

Models for the generation $G(x)$ and the spectrum $S(\lambda)$ in SCAPS

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1. Introduction

The SCAPS application discussed in this document uses:

- SCAPS version 3.3.05 of december 2016, or more recent.
- The following files:
 - Definition files and all-SCAPS files that must be present in the folder [your SCAPS]\def:
 - ✓ the all SCAPS file Numos baseline with gaussian EBIC beam.scaps

2. The internal optical model of SCAPS

In its default mode, SCAPS calculates the generation of eh -pairs $G(x)$ from the incident photon flux $N_{\text{phot0}}(\lambda)$ from a very coarse optical model. This model contains only reflection/transmission at the two contacts, and absorption in the semiconductor layers. Thus: no interference, no scattering, no intermediate reflectors... For a single layer of thickness d , with uniform optical absorption constant $\alpha(\lambda)$ (uniform here means that α does not depend on position within the layer, thus $\alpha(\lambda, x) = \alpha(\lambda)$), and for light incident from the left with photon flux $N_{\text{phot0}}(\lambda)$, the photon flux $N_{\text{phot}}(\lambda, x)$ at each position in the layer is given by

$$N_{\text{phot}}(\lambda, x) = N_{\text{phot0}}(\lambda) \cdot T_{\text{front}}(\lambda) \cdot \exp(-x\alpha(\lambda)) \cdot \frac{1 + R_{\text{back}}(\lambda) \exp(-2(d-x)\alpha(\lambda))}{1 - R_{\text{back}}(\lambda) R_{\text{int}} \exp(-2d\alpha(\lambda))} \quad (1)$$

where

$T_{\text{front}}(\lambda)$ is the (possibly wavelength dependent) transmission of the front contact; the front contact is where the light is incident, here the left contact. T_{front} is in SCAPS a property of the contact, and thus is input in the Contact Properties Panel of the front contact.

$R_{\text{back}}(\lambda)$ is the (possibly wavelength dependent) reflection at the back contact; the back contact is at the opposite side from where the light is incident, here the right contact. R_{back} is in SCAPS a property of the contact, and thus is input in the Contact Properties Panel of the back contact.

R_{int} is a (not wavelength dependent!) internal reflection at the front contact. In SCAPS, the value of R_{int} or its complement $T_{\text{int}} = 1 - R_{\text{int}}$, should be input in the Solar Cell Definition Panel, see Fig. 1.

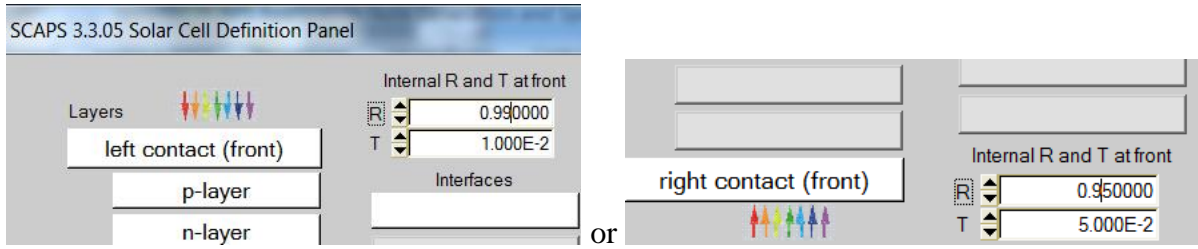


Fig. 1 Input fields for the internal reflection R_{int} , or its complement the internal transmission $T_{\text{int}} = 1 - R_{\text{int}}$, in the Solar Cell Definition Panel. The position of the input fields depend on the side where the light is incident. These input fields are only visible if a reflection at the back contact R_{back} is set.

Eq. (1) is simple to interpret: If there is no reflection at the back contact ($R_{\text{back}} = 0$), there is only one pass of light through the cell, and the light is extinguished with the familiar exponential function $\exp(-\alpha x)$. If $R_{\text{back}} \neq 0$, but the internal reflection at the front contact is zero, $R_{\text{int}} = 0$, there is a second pass of the light reflected at the back contact, and an additional extinguishing function $\exp(+\alpha x)$ appears in (1) for the reflected light. If there is internal reflection $R_{\text{int}} \neq 0$, there is an infinite number of passes of the light, that are summed up in (1) yielding the denominator.

In SCAPS, this model is extended to more than one layer, to layers with non-uniform (= position dependent) absorption $\alpha(\lambda, x)$, and to the possibility of light to be incident on the other contact. But there is no more physics than that already described in Eq. (1).

From the photon flux $N_{\text{phot}}(\lambda, x)$ at each position and for each wavelength, the generation of eh pairs is then calculated as

$$G(\lambda, x) = \alpha(\lambda, x) \cdot N_{\text{phot}}(\lambda, x) \quad (2)$$

This is then integrated over all wavelengths of the incoming photon flux:

$$G(x) = \int_{\lambda_{\text{min}}}^{\lambda_{\text{max}}} G(\lambda, x) d\lambda = \int_{\lambda_{\text{min}}}^{\lambda_{\text{max}}} a(\lambda, x) \cdot N_{\text{phot}}(\lambda, x) d\lambda \quad (3)$$

where λ_{min} and λ_{max} are the short and long wavelength limits of the incoming photon spectrum $N_{\text{phot}}(\lambda)$, as it is specified in the spectrum input file.

Users that are not satisfied with the optical model of SCAPS, can directly specify the eh generation $G(x)$ at each position. The optical model of Eqs. (1)-(3) is then not used. Since the impurity photovoltaic effect (IPV) relies on this internal optical model (with extensions), assigning IPV properties to defects is incompatible with a user specified generation $G(x)$. Precautions in SCAPS prevent the user to define both in one problem.

3. Analytical models for the generation and for the spectrum: motivation

Direct specification of $G(x)$ through an input file with extension .gen is intended for users who want to use SCAPS for the electrical calculations, but prefer to do the optical calculations themselves. A number of users have applied SCAPS with a file input for $G(x)$ to simulate electron beam induced current (EBIC) measurements. Typically, they would define intense

generation in a small sheet of the cell, and 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 proves to be a rather complicated and time consuming procedure. There was a little improvement for those brave users with SCAPS 3.3.02 of July 2015, where script commands were introduced that called one file from a list of file names, but still it was labour intensive work.

Another problem is the 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. For example, 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...

That is why we introduced in SCAPS 3.3.05 of December 2016 the possibility of defining $G(x)$ from an analytical model, where all parameters of the model (e.g. ‘central beam position’) can be manipulated in the SCAPS batch, recorder and script facilities. And in the same move, analytical models for the spectrum were implemented.

4. New facilities in SCAPS 3.3.05

The main SCAPS panel, the Action Panel was modified somewhat.

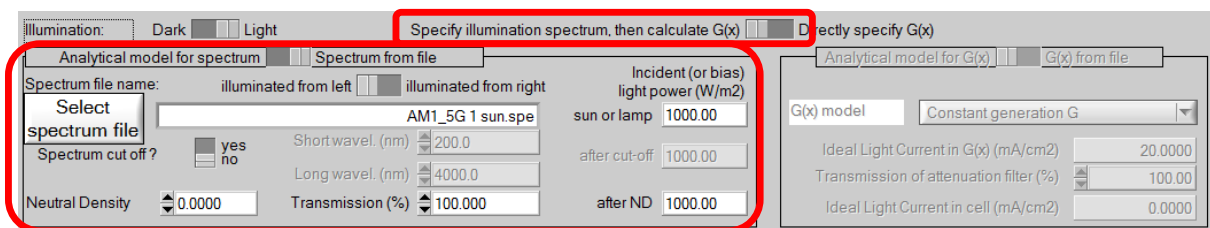


Fig. 2 Using the internal optical model of SCAPS: define a spectrum, let SCAPS calculate $G(x)$ with Eqs. (1) - (3). The selection switch marked on top of this figure is only active when the light is switched on.

The default setting is shown in Fig. 2: a spectrum is specified from a file, and the internal optical model of SCAPS is used. External optical filters can be applied: two spectrum-cut-off filters and a neutral density filter. When the model/file switch in the spectrum part of Fig. 2 is set to ‘Analytical model for spectrum’ (instead of ‘Spectrum from file’), the new facilities to calculate a spectrum from a (simple) model are enabled, see Fig. 3. The available spectrum models are discussed below.

When in Fig. 2 the option ‘Directly specify $G(x)$ ’ is set, one can set the generation $G(x)$ from an input file or from analytical model, see Fig. 4. The available generation models are discussed below.

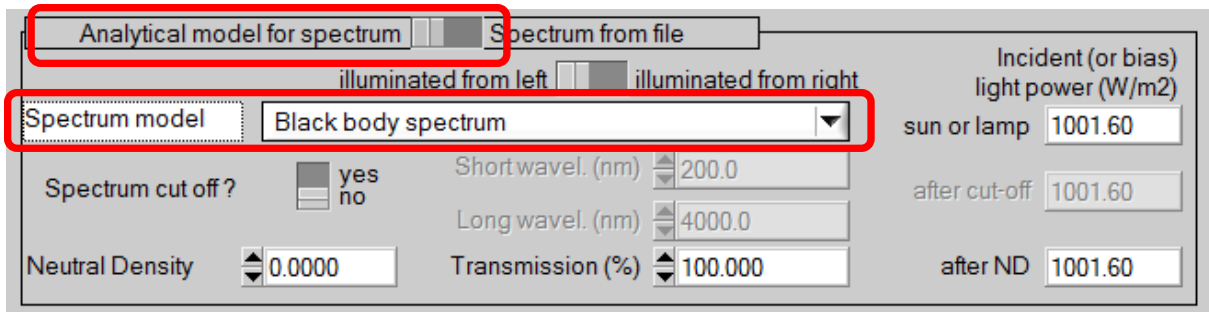


Fig. 3 Setting an analytical model for the spectrum, here a black body spectrum is selected.

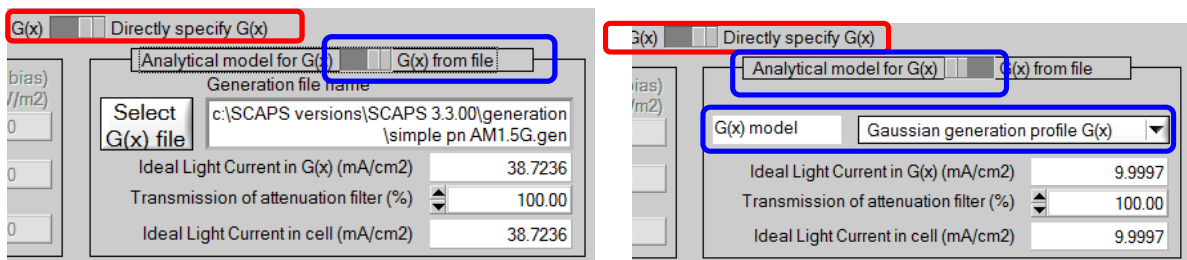


Fig. 4 Directly specifying the generation $G(x)$. Left: take $G(x)$ from an input file with extension .gen (as in previous SCAPS versions). Right: calculate $G(x)$ from an analytical model (new in SCAPS 3.3.05). The selection switch marked in red is only active when the light is switched on.

5. Analytical models for the generation $G(x)$

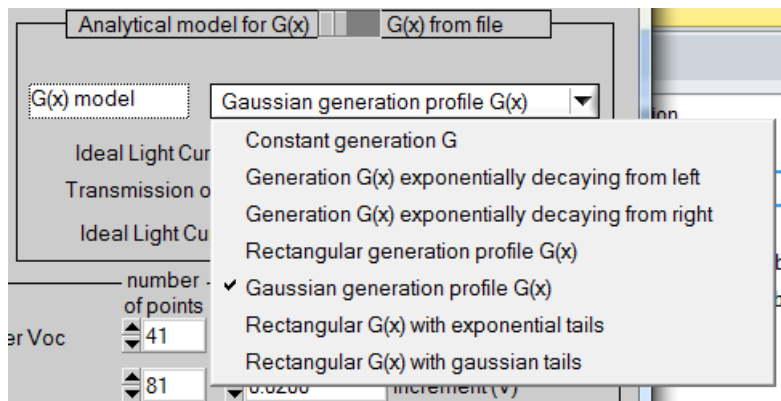


Fig. 5 The available generation models

As of now, the user can select one from seven models as shown in Fig. 5. When selecting one of them, e.g. here a Gaussian generation profile $G(x)$, the new SCAPS Model Panel opens, see Fig. 6. The panel is operated in much the same way as the SCAPS Grading Panel, that is maybe familiar to many users.

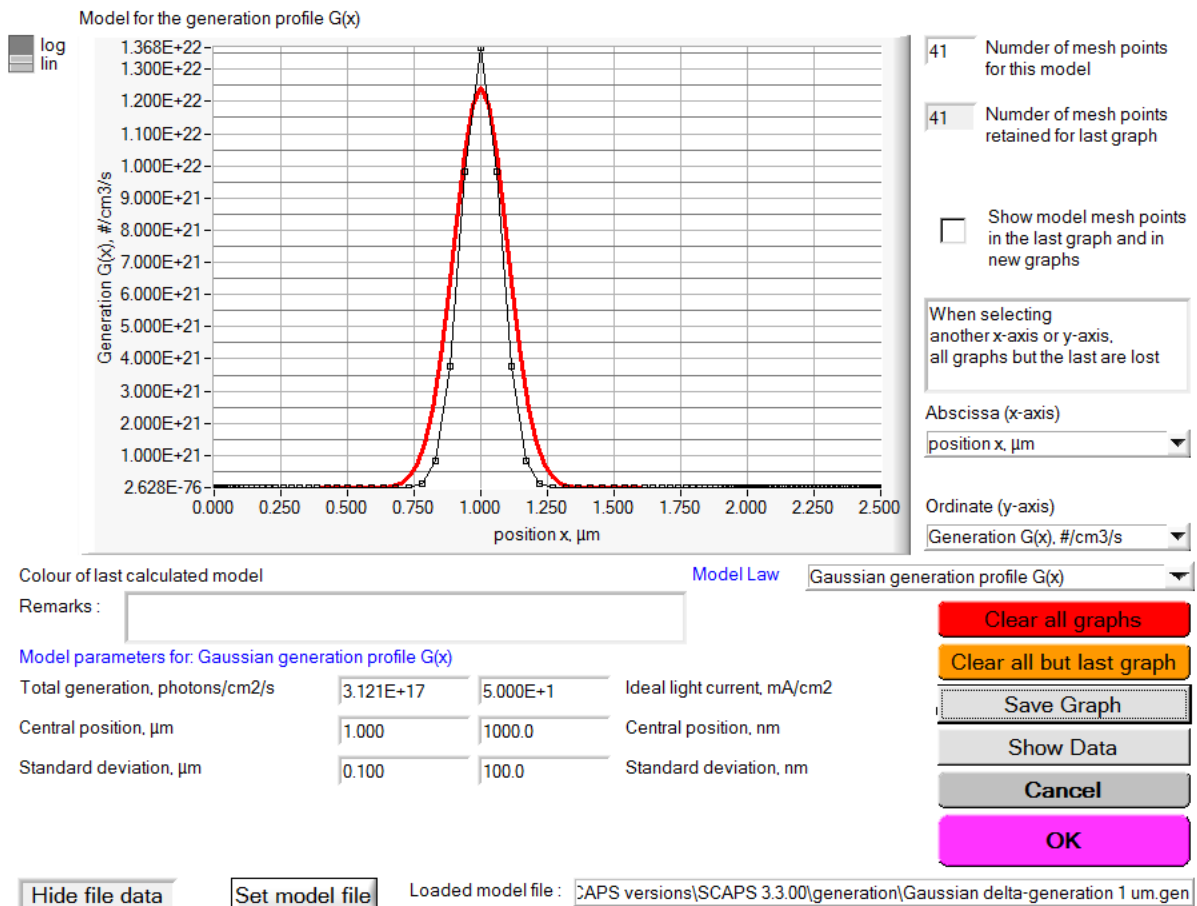


Fig. 6 The SCAPS Model Panel, showing a modelled gauss curve $G(x)$, and also the generation profile from an input file, that can be used for comparison with the $G(x)$ model. The meaning parameters is (should be, I hope) self-understood.

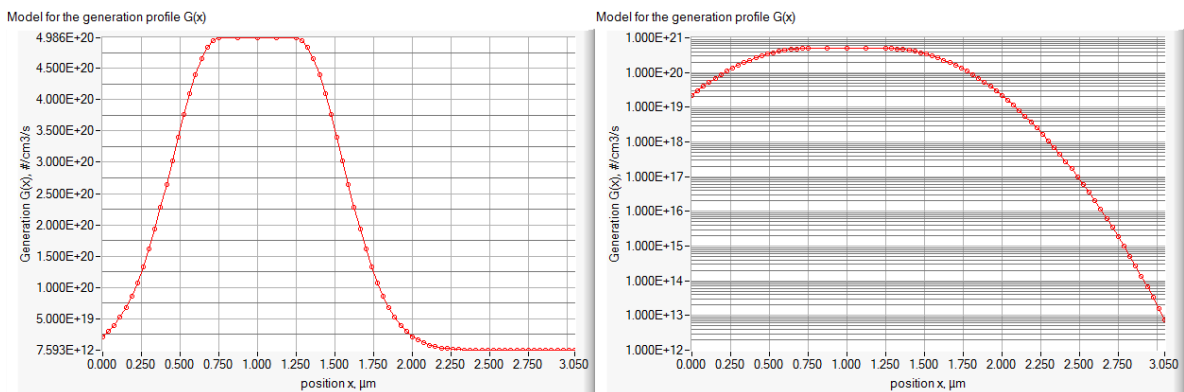


Fig. 7 Linear and logarithmic view of the generation model 'rectangular with Gaussian tails', with parameters: central position 1 μm , total width of rectangle 0.5 μm , standard deviation of Gaussian tails 0.3 μm . Ideal light current: 10 mA/cm².

5.1 The SCAPS Model Panel

The number of x points is set at the top right of the Model Panel (Fig. 6, $n = 41$ is set). But modelled points with $x < 0$ are discarded. The remaining number of points is displayed for information. In the example of Fig. 7, 101 x -points were asked, but only 73 have $x > 0$ and are retained. x points beyond the cell thickness d , thus points with $x > d$, are not discarded, although they are not used in the SCAPS calculations of course. But when one would increase the thickness of a layer, points beyond the original thickness could fall inside the cell, and they will be accounted for. The x -mesh of the generation profile $G(x)$ is independent from the x -mesh of the SCAPS calculations, and usually contains much less points. One can or cannot include the $G(x)$ mesh points into the SCAPS mesh by clicking this option in the Numerical Panel, see Fig. 8.

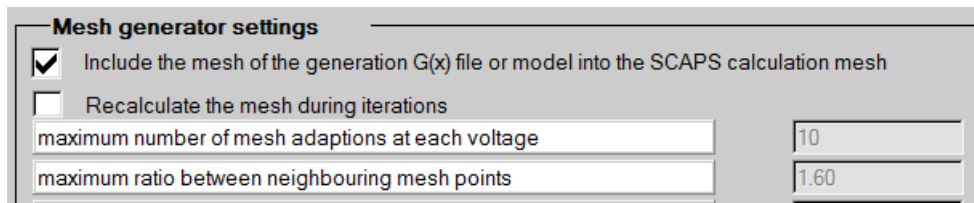


Fig. 8 In the Numerical Panel, one can ask (or not) to include the mesh points of $G(x)$ into the SCAPS mesh.

Also in the right part of the Model Panel of Fig. 6, one can select the abscissa (x -axis) and the ordinate (y -axis) of the plot, see Fig. 9.

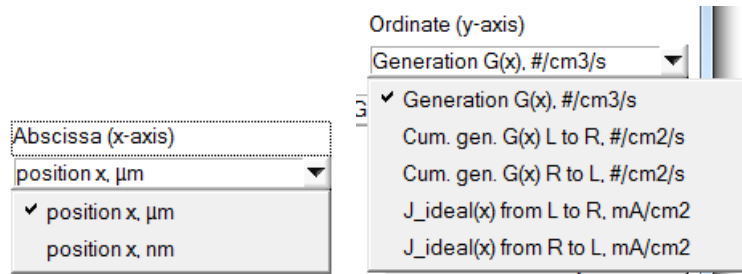


Fig. 9 Possible choices for the abscissa (x -axis) and ordinate (y -axis) to be displayed in the Model Panel for generation models.

The x -axis options are trivial (micrometer or nanometer units), but the y -axis options are more interesting. The definitions are:

$$\begin{aligned}
 G_{\text{cumul, L} \rightarrow \text{R}}(x) &= \int_0^x G(x') dx' & \text{and} & & J_{\text{ideal, L} \rightarrow \text{R}}(x) &= q \cdot \int_0^x G(x') dx' \\
 G_{\text{cumul, R} \rightarrow \text{L}}(x) &= \int_x^d G(x') dx' & \text{and} & & J_{\text{ideal, R} \rightarrow \text{L}}(x) &= q \cdot \int_x^d G(x') dx'
 \end{aligned} \tag{4}$$

These integrals are calculated numerically. The total generation, expressed as a light current, thus

$$J_{\text{ideal}} = J_{\text{ideal}, L \rightarrow R}(d) = J_{\text{ideal}, R \rightarrow L}(0) = q \cdot G_{\text{tot}} = q \cdot \int_0^d G(x) dx \quad (5)$$

is displayed in the Action Panel, see Fig. 4 right (the value 9.9997 mA/cm² indeed slightly deviates from the parameter value 10.0 mA/cm² that was set). If e.g. a substantial fraction of the $G(x)$ profile modelled would have $x < 0$ and thus lay outside the cell, the displayed J_{ideal} value would substantially be lower than the J_{ideal} parameter value set.

The name of the model parameters is self-evident, we hope. For most parameters, you have two alternative forms of the same parameter; input one and the other is adapted automatically. Examples are: positions in μm or in nm; total (integrated over cell thickness) G_{tot} values as a photon flux (# photons.s⁻¹cm⁻²) or as an ideal current (mAcm⁻²). And finally, as is customary in SCAPS, there is only one mouse click between you and your logarithmic thoughts ☺.

You can display also the $G(x)$ data from an input file, but that is only for information: it allows to compare a modelled $G(x)$ with $G(x)$ data from a file. To actually set $G(x)$ from an input file, proceed as in Fig. 4 left. (And don't forget, SCAPS is expecting the input files as a table of x (in μm) G_{eh} (in #/m³.s), separated by white space (blanc or tab)).

5.2 The generation models

5.2.1 Constant generation G

There is only one parameter, G_{tot} , expressed either as a photon flux or as an ideal current. This generation is smeared out uniformly over the cell thickness. Thus, if the cell thickness is changed subsequently, the generation $G(x)$ is changed accordingly, but G_{tot} remains the same.

5.2.2 Exponentially decaying $G(x)$

The first parameter is G_{tot} or J_{ideal} , as in the previous model. The other parameter is the characteristic length of the exponential decay. The $G(x)$ laws are

$$G(x) = \frac{G_{\text{tot}}}{L_{\text{decay}, L}} \exp\left(-\frac{x}{L_{\text{decay}, L}}\right) \quad \text{or} \quad G(x) = \frac{G_{\text{tot}}}{L_{\text{decay}, R}} \exp\left(-\frac{d-x}{L_{\text{decay}, R}}\right) \quad (6)$$

In these equations, d is the actual cell thickness.

5.2.3 Gaussian generation profile $G(x)$

The parameters are: G_{tot} or J_{ideal} , the central position x_{central} and the standard deviation σ . Part of the profile could fall left of the cell (thus $x < 0$), and then will be discarded. When the cell is too thin for the defined profile, part of the Gauss curve with $x > d$ will not be accounted for.

5.2.4 Rectangular generation profile $G(x)$

The first parameter is G_{tot} or J_{ideal} , as in the previous models. The other parameters are the central position of the rectangle, and the full width. When you specify e.g. $x_{\text{central}} = 1 \mu\text{m}$ and $w_{\text{full}} = 0.3 \mu\text{m}$, the generation will be a constant between $x = 0.7 \mu\text{m}$ and $1.3 \mu\text{m}$ and 0 outside. When the cell thickness was only $1 \mu\text{m}$, or you set a total thickness of $1 \mu\text{m}$ afterwards, only the left half of the generation profile will lay within the cell.

5.2.5 Rectangular generation profile $G(x)$ with tails

This works like a rectangular profile, but with a tail left and a tail right; both tails are symmetric. They can be exponential (then define the decay length), or (half) Gaussian (then define the standard deviation).

For all $G(x)$ profiles with exponentials or Gauss curves, it might be worth while to look at the logarithmic graph!

6. The spectrum models

The available spectrum models are shown in Fig. 10.

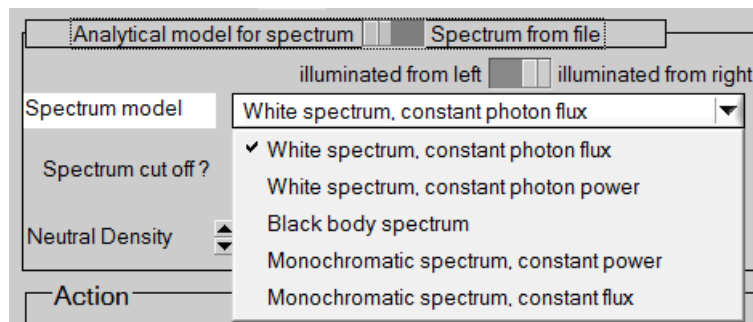


Fig. 10 The available spectrum models

Again the SCAPS Model Panel opens upon selecting a spectrum model. The options for the x -axis and y -axis for spectra are shown in Fig. 11.

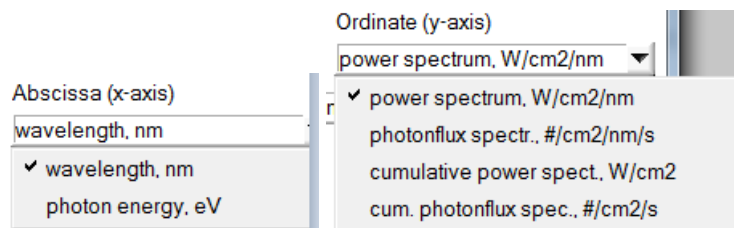


Fig. 11 Possible choices for the abscissa (x -axis) and ordinate (y -axis) to be displayed in the Model Panel for spectrum models.

The abscissa can be switched between wavelength and photon energy. The ordinate can be based on the photon flux (the number of photons incident at each wavelength) or the photon power (the photon power incident at each wavelength). Both can be shown as such, or integrated from the short wavelength limit of the spectrum ('cumulative spectrum').

There are two versions of white spectra: one has a constant photon flux over the specified wavelength range (expressed as a total photon flux or ideal current), the other has a constant photon power over the wavelength range (expressed as total incoming power, in suns or in mW/cm^2 ; $1 \text{ sun} = 100 \text{ mW}/\text{cm}^2 = 1000 \text{ W}/\text{m}^2$). Similarly, there are two versions of monochromatic spectra, one with specified total photon flux, and one with specified total photon power. The black body spectrum is there to please our colleagues more oriented towards fundamental theory. Of course, the black body temperature is the main parameter

(input $T_{\text{blackbody}}$ or the wavelength of the maximum, according to Wien's displacement law). As you will observe when playing with this model, black body radiation extends very far in the infrared wavelength range. To avoid spending many λ -mesh points on not-useful wavelengths, one can limit the λ range of interest.

7. Application example: simulating an EBIC measurement

We load the cell problem Numos CIGS baseline.def. We model the e -beam of the cross-sectional EBIC measurement by a Gaussian generation profile, with standard deviation $0.02 \mu\text{m} = 20 \text{ nm}$, and a total generation corresponding with an ideal current $J_{\text{ideal}} = 1 \text{ mA/cm}^2$; thus, the numerical value of the short circuit current will be the collection efficiency. See Fig. 12 for a linear and a logarithmic view of the beam profile (figure from the SCAPS Model Panel). We let the central position of the beam slide over the cell thickness, with $x_{\text{central}} = 0, 0.05 \mu\text{m}, 0.1 \mu\text{m}, 0.15 \mu\text{m}, \dots 3.1 \mu\text{m}$ (the total cell thickness of Numos CIGS baseline.def). A few beam positions are shown in Fig. 13.

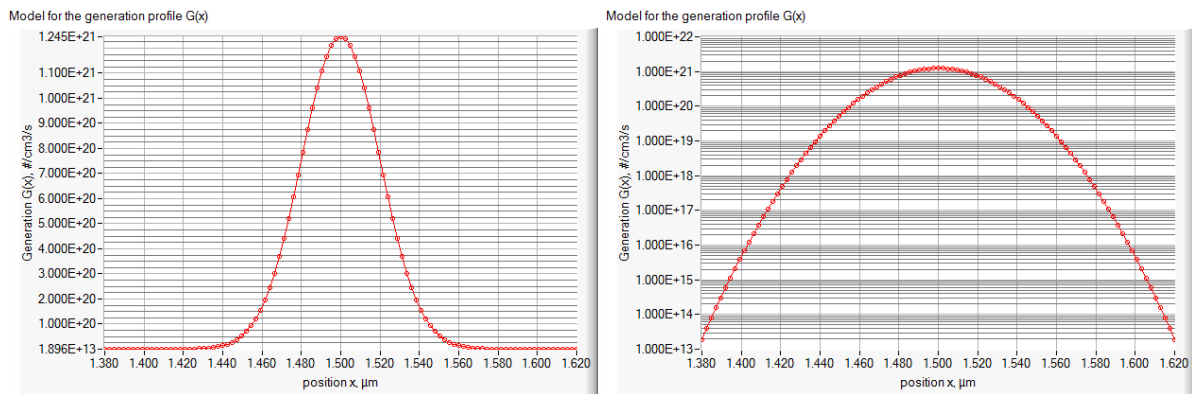


Fig. 12 The Gaussian generation profile $G(x)$ to simulate an EBIC e -beam with central position $1.5 \mu\text{m}$.

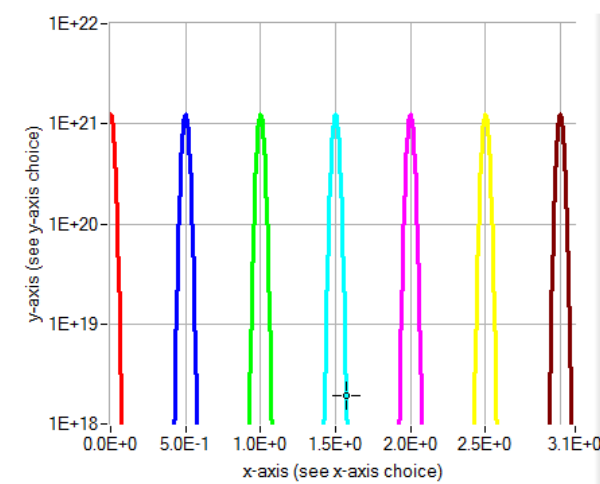


Fig. 13 Seven of the Gaussian e -beam profiles. The beam with central position 0 is only for one half incident on the cell, the left half is outside.

This Fig. 13 was made with a SCAPS script, only to convince myself that the new generation facilities are correctly working in the script ☺.

And here is the result, in Fig. 14, once in a linear, once in a logarithmic view.

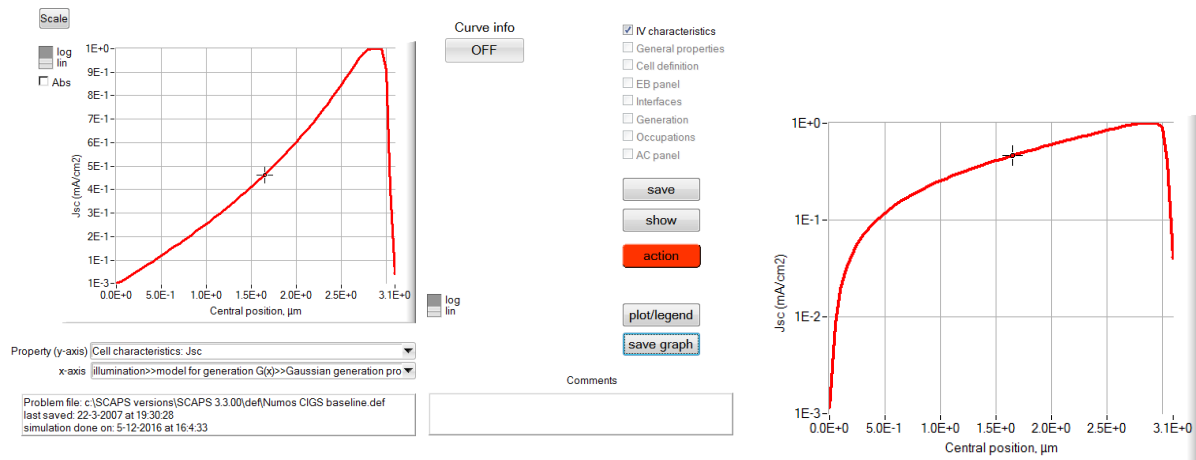


Fig. 14 Result of the EBIC simulation for the Numos CIGS baseline cell: the short circuit current *versus* the central position $x_{central}$ of the beam. $x_{central}$ was varied in the Batch set-up, and J_{sc} was recorded with... the Record set-up. Left in a linear view of J_{sc} , right in a logarithmic view.

One can nicely see the space charge layer SCL (roughly at $2.7 \mu\text{m} < x < 3 \mu\text{m}$) 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 ($x < 2.7 \mu\text{m}$) 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. But that is not the case. This is of course the influence of recombination at the back contact, that is set very high in the Numos GIGS baseline: $S_n = 10^7 \text{ cm/s}$ at the back contact. All settings to run this simulation have been saved in Numos baseline with gaussian EBIC beam.scaps.

We have redone the calculation for other values of S_n , specifically $S_n = 1 \text{ cm/s}$ (that can be considered as very, very low, say zero back contact recombination, and for an intermediate value $S_n = 10^4 \text{ cm/s}$, Fig. 15. We see that the cell with S_n about 10^4 cm/s behaves as an infinitely thick cell. And we quickly check that for this value $S_n L_n / D_n = 1$, hurry, we should not throw away the textbook theories, they are relevant!

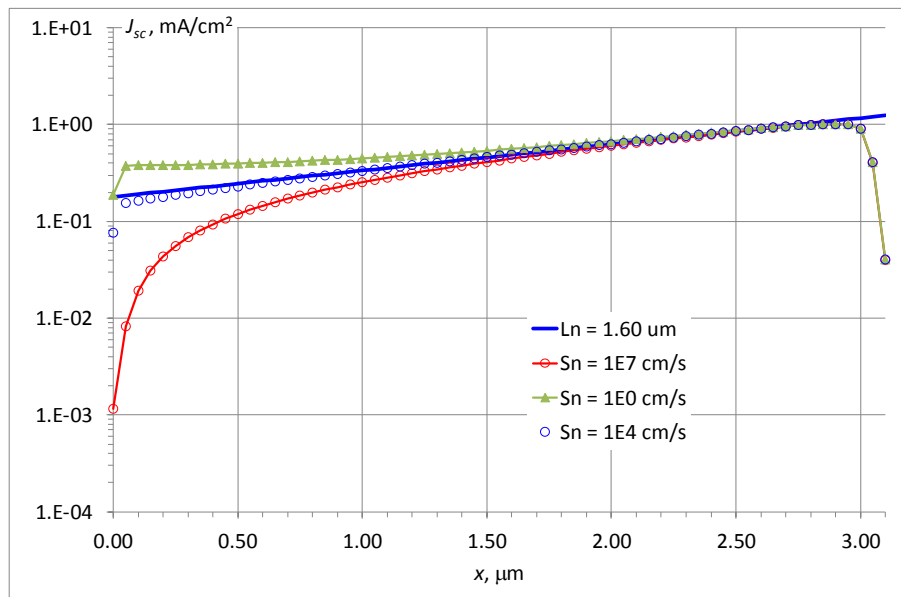


Fig. 15 Simulated EBIC experiment for the Numos CIGS baseline cell, for three values of the back contact minority carrier recombination velocity $S_n = 0, 10^4$ and 10^7 cm/s. The straight blue line corresponds to the basic theory for an ‘infinite cell’ (thus CIGS very thick) with diffusion length $L_n = 1.6 \mu\text{m}$. The numerical artefact at $x = 0$ is because the beam at this position is only half in the cell.

8. Application example with theoretical spectra

Since the spectrum model facilities were primarily meant for users oriented towards theoretic, we can release our pragmatism for a while and follow a wild fantasy: What if we could move to another star, but take our favourite solar cells with us? How could we choose a star with the optimal surface temperature for our cells? So, we set the spectrum to the black body model, and vary the black body temperature from 2000 K to 12000 K (with Batch Set-up), and we record the solar cell efficiency parameters (with Recorder Set-up).

We see that the three cells simulated (*c*-Si, CIGS and CdTe) all have their own optimal temperature. Should the adepts of these cells each move to a different star? Well no, it is not worth while: the optimum is very flat, and our own good old sun with $T = 5800$ K isn’t performing badly at all!

But can we do better? What if we could move to a monochromatic star? Painters and other artists would passionately oppose the idea, and since Planck no physicist in the world would even think of a ‘monochromatic star’. But the slogan of our University is **Durf denken** (dare to think), so it won’t harm to show this simulation in Fig. 17. Persons who are too much shocked by this idea maybe better could think of assemblies of multiple cells with optical spectrum splitters: such devices have been proposed, studied and even made.

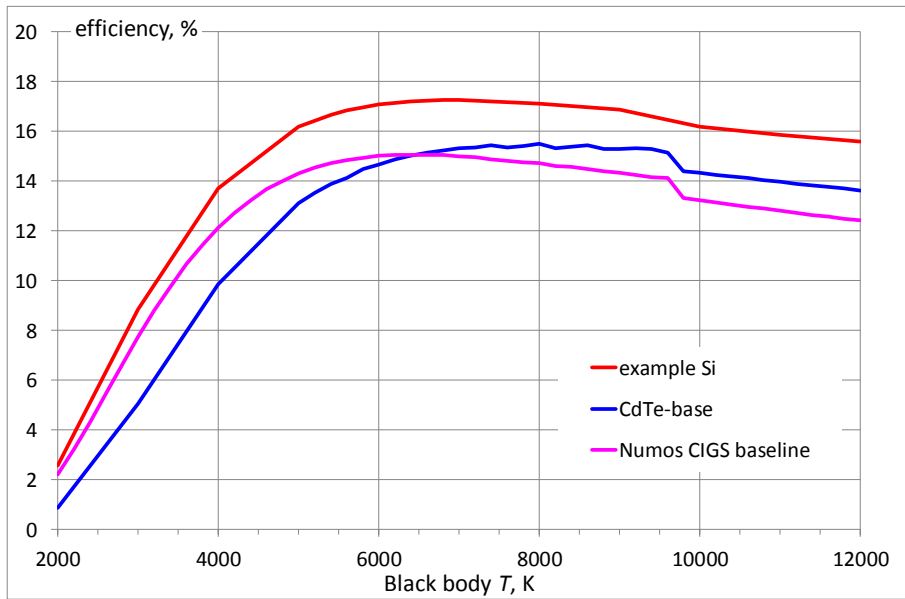


Fig. 16 Cell efficiency for black body spectra with varying temperature, but with constant total power = 1 sun. The three cells are simulated with the simplified definition files included in the SCAPS distribution.

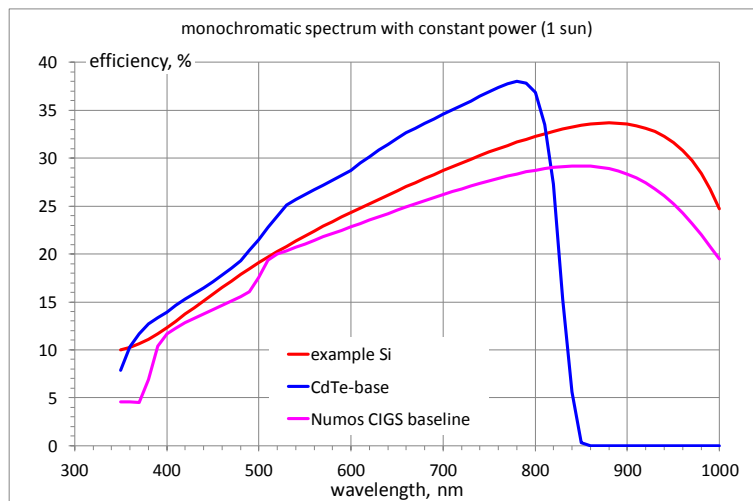


Fig. 17 Cell efficiency for monochromatic radiation with constant total power = 1 sun. The three cells are simulated with the simplified definition files included in the SCAPS distribution.