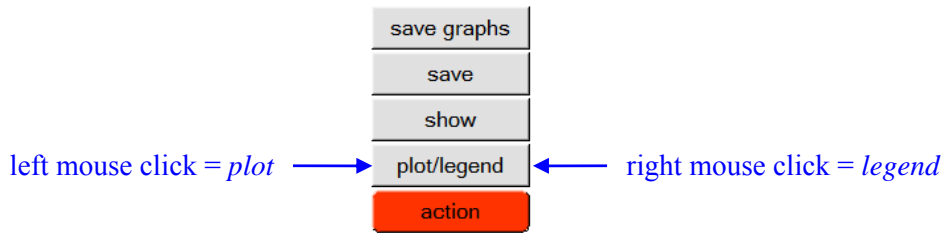


Figure 14 The new legend facility is available on all panels where there is a 'plot/legend' button is present. A right mouse click activates the legend and curve selection facility.

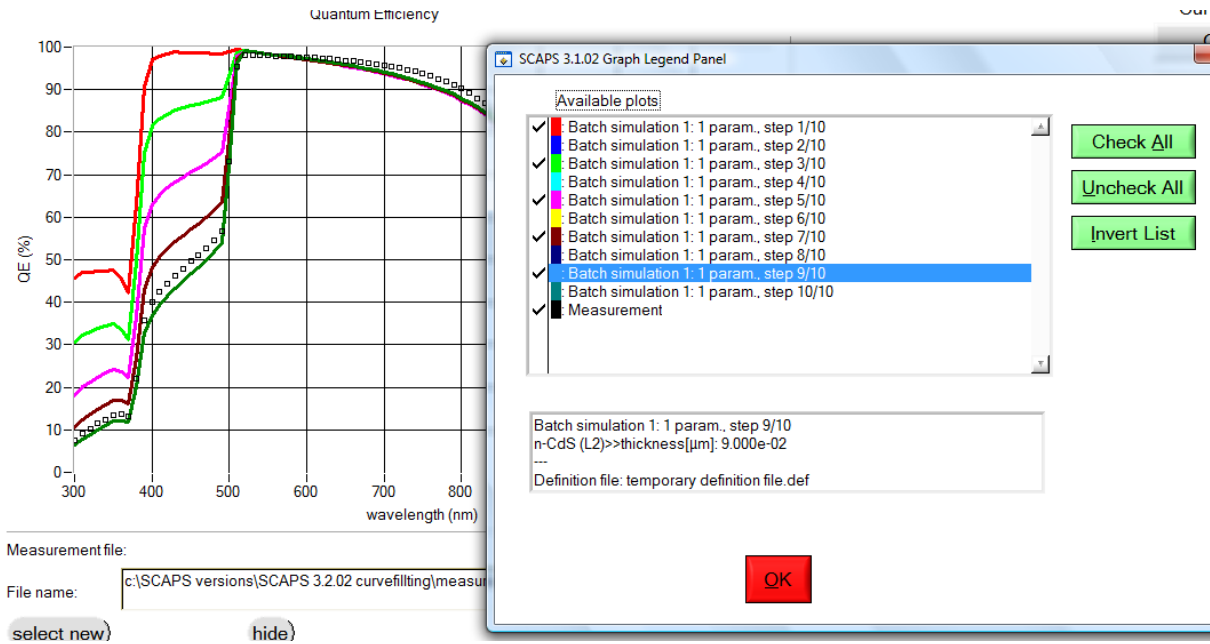
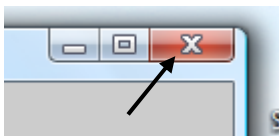


Figure 15 Example of the new legend facility. Only the curves checked are shown (checking/unchecking has immediate effect). The detailed information at the bottom (here $d_{CdS} = 90$ nm) is for the selected curve.

3.4 The Window close button is working now



We made the Windows close button active in all SCAPS panels – at last! When there is a cancel button on the panel, closing is equivalent to pressing 'cancel'. When not, and there is an OK button, closing has the same effect as clicking 'OK'. When not, it is equivalent to clicking 'action'. And finally, on the action panel, it means 'quit SCAPS'.

UGent – ELIS, October 2011

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