Simulator of charge transport in multi-layer systems (GraphiXT plug-in)

v0.75

User‘s Manual

by Andrius Poškus (Vilnius University, Faculty of Physics)

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E-mail: andrius.poskus@live.com
Web: http://www.graphixt.com

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1. Simulation method

The charge carrier kinetics is simulated by numerically solving the following system of partial differential equations:

$$\frac{\partial n_i}{\partial t} = -\frac{1}{q_i}\frac{\partial j_i}{\partial x} + \alpha_{i0} + \sum_{k \neq i} \alpha_{ik} c_k - n_i \sum_{k \neq i} \beta_{ik} p_k \ , \tag{1.1}$$

$$j_i(x,t) = | q_i | \mu_i n_i E - q_i D_i \frac{\partial n_i}{\partial x} \ , \tag{1.2}$$

$$\frac{\partial E}{\partial x} = \frac{\rho(x,t)}{\varepsilon_0 \varepsilon} \ , \tag{1.3}$$

where the following notations are used:

t – time,
x – coordinate,

n_i – concentration of the charge carriers of i-th type,
q_i – electric charge of the charge carriers of i-th type,
α_{i0} – the rate of bipolar generation (including photogeneration) of the charge carriers of i-th type,
c_k – concentration of the “filled” states of k-th type, which act as a source of charge carriers of i-th type,
α_{ik} – the rate coefficient of generation of the charge carriers of i-th type from the states of k-th type,
p_k – concentration of the “empty” states of k-th type, which can accept charge carriers of i-th type,
β_{ik} – the rate coefficient of capture of the charge carriers of i-th type to the states of k-th type,
j_i – the conduction current density of the charge carriers of i-th type,
μ_i – mobility of the charge carriers of i-th type,
D_i – diffusion coefficient of the charge carriers of i-th type,
E – electric field strength,
ρ – the total space charge density,
ε – the high-frequency dielectric permittivity,
ε_0 – the electric constant.

For brevity, the term “charge carriers” will be applied not just to free charge carriers, but to traps of a particular charge state as well. The program can simulate interface traps, too (in order to simplify Equations (1.1) and (1.2), the terms corresponding to interface traps have been omitted). Charge carrier capture to interface traps and release from them causes an additional term in the expression of charge carrier flux density at the given interface. The value of that term depends on the charge carrier concentration at that interface and on the surface density of interface traps of the given charge state.

The number of free charge carriers of a given type in a given space region can change due to their transport through the boundaries of that region, or due to their bipolar generation or recombination, or due to their capture or release, or due to their transmutation into other free charge carriers. The number of bulk or interface traps of a given charge state can only change due to capture or release of free charge carriers. Consequently, equations that describe the time dependence of the trap concentration of each charge state do not contain the first two terms that are present on the right-hand side of Equation (1.1), and summing is done over free charge carriers that can be captured into those traps or released from them.

The system of equations (1.1) – (1.3) is solved by the finite difference method. The entire range of x values corresponding to each layer of the system is discretized by replacing it with a set of fixed values, which will be referred to as “nodes”. The partial derivative of current density, which appears in Equation (1.1), at the k-th node of the layer is calculated as follows:

$$\left.\frac{\partial j}{\partial x}\right|_{x=x_k} \approx \frac{(j_{k+1} - j_k)r + (j_k - j_{k-1})\frac{1}{r}}{x_{k+1} - x_{k-1}} \ , \tag{1.4}$$

where j_{k-1}, j_k and j_{k+1} are the values of current density at three adjacent nodes, x_{k-1}, x_k and x_{k+1} are the coordinates of those nodes, and r is the ratio of the two adjacent inter-node intervals:

$$r \equiv \frac{x_k - x_{k-1}}{x_{k+1} - x_k} \ .$$

In a special case when $r = 1$, i.e., when both adjacent intervals are of equal width, the expression (1.4) becomes

$$\left.\frac{\partial j}{\partial x}\right|_{x=x_k} \approx \frac{j_{k+1} - j_{k-1}}{x_{k+1} - x_{k-1}}. \tag{1.5}$$

Similar expressions are used when calculating the derivative of the charge carrier concentration, which is used in the expression of the conduction current density (1.2). The expression (1.4) or (1.5) is called the "two-sided derivative", because its value at the k-th node depends on function values at two adjacent nodes (with numbers $k - 1$ and $k + 1$). At the edges of the system and at interfaces between different layers of the system, "one-sided derivatives" are used. For example, the derivative of the charge carrier concentration at the left edge of the layer (which corresponds to the minimum value of x, i.e., to the first node $x = x_1$) is calculated as follows:

$$\left.\frac{\partial n}{\partial x}\right|_{x=x_1} \approx \frac{n_2 - n_1}{x_2 - x_1}. \tag{1.6}$$

The system of equations (1.1) – (1.3) is solved using the so-called explicit algorithm. I.e., increments of the charge carrier concentrations during one time step of simulation are calculated by multiplying the time derivatives of the concentrations by the simulation time step Δt. For example, if the concentration of a given type of charge carriers at the k-th node at the l-th moment of time ($t = t_l$) was $n(x_k, t_l)$, then after one time step (i.e., at the moment of time $t = t_{l+1} = t_l + \Delta t$) that concentration will be

$$n(x_k, t_{l+1}) = n(x_k, t_l) + \left.\frac{\partial n}{\partial t}\right|_{x_k, t_l} \Delta t\ . \tag{1.7}$$

Thus, it is assumed that the charge carrier concentrations at all nodes during the time interval from t_l to $t_l + \Delta t$ depend on time linearly, and the rate of that dependence is determined by the state of the system at the moment of time t_l (because the right-hand sides of Equations (1.1) – (1.3) are computed using the charge carrier concentrations at the moment of time t_l). The simulation time step Δt is computed based on the rate of change of the charge carrier concentrations (the faster the change, the less the time step Δt).

The precision of finite-difference estimates of the derivatives with respect to the coordinate can be increased by decreasing the inter-node interval Δx, but this would also cause an increase of the number of nodes and of the computer memory usage. Δx may depend on the coordinate. For example, the node density may be largest at the edges of the layer and smallest at its center (this option is in the parameter sheet "Simulation algorithm parameters"). However, in the current version of the model (v0.75), the node positions do not depend on time, i.e., they do not change during the entire simulation.

Since the explicit algorithm becomes unstable at large time steps Δt, better results are sometimes obtained by smoothing the concentrations of free charge carriers. The dependence of the free carrier concentration on the coordinate is smoothed when a "seesaw"-type sequence of concentration values is detected, with inflection points spaced periodically. One of two smoothing methods can be chosen. If the three-point smoothing method is used, then the mentioned sequence is only smoothed when its inflection points are at adjacent nodes. If the five-point smoothing method is used, then the mentioned sequence is also smoothed when its inflection points are at every other node. Only the concentration values corresponding to the mentioned sequence are smoothed, and only when the number of inflection points is 2 or greater. The smoothing methods ensure that the smoothing does not affect the average charge carrier concentration inside the smoothing range. The user can specify the smoothing frequency (this is done in the parameter sheet "Simulation algorithm parameters").

The rate coefficients α_{ik} and β_{ik} (see Equation (1.1)), mobilities and diffusion coefficients can be either constant or computed according to a user-specified model. For example, charge carrier mobility can be calculated according to the formula $\mu = a\exp(b\sqrt{|E|})$ (such dependence is a result of the so-called "Poole-Frenkel effect").

The number of charge carrier types, trap types and processes that can be simulated using the programs CarrierFunc.dll and CarrierParms.exe is practically unlimited. In the current version (v0.75), the only limitation is the requirement that the total number of parameters corresponding to one layer can not exceed 5000, and the total number of layers can not exceed 10.

2. Introduction to user interface

The GraphiXT plug-in for simulation of charge transport in multi-layer systems consists of two files: the function file CarrierFunc.dll and the model parameter editor CarrierParms.exe. If the function file and the parameter editor are loaded, then the parameter editor can be invoked using the GraphiXT menu command "Simulation options / Model parameters…", and simulation can be started (resumed) or stopped using the menu command "Start simulation" or "Stop simulation". In order to load the function file, the GraphiXT menu command "Simulation options / Model function file…" must be selected (this action also causes the reference to the plug-in user's manual to be added to the help system). The parameter editor is loaded using the menu command "Simulation options / Parameter editor file…". Prior to starting simulation with the currently loaded plug-in, the user has to set the initial and final times of simulation (the GraphiXT menu command "Simulation options / Time limits and amount of data…"). [The GraphiXT user's manual is in a separate file. Further on, only the GraphiXT plug-in for simulation of charge transport will be described.]

In the parameter editor window, all parameters of the simulated system are grouped into "parameter sheets", which are accessed by left-clicking a corresponding tab (see Fig. 1). Each sheet corresponds to a particular category of model parameters. In the current version of the model (v0.75), there are 9 parameter sheets. Their titles are seen in Fig. 1. Parameter sheets contain controls of various types: edit controls for entering parameter values and parameter set names, drop-down lists for selecting layers and parameter sets, push buttons, radio buttons and checkboxes.

Each physical material parameter (e.g., charge carrier mobility, trap concentration, etc.) "belongs" to one layer of the simulated system. All material parameters that are visible in each parameter sheet correspond to a particular layer – the "current layer". The current layer can be selected using the drop-down list "Selected layer", which is on the left side of most parameter sheets (see Fig. 1). Above that drop-down list, there is a button "Add or delete a layer". That button is used to open a dialog window where one of three actions can be selected: addition of a new layer "on the right", i.e., after the layer with the greatest value of the *x* coordinate (this is the default action), insertion of the new layer before the current layer, and deletion of the current layer. A layer can only be deleted when the simulated system consists of two or more layers. After inserting a new layer, it is "empty", i.e., there are no free charge carriers or traps in it.

If there can be several parameter sets of a given type (e.g., free charge carriers of several types, or traps of several types), then a parameter set of that type can be added or removed using a corresponding button. For example, four such buttons are visible in Fig. 1. Under each such button, there is a drop-down

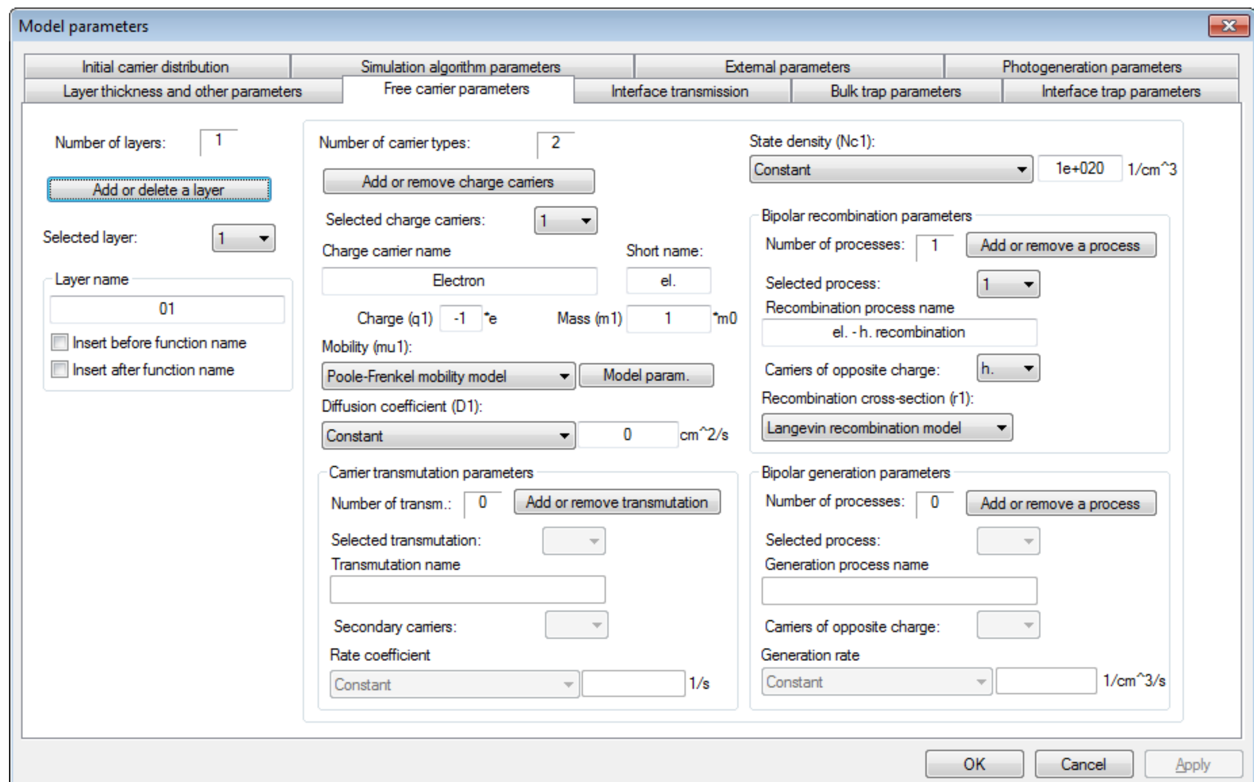


Fig. 1. An example of the parameter editor window (the parameter sheet "Free carrier parameters" is active)

list for selecting a parameter set of the corresponding type. The parameter values corresponding to the selected parameter set are under that drop-down list. Thus, only one set of parameters of each type is shown at a time.

Some simulation parameters do not belong to any layer of the simulated multi-layer system. Those are the simulation algorithm parameters (e.g., the parameters that control the time step of the simulation) and external parameters (e.g., temperature and external illumination parameters). ***Note***: The program assigns those parameters to the layer No. 0. This "layer" is not included in the total number of layers that is shown above the button "Add or delete a layer" (see Fig. 1). The "real" layers, which compose the simulated system, are numbered starting from 1 (only such layers can be added or removed).

In the parameter editor window, units of all parameters are shown to the right of their values. Values of layer thickness and coordinates of various points of the system are given in microns (µm, „um"), the unit of length that is used in derived units is centimeter ("cm"), the unit of energy is electronvolt ("eV"), the unit of mass is the electron rest mass in vacuum (m_0, "m0"), the unit of electric charge is the elementary charge (e, "e"), other units correspond to the SI system of units. The character "^" in unit notations means raising to a power.

The parameter values must be entered according to the following rules: the number of significant digits must be such that all digits are visible, and the decimal exponent must be specified using the format „x.xxxxxe±y" (for example, the number $1.234 \cdot 10^9$ should be written „1.234e9"). ***Note***: When displaying the previously-entered or default parameter values with the decimal exponent, the program uses the standard format of the C programming language, where the exponent always consists of three digits and is preceded by the sign "+" or "–" (for example, the mentioned number would be displayed as "1.234e+009"), but there is no need to insert zeros or the sign "+" at the beginning of the exponent when entering a new value.

Some edit controls are used to specify the name of a particular parameter set (i.e., of a particular type of charge carriers or traps, or of a particular process). Some default names contain names of other objects or charge values. For example, the name of a process of electron capture into traps could be the following: „don. (+1) <- el. capture". This name consists of the following components: 1) the short name of the traps "don." (meaning "donors"), 2) the initial trap charge prior to capture, expressed in elementary charges (+1), 3) the short name of the captured charge carriers "el." (meaning "electrons"). Since the mentioned three components of the process name are read from other fields, they are represented by special character sequences, which indicate the place where a given component must be inserted. Therefore, when entering the mentioned name into a corresponding text box, the following character sequence must be entered: "%s (%+d) <- %s capture". This is a format sequence of the C programming language: "%s" means any string (i.e., any sequence of characters), and "%+d" means an integer number with the sign "+ " or "–". This example is one of default names. Any name can be modified. For example, one or two last format specifiers can be removed. In the mentioned example, the format string could be modified to contain only the first two format specifiers ("%s" and "%+d"), or only the first one ("%s"). The name may also be entered without any format specifiers. In such a case, it would not depend on the content of any other input fields.

Note: Since a single percent character "%" in the format specification has a special meaning (it indicates that a value of a certain variable must be inserted in its place), in order to display a single percent character in the final text, it must be entered twice: "%%".

The rate coefficients α_{ik} and β_{ik} (see Equation (1.1)), mobilities and diffusion coefficients can be either constant or computed according to a user-specified model. For example, in the case of Fig. 1, electron mobility is calculated according to the formula $\mu = a\exp(b\sqrt{|E|})$ (such dependence is a result of the so-called "Poole-Frenkel effect"). If a coefficient is computed according to a particular model, then parameters of that model can be modified by clicking the button "Model param.", which is to the right of the model name (see Fig. 1). If the selected model does not have user-adjustable parameters, then the mentioned button is absent. For example, if the model "Einstein relation" is selected in the list of diffusion coefficient models, then the diffusion coefficient is calculated from the values of mobility and temperature, which are specified elsewhere.

In order to apply parameter changes, the button "OK" or "Apply" must be clicked. Some parameters (e.g., some simulation algorithm parameters, external voltage, etc.) can be modified without stopping the simulation process. In the case of a major change (such as adding or deleting a parameter set, or changing a parameter that is used to define the initial state of the system), the simulation process will be terminated and all stored model data will be deleted. In this case, prior to applying the changes, a warning message will appear, with an option to discard the latest modifications of parameter values.

3. Simulation algorithm parameters

An example of the parameter sheet "Simulation algorithm parameters" is shown in Fig. 2. All parameters of this sheet are explained below.

- The parameter "maxChange" is the maximum allowed relative change of concentrations of free charge carriers and traps of each type and of each charge state during a single time step of simulation. For example, if its value is 0.001 (as in Fig. 2), then the simulation time step Δt will be chosen such that the concentration of each carrier type at each node of the system does not change more than by 0.1 % relative to charge carriers or traps whose charge density at that node is greatest or whose charge density at that node varies fastest (see below for a more detailed explanation). In order to increase accuracy of simulation, this parameter must be decreased (however, then the processing time would increase). The final value of Δt depends on other parameters, too (see below). ***Note***: If "maxChange" is zero, then it will not be used during simulation, i.e., Δt will be computed from other parameters.
- The parameter "dtMax" is the maximum value of the simulation time step Δt. If the value of Δt computed only from the mentioned parameter "maxChange" exceeds "dtMax", then Δt is decreased to the value of "dtMax". ***Note***: If the parameter "dtMax" is zero, then it will not be used during simulation, i.e., the simulation time step Δt will be computed from other parameters.
- The parameter "minR" is the minimum value of the ratio of the time interval between adjacent argument values of computed $f(t)$ functions (i.e., between two adjacent points of their graphs) and the simulation time step Δt. When that ratio is increased, the minimum number of the simulation time steps that can "fit" between two adjacent argument values of a computed $f(t)$ function increases as well. If neither "maxChange" nor "dtMax" is used, then at first the maximum graph time step is computed, then it is divided by „minR". The result is the maximum simulation time step Δt.
- The parameter "maxR" is the maximum value of the ratio of the time interval between adjacent argument values of computed $f(t)$ functions (i.e., the "graph time step") and the simulation time step Δt. If at least one of the mentioned parameters "maxChange" and "dtMax" is used, then at first Δt is computed, then it is multiplied by "maxR". The result is the maximum graph time step (later on, it can be decreased on the basis of other parameters, which are described below). An increase of "maxR" causes an increase of the maximum number of simulation time steps between adjacent argument values of computed $f(t)$ functions. As a result, the spacing of the points in $f(t)$ plots increases. In order to decrease computer memory requirements, that parameter should be increased. The final value of the spacing between adjacent points in $f(t)$ plots depends on another parameter, too (see below).

Fig. 2. An example of the parameter sheet "Simulation algorithm parameters"

- The parameter "dtMax_graph" is the maximum spacing between adjacent points of computed *f*(*t*) functions (i.e., the "graph time step"). If the value of the graph time step, computed only from the previously mentioned parameters, exceeds "dtMax_graph", than that value is decreased to "dtMax_graph". Consequently, if the parameter "maxChange" or "dtMax" is used (i.e., non-zero) and if it is desirable to use constant spacing between computed points of *f*(*t*) functions, then the required value of the spacing must be assigned to "dtMax_graph", and the parameter "maxR" must be assigned a very large value (such that the value of the graph time step computed from "maxR" is always greater than the required value). ***Note***: If the parameter "dtMax_graph" is zero, then it will not be used during simulation, i.e., the graph time step will be computed from other parameters. However, at least one of parameters "maxChange", "dtMax" and "dtMax_graph" must be used, i.e., non-zero.
- The parameter "minR_graph" is the minimum ratio of the duration of the simulated process and the graph time step. In other words, it is approximately equal to the minimum total number of points in *f*(*t*) function graphs. If the parameter "dtMax_graph" is not used (i.e., zero) or if it is greater than the ratio *T* / minR_graph, then the latter ratio has the same role as dtMax_graph, i.e., it is approximately equal to the maximum value of the graph time step. In this case, minR_graph is approximately equal to the final number of points in *f*(*t*) function graphs.

  Important! Parameters "maxR" and "dtMax_graph" must be chosen carefully, trying to avoid too small values, because otherwise there is a risk of insufficient computer memory during simulation. For the same reason, one should avoid too large values of the parameter "minR_graph". During simulation, it is possible to check how fast the amount of used computer memory is growing (this is done using the GraphiXT menu command "Simulation options / Time limits and amount of data…"). If the simulation is done in the "current-voltage characteristic mode" (see below), then the mentioned parameters do not affect the memory requirements.
- The first two radio buttons of this parameter sheet are used to specify the reference charge carriers or traps whose concentration is used to define the maximum allowed relative change of the charge carrier concentration during one time step of simulation. That relative change may be defined relative to charge carriers or traps of one charge state whose concentration at a given node either is greatest, or varies fastest. This is done in the following way. First, at each node of the layer, the program determines charge carriers whose space charge density varies fastest in time (those charge carriers could be electrons, holes, traps of a particular type and charge state, etc.). If the button "varies fastest" is selected, then the value of Δt for that node is calculated by dividing the space charge density of those charge carriers by the absolute value of its time derivative, and multiplying the result by the mentioned parameter "maxChange". If the button "is greatest" is selected, then the program determines charge carriers whose space charge density is largest at that node and divides that charge density by the absolute value of the same time derivative as in the previous case. Thus, this option only affects the numerator of the ratio, but not its denominator (the denominator is always equal to the absolute value of the time derivative of the fastest-varying space charge density component, multiplied by "maxChange"). In this manner, the value of Δt is computed for each node of the system, and then the minimum value of Δt is used as the simulation time step (at interface nodes, the surface charge and its variation rate are also taken into account).

  The optimal value of that parameter depends on the simulated system. For example, if the simplest Schottky diode is being simulated, then there are free charge carriers of one type (electrons) and traps of one type and one charge state (positive donor ions). The Schottky diode current is governed by conditions of electron transfer across the interface between the electrode and the semiconductor. At that interface, the electron concentration is much less than the donor concentration. However, the donor ion concentration stays constant (assuming that all donor atoms are ionized and do not capture electrons); only the electron concentration varies with time. Thus, in this case the denominator of the mentioned ratio would be equal to the absolute value of the time derivative of electron space charge density. If the relative change of electron concentration were defined with respect to charge carriers whose space charge density is greatest (i.e., donor ions), the simulation time step would be too large and consequently large simulation errors would be possible (for example, negative values of electron concentration could be obtained). Therefore, in this example the preferred option is "varies fastest". However, if the magnitude of the conduction current is determined by charge carriers whose concentration is greatest (for example, in the case of discharge of an electrophotographic layer), then this option has no significant effect on simulation accuracy, hence the more appropriate option is "is greatest", because then the simulation is shorter.

- At some points of the system, the concentration of some types of charge carriers can become so small that it will have practically no effect on the simulated physical phenomena. In such a case, there is no need to use the concentration of those charge carriers during simulation. In order to be able to detect such situations, the so-called "threshold concentration" is defined. It is the concentration value that must be exceeded for the given charge carriers to be taken into account at any given node. Otherwise, the concentration of those charge carriers is assumed to be zero and is not used for simulation (for example, it is not taken into account when calculating the mentioned relative change of charge carrier concentrations). The threshold concentration is defined using the parameter "f" (see Fig. 2) as follows. First, the program computes the average space charge densities of free charge carriers of each type and of traps of each type and each charge state (the average space charge density of *interface* traps of a given type and charge state is defined as the ratio of the surface charge density of those traps and the width of the system). Next, the maximum absolute value of all those averages is determined, taking into account not only free charge carriers and traps, but also the "free surface charges" of the interfaces (see Section 8) and the electrode surface charges. Finally, that maximum value is multiplied by the parameter "f", which is specified in the parameter sheet "Simulation algorithm parameters", and divided by the absolute value of the charge of a single charge carrier of that type. The result is the threshold concentration for that type of carriers.
- The next parameter defines the smoothing frequency of free charge carrier concentrations as functions of the coordinate (see Section 1 "Simulation method"). The smaller this parameter, the more frequent the smoothing. When the simulation time step is sufficiently small, smoothing is not needed. In order to turn off smoothing, this parameter must be assigned a zero value.
- The next two radio buttons allow selection of the concentration smoothing method: three-point smoothing or five-point smoothing (see Section 1 "Simulation method"; the three-point smoothing is also briefly described in the GraphiXT user's manual, Section "Data smoothing").
- The checkbox "Smooth time dependences of concentration rates" is used to turn on or turn off exponential smoothing of time derivatives of charge carrier concentrations as functions of time. When this checkbox is checked, then time derivatives of concentrations of free charge carriers and traps of all types and all charge states at each node are replaced by their smoothed values, which are calculated according to the formula $\overline{f}_{l+1} = \beta f_l + (1-\beta)\overline{f}_l$, where $\overline{f}_l$ is the smoothed value at the moment of time t_l, $\overline{f}_{l+1}$ is the smoothed value at the moment of time $t_{l+1} = t_l + \Delta t$, and f_l is the original (non-smoothed) value at the moment of time t_l. The value of the smoothing factor β is always between 0 and 1. When β is close to 1, then $\overline{f}_{l+1} \approx f_l$. When β is close to 0, then the smoothed value is close to the average of all previous values (i.e., its time dependence is weak). The smoothing factor β is the same for all nodes and all types of charge carriers. This parameter is re-calculated at each time step of simulation so as to ensure that smoothed values accurately represent systematic (i.e., non-random) variation of concentration time derivatives (i.e., systematic increase or decrease) and that their random component is as small as possible. [A similar approach is used when computing smoothed values of concentrations themselves (rather than their time derivatives), which are used to determine if the system has reached the stationary state (see below).] When this option is selected, computation time usually decreases, especially in the stationary state simulation mode, which is described below.
- The next checkbox is used to turn on or turn off the stationary state simulation mode. In this mode, simulation is stopped when either of these two conditions is satisfied: 1) the largest duration of the simulated process is reached (that duration is entered using the GraphiXT menu command "Simulation options / Time limits and amount of data…"); 2) the stationary state is reached (it is such a state when all bulk and interface charges of the system stop depending on time).
- In the stationary state simulation mode, it is possible to modify the stationarity criterion ("alphaMin"). The stationary state is defined as the state when all charge densities of all types of bulk and interface charges at all nodes of the system do not depend on time. The stationarity can be exact or approximate. Under conditions of exact stationarity, the increments of all types of charge densities at all nodes during a single time step of simulation are less than the round-off error (the relative round-off error is approximately 10^{-15}), so that the newly computed values are exactly equal to the old ones. Under conditions of approximate stationarity, the charge densities fluctuate with time, but those variations are random, i.e., the average of several last values is approximately constant. The approximate stationarity is detected as follows. Time dependences of concentrations of free charge carriers, bulk and interface traps of all types and charge states at all nodes, as well as "free" interface charges and

electrode surface charges are smoothed by the method of adaptive exponential smoothing. The definition of exponential smoothing is $\overline{f}_{l+1} = \alpha f_l + (1-\alpha)\overline{f}_l$, where $\overline{f}_l$ is the smoothed value at the moment of time T_l, $\overline{f}_{l+1}$ is the smoothed value at the moment of time T_{l+1}, and f_l is the original (non-smoothed) value at the moment of time T_l. The smoothing factor α is always between 0 and 1. A decrease of α makes the resulting smoothed time dependence of $\overline{f}$ more smooth. In this way, random fluctuations of f are eliminated. However, along with random fluctuations, the systematic changes of f are decreased, too. *Adaptive* exponential smoothing attempts to adjust the value of the smoothing factor α at each smoothing step so that the time dependence of $\overline{f}$ represents the systematic changes of f as accurately as possible. I.e., if the systematic dependence of f on time becomes more pronounced, then α is increased, and if the time dependence of f becomes more random, then α is decreased (adaptive exponential smoothing is described in more detail in the GraphiXT user's manual, Section "Data smoothing"). In this manner, values of α are computed for each node and for each charge type. Then the average α is computed. That average is used as the stationarity criterion. Simulation is stopped when the average α decreases below the given threshold value "alphaMin".

Notes: 1) The exponential smoothing of time dependences of concentrations is only used to check if the state of the system is stationary. All stored values of model functions are computed using original (non-smoothed) concentrations. In this respect, this type of smoothing differs from the previously mentioned smoothing of concentration dependences on the coordinate, which modifies concentrations of free charge carriers, and the exponential smoothing of concentration time derivatives, which also modifies those time derivatives.

2) Sometimes, when the state of the simulated system is close to stationary, charge carrier concentrations begin oscillating in time. If those oscillations are relatively "smooth", i.e., if their period is at least several times longer than the time interval between the smoothed values, then the smoothing factor α will begin oscillating as well and its decrease will slow down significantly. In order to avoid such a situation, the smoothed sequence of values only includes the points where the concentration time derivative changes sign, i.e., the concentration maxima and minima. Then the smoothing factor continues decreasing even in the presence of the mentioned oscillations, hence it eventually becomes less than the user-specified threshold value ("alphaMin") and simulation of the stationary state is stopped.

3) Another difference between exponential smoothing of concentrations and the previously mentioned exponential smoothing of concentration time derivatives is that values of α are different for different nodes and different types of charge carriers, and that concentrations are smoothed not at every time step of simulation, but at every time step of the graph (specified by the parameter "dtMax_graph").

- The next checkbox is used to turn on or turn off the "current-voltage characteristic mode" ("I-V mode"). In this mode, the program computes a sequence of stationary states corresponding to a specified sequence of fixed values of external voltage or external illumination intensity. Each of the mentioned fixed values is computed from corresponding time dependences, which are defined in parameter sheets "External parameters" and "Photogeneration parameters". Thus, in this mode, the term "simulation time" has dual meaning: one time is used to compute values of external factors (i.e., external voltage and illumination intensity), and the other time is the true duration of the simulated physical process. Those two times are independent of each other. The first mentioned time is displayed in the graphs (i.e., it is used as the argument of the plotted model functions), hence it may be called "graph time", whereas the second mentioned time ("process time") is shown during simulation in the status bar of the GraphiXT main window and in the GraphiXT dialog window "Time limits and amount of data…". A point is added to the stored model data only when the process time exceeds a given maximum value (see description of the parameter "maxTime" below), or when a stationary state is reached. Then the graph time is incremented by a given amount (see description of the parameter "interval" below), and simulation of another stationary state starts, using the previous stationary state as the initial state of the system. ***Notes***: 1) In order to stop the simulation upon reaching the stationary state, the previously mentioned stationary state simulation mode must be turned on. In this mode, the mentioned parameters "minR", "maxR" and "dtMax_graph" are only used to define the smoothed sequence of charge densities (and not the points plotted in the graphs), hence they do not affect the computer memory requirements. 2) Intermediate computation results are also displayed in the graphs.
- The parameter "interval" defines the interval between time values used to compute values of external factors according to corresponding time functions. For example, let us assume that: 1) zero initial voltage is specified in the parameter sheet "External parameters", 2) the chosen time dependence of the voltage is linear growth with rate 1 V/s, starting at the moment of time 0, 3) the parameter

"interval" is 1 s, 4) the initial and final times of simulation (specified in the GraphiXT dialog window "Time limits and amount of data") are 0 and 10, respectively. Then the program will compute a sequence of 11 stationary states, corresponding to external voltage values 0 V, 1 V, 2 V, …, 10 V. The corresponding argument values of *f*(*t*) model functions (i.e., abscissas of the corresponding curves plotted in time graphs) in this case would be equal to 0 s, 1 s, 2 s, …, 10 s.

- The parameter "maxTime" is the maximum duration of the simulated physical process corresponding to a single value of the varied external factor (external voltage or illumination intensity).
- The parameter group "Adjacent node interval calculation parameters" contains parameters that define the rule for computing node coordinates in each layer of the simulated system. If all inter-node intervals were equal to each other, then it would be sufficient to specify the total number of nodes in each layer (the first and the last nodes are on the opposing surfaces of the layer). The corresponding parameter is denoted "nX" (see Fig. 2). However, this program can also use coordinate-dependent inter-node intervals, which are either monotonously increasing or monotonously decreasing with distance to the layer surface. For example, the interval could be largest at one surface and smallest and the opposite surface, or smallest at the layer center and largest at its surfaces, or largest at the layer center and smallest at its surfaces. The remaining parameters of that parameter group define the rule for computing inter-node intervals, when nodes are not equidistant. The parameter "dxR" is the ratio of the maximum and minimum intervals (in the case of equal intervals, it should be equal to 1). In the example of Fig. 2, the maximum inter-node interval is 50 times larger than the minimum interval. The next four radio buttons define the points of the layer where the interval is largest and where it is smallest. For example, in the case of Fig. 2, the maximum interval is between the node that is on the right surface of the layer and the adjacent node on the left, and the minimum interval is between the node that is on the left surface of the layer and the adjacent node on the right. If it were specified that the interval is smallest at both surfaces of the layer, then the maximum interval would be between the central nodes (there it would be 50 times larger than near the surface of the layer).

  Important! The parameter "nX", as well as the previously mentioned parameters „maxR", „dtMax_graph" and „minR_graph", strongly affects the amount of used computer memory during simulation. One should avoid too large values of that parameter, because otherwise there is a risk of computer memory shortage during simulation.
- Parameters of the parameter group "Multithreading parameters" control the multithreading mode. The essence of multithreading is splitting the simulation into several "threads", which run in parallel. The Windows operating system distributes the computer resources equally among all those threads. If the computer has more than one processor and if the number of threads does not exceed the number of processors, then each thread that is not in a suspended state fully utilizes one processor (here, the term "processor" is used synonymously with the term "core", if a multi-core processor is used). Consequently, if, for example, the computer has four processors and only one thread is used for simulation, then simulation would only utilize 25 % of available computing power, and if 4 threads were used, then all available computing power would be utilized, so that processing time could decrease 3 or 4 times. However, this would be only possible in the ideal case, when different threads are practically independent (i.e., communication between threads and their synchronization is relatively infrequent) and when absolutely all operations are equally distributed among the threads. In this respect, simulation of charge carrier kinetics is not very amenable to multithreading, because different threads must be synchronized several times during each time step of simulation. Besides, some steps are done by a single thread. Threads are synchronized with each other as follows. Each thread that has finished the current stage of simulation checks if the other threads have finished their tasks, too. If not, then the thread enters the suspended state and waits until all other threads finish their tasks. Threads are suspended and resumed using special "signals" of the operating system. The mentioned periodic checks for task completion and thread response to the mentioned signals are not instantaneous, hence, when synchronization is especially frequent, the multithreading mode can become slower than single-threaded mode. This is the case when the processing time of a single time step of simulation is especially short, i.e., when the simulated system is especially simple (i.e., has few nodes and few processes to simulate), or when a very fast computer is used. ***Note***: Another reason why the multi-threaded mode can become slower than the single-threaded mode is running other programs during simulation. Each executed program consists of at least one thread. If the total number of processor-intensive threads exceeds the number of processors, then the operating system can slow down.

Each thread processes a part of the nodes of the simulated system. For example, if two threads are active, then one thread processes the data corresponding to even-numbered nodes, and the other thread processes the data corresponding to odd-numbered nodes. If three threads are used, then each of them processes every third node, etc. This ensures that all threads have approximately equal “work-loads”, even when simulating an asymmetric system. In multithreading mode, the program can use a user-specified constant number of threads. This is done by selecting the radio button “Use constant number of simulation threads” (see Fig. 2) and entering the required number of threads (“nThreads”) in the corresponding text box. Alternatively, the program can optimize the number of threads (this is done by selecting the radio button “Optimize the number of simulation threads”). In the latter case, the program determines the number of threads that corresponds to the maximum processing speed, i.e., to the minimum processing time of a single simulation time step. This is done as follows. The number of active threads is periodically (every 5000 simulation time steps) increased or decreased by 1, then the processing time corresponding to 100 time steps is measured and the average processing time of a single simulation step is calculated and compared with the previous value. Based on the result of this comparison, it is determined if the simulation should continue using the new number of threads or if the previous number of threads should be restored. When optimization of the number of simulation threads is turned on, the number of threads can not exceed the number of processors in the computer.

4. Free charge carrier parameters

The parameter sheet “Free carrier parameters” is used to enter parameters of each type of free charge carriers, as well as parameters that define processes of bipolar recombination, bipolar generation and charge carrier transmutations. An example of this parameter sheet is shown in Fig. 3. Below are explanations of all controls of this parameter sheet:

- The button “Add or remove charge carriers” is used to open a dialog window where one of three actions can be selected: addition of a new type of free charge carriers to the end of the list (this is the default action), insertion of the new carrier type before the current type of free charge carriers, and deletion of the current type of free charge carriers.
- The drop-down list “Selected charge carriers” is used to select charge carriers when there are two or more types of charge carriers in the current layer. All parameters shown in this parameter sheet correspond to the selected type of free charge carriers.
- The next two text boxes are used to enter the full name and the abbreviated name of the carriers.
- The next two text boxes are used to enter the charge value of the current charge carriers (in units of the elementary charge) and the carrier effective mass (in units of the electron rest mass in vacuum). ***Note***: In the current version of the program (v0.75), the carrier effective mass in only used in these cases: (a) to compute the thermionic emission flux (see Section 8), (b) to compute the average thermal velocity (it is used to compute the rate of bipolar recombination or capture into traps when the corresponding cross-section is known), (c) to compute the state density when the free particle approximation is applied.

Fig. 3. An example of the parameter sheet „Free carrier parameters “

- The drop-down list “Mobility” is used to select the carrier mobility computation method. Four choices are available:
  1) constant mobility,
  2) exponential dependence on the square root of electric field strength:
  $$\mu = a\exp(b\sqrt{|E|}), \tag{4.1}$$
  3) the bipolar mobility model for electrons in silicon,
  4) the bipolar mobility model for holes in silicon.

The bipolar mobility model for electrons in silicon is defined by the following two formulas:

$$\mu_{S,n}(N) = \mu_n^{\min} + \frac{\mu_n^{\max}\left(\frac{T}{300}\right)^{\nu_n} - \mu_n^{\min}}{1+\left(\frac{T}{300}\right)^{\xi_n}\left(\frac{N}{N_{\mathrm{ref},n}}\right)^{\alpha_n}}, \qquad \mu_n(N,E) = \mu_{S,n}(N)\left[1+\left(\frac{\mu_{S,n}|E|}{\upsilon_{\mathrm{sat},n}}\right)^{\beta_n}\right]^{-\frac{1}{\beta_n}}, \tag{4.2}$$

where N is the total concentration of impurities (donors and acceptors), measured in units of cm^{-3}, T is the absolute temperature (measured in kelvins), and E is the electric field strength (V/cm). The definition of the bipolar mobility model for holes in silicon is similar (in the case of holes, the subscript "n" should be replaced by "p"). The values of the bipolar mobility model parameters are listed in Table 4.1 (data from the software package "MicroTec" user's manual „*MicroTec Software Package for Two-Dimensional Process and Device Simulation. Version 4.0 for Windows. User's Manual. – Siborg Systems Inc.– 1998*").

Table 4.1. Bipolar mobility model parameters for electrons and holes in silicon

Symbol	Value	Units	Meaning
$\mu_n^{\min}$	55,2	$\mathrm{cm^2\,V^{-1}\,s^{-1}}$	Minimum electron mobility
$\mu_n^{\max}$	1430	$\mathrm{cm^2\,V^{-1}\,s^{-1}}$	Maximum electron mobility
$N_{\mathrm{ref},n}$	$1{,}07 \cdot 10^{17}$	$\mathrm{cm^{-3}}$	Reference impurity concentration for electrons
$\upsilon_{\mathrm{sat},n}$	$1{,}07 \cdot 10^{7}$	cm/s	Electron saturation velocity
ν_n	−2,3	–	Exponent of normalized temperature in the numerator for electrons
ξ_n	−3,8	–	Exponent of normalized temperature in the denominator for electrons
α_n	0,733	–	Exponent of impurity concentration for electrons
β_n	2,0	–	Exponent of electric field for electrons
$\mu_p^{\min}$	49,7	$\mathrm{cm^2\,V^{-1}\,s^{-1}}$	Minimum hole mobility
$\mu_p^{\max}$	479	$\mathrm{cm^2\,V^{-1}\,s^{-1}}$	Maximum hole mobility
$N_{\mathrm{ref},p}$	$1{,}6 \cdot 10^{17}$	$\mathrm{cm^{-3}}$	Reference impurity concentration for holes
$\upsilon_{\mathrm{sat},p}$	$1{,}06 \cdot 10^{7}$	cm/s	Hole saturation velocity
ν_p	−2,2	–	Exponent of normalized temperature in the numerator for holes
ξ_p	−3,7	–	Exponent of normalized temperature in the denominator for holes
α_p	0,7	–	Exponent of impurity concentration for holes
β_p	1,0	–	Exponent of electric field for holes

- The drop-down list "Diffusion coefficient" is used to select the carrier diffusion coefficient computation method. Two choices are available:
  1) a constant diffusion coefficient,
  2) Einstein relation, which states that the diffusion coefficient (D) is directly proportional to mobility (μ):
  $$D = \frac{kT}{|q|}\mu, \tag{4.3}$$
  where k is the Boltzmann constant, T is the absolute temperature, and q is the carrier charge.
- The drop-down list "State density" is used to select the method that should be used when computing the state density of the selected free charge carriers. Two choices are available:
  1) constant state density,
  2) free particle approximation. According to this approximation, the free carrier state density is
  $$N_c = \left(\frac{2\pi kTm^*}{h^2}\right)^{3/2}, \tag{4.4}$$
  where k is the Boltzmann constant, T is the absolute temperature, m^* is the carrier effective mass, and h is the Planck constant. If the carrier spin is 1/2, then the actual state density is greater than (4.4) by a factor of 2 (this is the so-called "spin factor"), because there are two different spin states of the charge carrier corresponding to each state of its spatial motion. However, when the free-particle approximation is selected, the spin factor is not used (i.e., it is assumed to be 1), because the state density is only needed to compute the rate of carrier release from traps according to the Shockley-Read-Hall model (this option is in the parameter sheets "Bulk trap parameters" and "Interface trap parameters"), and the carrier spin state does not change during its release from a trap.
- The parameter group "Bipolar recombination parameters" contains the controls that are used to specify names and cross-sections of bipolar recombination processes. Such a process can be added or removed

using the button "Add or remove a process". When defining a new recombination process, the "secondary" carriers, whose charge is opposite to the charge of the currently selected "primary" carriers (specified in the previously mentioned drop-down list "Selected charge carriers"), must be selected in the drop-down list "Carriers of opposite charge".

Note: When defining a bipolar recombination process, it does not matter which charge carriers are treated as "primary" ones, and which are treated as "secondary" ones. In any case, each such process must be defined *only once*. For example, if the recombination process has been defined using electrons as the primary charge carriers (as in Fig. 1 and Fig. 3), then, after selecting holes in the drop-down list "Selected charge carriers", that recombination process must not be defined again (otherwise there would be two identical recombination processes and the total recombination rate would increase by a factor of 2). This note also applies when defining bipolar generation and photogeneration processes, excluding impact ionization (see below).

- The drop-down list "Recombination cross-section" is used to select the recombination cross-section computation method. The recombination cross-section σ_r appears in the expression of the recombination rate R:

$$R = \sigma_r \upsilon_{rel} n_1 n_2 , \tag{4.5}$$

where n_1 and n_2 are concentrations of the recombining charge carriers, and υ_{rel} is their average relative velocity (i.e., the average absolute value of their velocity with respect to each other). In the case of the Maxwell distribution of speeds,

$$\upsilon_{rel} = \sqrt{\frac{8kT}{\pi m_r}} , \tag{4.6}$$

where m_r is the reduced mass:

$$m_r = \frac{m_1 m_2}{m_1 + m_2} , \tag{4.7}$$

where m_1 and m_2 are effective masses of both charge carriers. Sometimes the recombination rate is expressed using the recombination coefficient β_r:

$$R = \beta_r n_1 n_2 . \tag{4.8}$$

By comparing (4.5) and (4.8), we see that

$$\beta_r = \sigma_r \upsilon_{rel} . \tag{4.9}$$

Four choices are available in the drop-down list "Recombination cross-section":

1) a constant value of the recombination cross-section,

2) Langevin recombination model. According to this model, the recombination coefficient depends on mobilities μ_1 and μ_2 of the recombining charge carriers:

$$\beta_r = \frac{|q|(\mu_1 + \mu_2)}{\varepsilon_0 \varepsilon} , \tag{4.10}$$

where $|q|$ is the absolute value of the charge, ε_0 is the electric constant, ε is the dielectric permittivity.

3) A known recombination coefficient. In this case, the user must specify not the recombination cross-section σ_r, but the recombination coefficient β_r, and the program calculates the recombination rate according to (4.8).

4) Shockley-Read-Hall recombination. This is recombination of free charge carriers via traps, which are called "recombination centers". Each SRH recombination process is a sum of four processes:

a) capture of primary charge carriers into bulk traps of charge state "B", forming charge state "A";

b) release of primary charge carriers from the traps of charge state "A", forming charge state "B";

c) capture of secondary charge carriers into the traps of charge state "A", forming charge state "B";

d) release of secondary charge carriers from the traps of charge state "B", forming charge state "A".

Since those four processes are defined in the parameter sheet "Bulk trap parameters" (described in Section 5), only the first of the mentioned processes has to be specified in the SRH recombination dialog window. The program will find the other three processes automatically. If the defined capture and release processes do not include all mentioned processes, or if there are several "candidate" processes defined, then a corresponding error message will appear. If an SRH recombination process has been defined, then the change of concentration of traps of a given charge state during one simulation time step Δt is calculated not in the usual way (i.e., not by multiplying the rate of concentration change by Δt), but on the basis of the requirement that the difference of the primary

carrier capture and release rates is equal to the difference of the secondary carrier capture and release rates. This condition implies that concentration of state “A” traps is equal to

$$n_{\mathrm{A}} = N \frac{\upsilon_{\mathrm{th},1}\sigma_1 n_1 + \upsilon_{\mathrm{th},2}\sigma_2 N_2 \exp\left(-\frac{E_2}{kT}\right)}{\upsilon_{\mathrm{th},1}\sigma_1\left[n_1 + N_1 \exp\left(-\frac{E_1}{kT}\right)\right] + \upsilon_{\mathrm{th},2}\sigma_2\left[n_2 + N_2 \exp\left(-\frac{E_2}{kT}\right)\right]}, \tag{4.11}$$

where N is the trap concentration ($N = n_{\mathrm{A}} + n_{\mathrm{B}}$), n_1 and n_2 are concentrations of primary and secondary free charge carriers, respectively, $\upsilon_{\mathrm{th},1}$ and $\upsilon_{\mathrm{th},2}$ are average thermal velocities of primary and secondary charge carriers, which in the case of the Maxwell distribution are given by

$$\upsilon_{\mathrm{th}} = \sqrt{\frac{8kT}{\pi m^*}}, \tag{4.12}$$

σ_1 and σ_2 are capture cross-sections of primary and secondary charge carriers, respectively, N_1 and N_2 are state densities of primary and secondary charge carriers, respectively, E_1 and E_2 are “energy depths” of the traps with respect to release of primary and secondary charge carriers, respectively. For example, if the simulated system is a semiconductor with two types of charge carriers – electrons and holes – and if the primary charge carriers are electrons, then E_1 is the difference between the conduction band edge and the trap energy level, and E_2 is the difference between the trap energy level and the valence band edge (i.e., the sum $E_1 + E_2$ is the width of the forbidden energy band, also called the “energy gap”). The energy level of recombination centers is usually assumed to be at the center of the energy gap. Then $E_1 = E_2 = E_{\mathrm{g}} / 2$, where E_{g} is the energy gap width.

The SRH recombination rate is defined as follows:

$$R_{\mathrm{SRH}} = R_1 - G_1 = R_2 - G_2, \tag{4.13}$$

where R_1 and R_2 are the rates of primary charge carrier capture and secondary charge carrier capture into the traps, respectively, and $G_1$and G_2 are the corresponding release rates. Thus, both positive and negative values of R_{SRH} are possible: a positive value means that the dominant process is the charge carrier capture (recombination), and a negative value means that the dominant process is the charge carrier release (generation).

During simulation of the time evolution of the system state, the SRH recombination model violates conservation of charge: if the difference of the primary carrier capture and release rates were equal to the difference of the secondary carrier capture and release rates, then concentrations of traps of both charge states would be constant, but the concentration of charge state “A” traps calculated according to (4.11) is not constant, because it depends on the free carrier concentrations n_1 and n_2, which are not constant. However, if the concentration of recombination centers is by several orders of magnitude less than concentrations of other traps and free charge carriers, then the space charge of recombination centers has only a weak influence on electric field strength. Consequently, in such a case the errors caused by the mentioned non-conservation of charge are small, too. The dialog window “Shockley-Read-Hall recombination parameters” provides an option to specify whether the space charge of recombination centers should be taken into account. If that charge is taken into account, then its variation with time is not compensated by a corresponding variation of the other types of charges present in the system, i.e., the total electric charge of the system is not conserved. If the space charge of recombination centers is not taken into account, then the overall effect is such as if that charge was zero. Hence, this eliminates the mentioned non-conservation of charge. Consequently, this is the default option (although in reality recombination centers have a certain charge).

Notes: 1. If concentration of recombination centers is comparatively small, then turning SRH recombination on or off has practically no effect on the simulation results (this option only affects the method of calculation of trap population by charge carriers). Besides, the formula (4.11) is exact in the stationary state. Therefore, if the aim of the simulation is characterization of the stationary state (rather than of the system relaxation to the stationary state), then it is recommended to turn SRH recombination on, because then the simulator “reaches” the stationary state faster. On the other hand, if the aim of the simulation is characterization of the time evolution of the system, then more accurate results are obtained when the SRH recombination is turned off.

2. In order to turn SRH recombination off, it is sufficient to enter zero recombination cross-section. This is done by selecting “Constant” in the drop-down list “Recombination cross-section” and entering zero in the nearby text box (it is also possible to remove the recombination process altogether, but then all previous simulation results will be lost and all plotted model curves will be removed from the graphs).

- The parameter group "Bipolar generation parameters" contains the controls that are used to specify names and rates of bipolar generation processes. Such a process can be added or removed using the button "Add or remove a process". When defining a new generation process, the "secondary" carriers, whose charge is opposite to the charge of the currently selected "primary" carriers (specified in the previously mentioned drop-down list "Selected charge carriers"), must be selected in the drop-down list "Carriers of opposite charge".
- The drop-down list "Generation rate" is used to select the generation rate computation method. Two choices are available:

  1) a constant value of the generation rate,

  2) impact ionization. The rate of impact ionization by charge carriers of *i*-th type (i.e., the number of carrier pairs generated in unit volume per unit time) at point x is calculated using the expression

$$G_{\text{ii}}(x) = c_i \exp\left(-\frac{d_i}{|E(x)|}\right)\left|\frac{j_i(x)}{q_i}\right|, \qquad (4.14)$$

  where c_i and d_i are positive constants (model parameters), E is electric field strength, j_i is the current density of carriers of *i*-th type, and q_i is their charge. Impact ionization is the only "asymmetric" process of bipolar generation-recombination, i.e., a process when primary and secondary carriers are not equivalent to each other. During an elementary event of an impact ionization process, the primary carrier is the one that creates a pair of new carriers (the primary carrier does not disappear in the process). Thus, the factor j_i in (4.14) is the current density of the *primary* charge carriers. Consequently, if charge carriers of both types can cause impact ionization, then at least two impact ionization processes must be defined. In general, c_i and d_i may depend on electric field strength. This dependence can be modeled by defining several impact ionization processes, each one corresponding to a given interval of electric field strengths. In order to define an impact ionization process completely, four parameters must be entered: the maximum and minimum electric field strength values (they define the electric field range where that process is "active"), and the corresponding values of c_i and d_i. The maximum electric field strength corresponding to the last interval is ∞. The corresponding entered value must be such that it is always greater than the actual electric field strength (for example, a number 10^{20} could be entered).

  The electric field intervals and the corresponding values of parameters c and d for impact ionization processes in silicon are given in Table 4.2 (data from the software package "MicroTec" user's manual „*MicroTec Software Package for Two-Dimensional Process and Device Simulation. Version 4.0 for Windows. User's Manual. – Siborg Systems Inc.– 1998*").

Table 4.2. Impact ionization model parameters for electrons and holes in silicon

Symbol	Value	Units	Meaning
$E_{\min,n}$	0	V/cm	Minimum electric field strength for electrons
$E_{\max,n}$	∞	V/cm	Maximum electric field strength for electrons
d_n	$1{,}4 \cdot 10^6$	V/cm	Field exponent for electrons
c_n	$7 \cdot 10^5$	1/cm	Pre-exponential factor for electrons
$E_{\min 1,p}$	0	V/cm	Lower bound of the first electric field interval for holes
$E_{\max 1,p}$	$6{,}07 \cdot 10^5$	V/cm	Upper bound of the first electric field interval for holes
$d_{1,p}$	$2{,}09 \cdot 10^6$	V/cm	Field exponent for holes in the first electric field interval
$c_{1,p}$	$1{,}3 \cdot 10^6$	1/cm	Pre-exponential factor for holes in the first electric field interval
$E_{\min 2,p}$	$6{,}07 \cdot 10^5$	V/cm	Lower bound of the second electric field interval for holes
$E_{\max 2,p}$	∞	V/cm	Upper bound of the second electric field interval for holes
$d_{2,p}$	$1{,}4 \cdot 10^6$	V/cm	Field exponent for holes in the second electric field interval
$c_{2,p}$	$4{,}4 \cdot 10^5$	1/cm	Pre-exponential factor for holes in the second electric field interval

- The parameter group "Carrier transmutation parameters" contains the controls that are used to specify names and rate coefficients of free carrier transmutation processes. Each transmutation is a process whereby a free charge carrier is replaced by a different free charge carrier, whose charge is equal to the charge of the original carrier. Thus, carrier transmutations are only possible when the given layer contains several types of charge carriers with equal charge. A carrier transmutation process can be added or removed using the button "Add or remove transmutation". When defining a new transmutation process, the "secondary" free charge carriers, whose charge is equal to the charge of the

currently selected "primary" carriers (specified in the previously mentioned drop-down list "Selected charge carriers"), must be selected in the drop-down list "Secondary carriers".

- The drop-down list "Rate coefficient" is used to select the transmutation rate calculation method. In the current version of the model (v0.75), only one choice is available – "Constant", which corresponds to a constant rate coefficient (its value must be entered in the nearby text box). The rate coefficient γ appears in the expression of the transmutation rate V:

$$V = \gamma n \,, \tag{4.15}$$

  where n is the concentration of the primary charge carriers. The transmutation rate V is defined as the number of elementary transmutation events in the unit volume per unit time.

5. Bulk trap parameters

The parameter sheet “Bulk trap parameters” is used to enter parameters of each type of bulk traps, as well as parameters that define processes of charge carrier capture into bulk traps and release from bulk traps. An example of this parameter sheet is shown in Fig. 4. Below are explanations of all controls of this parameter sheet:

- The button “Add or remove bulk traps” is used to open a dialog window where one of three actions can be selected: addition of a new type of bulk traps to the end of the list (this is the default action), insertion of the new trap type before the current type of bulk traps, and deletion of the current type of bulk traps.
- The drop-down list “Selected bulk traps” is used to select bulk traps when there are two or more types of bulk traps in the current layer. All parameters shown in this parameter sheet correspond to the selected type of bulk traps.
- The next two text boxes are used to enter the full name and the abbreviated name of the traps.
- The drop-down list “Trap concentration” is used to select the trap concentration computation method. In the current version of the model (v0.75), only one choice is available – “Constant”, which corresponds to a constant trap concentration (its value must be entered in the nearby text box). However, this value is not the total concentration, but just a constant term in the total concentration (see below).
- The parameter group “Trap region parameters” is used to specify non-uniform trap distribution in the layer. This is achieved by defining the so-called “bulk trap regions”. Each region corresponds to one coordinate-dependent term in the total dependence of the trap concentration on the coordinate x:

$$N(x) = N_0 + \sum_{i=1}^{I} f_i(x), \tag{5.1}$$

where N_0 is the mentioned constant term, $f_i(x)$ is a coordinate-dependent term corresponding to the i-th region of the current traps, and I is the total number of regions. A trap region consists of three parts: the region of increasing concentration on the left, the constant concentration region in the middle and the region of decreasing concentration on the right. The dependence of concentration on the coordinate in the first and third mentioned parts is Gaussian. Thus, the general expression of the term $f_i(x)$ is

Fig. 4. An example of the parameter sheet „Bulk trap parameters “

$$f(x)=\begin{cases} N_{\max}\exp\left[-\dfrac{(x-a)^2}{(H_a^2/\ln 2)}\right]\equiv N_{\max}2^{-(x-a)^2/H_a^2} & \text{when } x<a, \\ N_{\max} & \text{when } a\le x\le b, \\ N_{\max}\exp\left[-\dfrac{(x-b)^2}{(H_b^2/\ln 2)}\right]\equiv N_{\max}2^{-(x-b)^2/H_b^2} & \text{when } x>b, \end{cases} \tag{5.2}$$

where $N_{\max}$ is the concentration in the central part of the trap region. Further on, the term "edge of the region" will mean the coordinate value corresponding to one of the boundaries of the central part of the trap region (with constant concentration), i.e., the parameter a or b in the expression (5.2). H_a is the left half-distance, i.e., the distance between the left boundary of the region (a) and the point $x < a$, where $f(x) = N_{\max} / 2$ (see Fig. 5). H_b is the right half-distance, i.e., the distance between the right boundary of the region (b) and the point $x > b$, where $f(x) = N_{\max} / 2$ (see Fig. 5).

A new region of bulk traps is defined by clicking the button "Add or remove a region", then clicking "OK" in the dialog window that is opened, and then entering the region parameters in the five text boxes that are below the drop-down list "Selected region" (see Fig. 4). Those parameters are:

a) the width of the trap region, which is equal to $b - a$ (it is denoted w in Fig. 5);
b) the distance between the left edge of the region and the left edge of the layer (sublayer), to which those traps belong (in the parameter sheet "Bulk trap parameters", this parameter is called "Region offset", and in Fig. 5 it is denoted a);
c) the maximum trap concentration in the region ($N_{\max}$);
d) the left half-distance H_a;
e) the right half-distance H_b.

In order to define a trap region with purely Gaussian profile (i.e., symmetric and without the intervening region of constant concentration), the width w must be set to zero and parameters H_a and H_b must be set equal to each other. In this case, the parameter a would mean the distance from the left edge of the current layer to the point of the maximum concentration.

- The group "Parameters of charge carrier capture to selected traps" contains the controls that are used to specify names and cross-sections of charge carrier capture to current bulk traps. A capture process can be added or removed using the button "Add or remove a process". When defining a new capture process, the captured carriers must be selected in the drop-down list "Captured carriers", and the trap charge prior to capturing a carrier must be specified in the text box "Initial trap charge" (in units of the elementary charge).

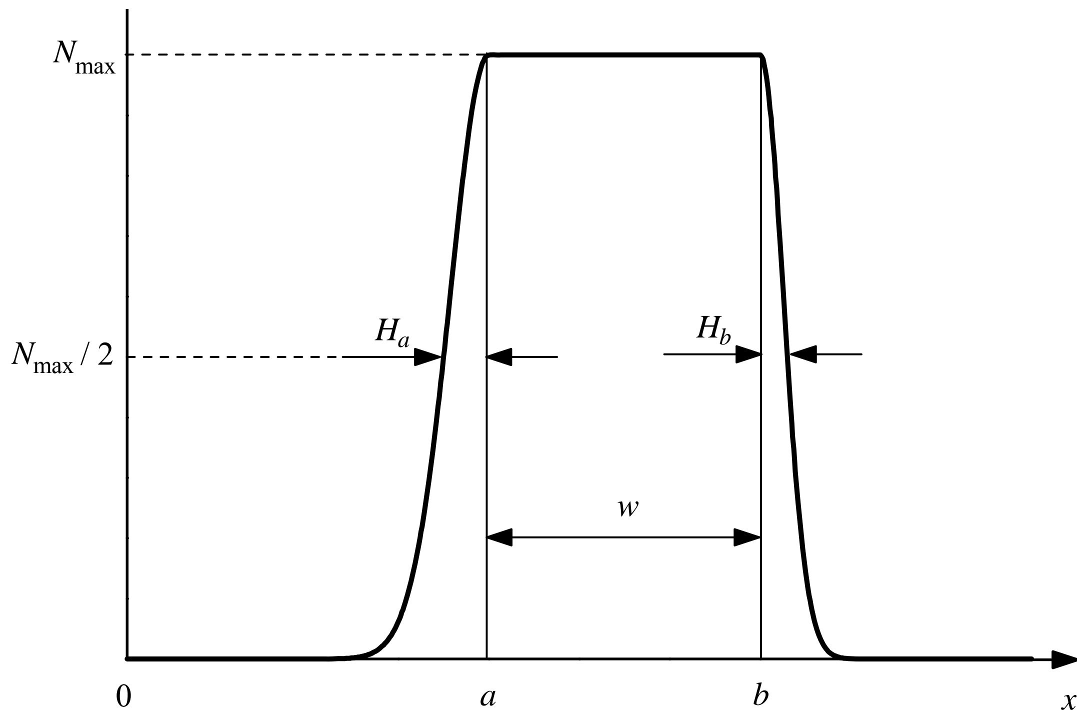


Fig. 5. Dependence of bulk trap concentration on coordinate in a single region, and the region parameters

- The drop-down list "Capture cross-section" is used to select the method that should be used to compute the cross-section of charge carrier capture into the bulk traps. The capture cross-section σ appears in the expression of the capture rate R_n:

$$R_n = \sigma \upsilon_{\text{th}} n p_{\text{t}}, \tag{5.3}$$

where υ_{th} is the average thermal velocity of the captured charge carriers (it is calculated according to (4.12)), n is their concentration, and p_{t} is the concentration of traps whose charge state corresponds to the charge value entered in the text box "Initial trap charge". The factor $\sigma\upsilon_{\text{th}}$ is sometimes called "the capture coefficient". In the current version of the model (v0.75), two choices are available in the drop-down list "Capture cross-section": a constant cross-section ("Constant") and a constant capture coefficient ("Known capture coefficient").

- The group of controls "Parameters of charge carrier release from selected traps" is used to specify names of release processes and parameters that define the release rates. A release process can be added or removed using the button "Add or remove a process". When defining a new release process, the released carriers must be selected in the drop-down list "Released carriers", and the trap charge prior to carrier release must be specified in the text box "Initial trap charge" (in units of the elementary charge).

- The drop-down list "Release coefficient" is used to select the method that should be used to compute the release coefficient. The release coefficient α appears in the expression of the release rate G_n:

$$G_n = \alpha n_{\text{t}}, \tag{5.4}$$

where n_{t} is the concentration of traps whose charge state corresponds to the charge value entered in the text box "Initial trap charge". Three choices are available in the drop-down list "Release coefficient":

1) A constant release coefficient;

2) The Shockley-Read-Hall model. According to this model, the release coefficient is proportional to the capture coefficient $\sigma\,\upsilon_{\text{th}}$ corresponding to the opposite process (charge carrier capture), where σ is the capture cross-section and υ_{th} is the average thermal velocity of the released charge carriers:

$$\alpha = \sigma \upsilon_{\text{th}} N_c \exp\left(-\frac{E_{\text{a}}}{kT}\right), \tag{5.5}$$

where N_c is the state density of free charge carriers, and E_{a} is the "energy depth" of the traps. For example, if the selected release process corresponds to liberation of electrons from donor atoms in a semiconductor, then N_c is the effective conduction band state density and E_{a} is the difference between the conduction band edge and the donor energy level. The factor N_c in (5.5) is computed using the method specified in the parameter sheet "Free carrier parameters" (drop-down list "State density").

Thus, the Shockley-Read-Hall model may only be selected when the opposite process (capture) exists. If there is no corresponding capture process, then a warning appears after an attempt to start simulation. If the selected traps act as recombination centers, then there must be two capture processes and two release processes defined, with two types of charge carriers participating in them (also see the part of Section 4 where the Shockley-Read-Hall recombination is described).

3) The SRH model with modified state density is also defined by (5.5), but with an arbitrary state density N_c, whose value must be entered by the user. In this case, the value of N_c may be different from the state density defined in the parameter sheet "Free carrier parameters".

6. Interface trap parameters

The parameter sheet "Interface trap parameters" is used to enter parameters of each type of interface traps, as well as parameters that define processes of charge carrier capture into interface traps and release from interface traps. Examples of this parameter sheet are shown in Fig. 6 and Fig. 7. Below are explanations of all controls of this parameter sheet:

- The button "Add or remove interface traps" is used to open a dialog window where one of three actions can be selected: addition of a new type of interface traps to the end of the list (this is the default action), insertion of the new trap type before the current type of interface traps, and deletion of the current type of interface traps. After selecting addition or insertion of new traps, the user has to specify the trap position. Three choices are available: left edge of the current layer, right edge of the current layer, or both edges of the layer (see Fig. 8). In the case of "both edges", the values of surface density of those traps on both edges of the layer will be equal to each other. If the adjacent layer of the simulated system has already interface traps defined, then it is possible to use the same traps when defining carrier capture and release processes of the current layer. In such case, the message box shown in Fig. 9 pops up before the mentioned trap position dialog. If the button "Yes" is clicked, the dialog window similar to the one shown in Fig. 10 is opened. It is used to select one of the previously defined interface trap types, which belongs to the adjacent layer of the system and which should "coincide" with the new traps that are being created. This option is necessary when the interface traps act as an intermediate state for charge carrier transfer from one layer to another. In this case, the interface traps do not "belong" to a particular layer, but "belong" to both adjacent layers (to be more precise, they characterize the interface between the two layers). Since this program requires each parameter set to belong to one layer, the concept of "coinciding" interface traps is used, i.e., interface traps belonging to one layer "coincide" with interface traps belonging to the adjacent layer.
- The drop-down list "Selected interface traps" is used to select interface traps when there are two or more types of interface traps in the current layer. All parameters shown in this parameter sheet correspond to the selected type of interface traps.
- The next two text boxes are used to enter the full name and the abbreviated name of the traps.
- The drop-down list "Surface density of the traps" is used to select the trap surface density computation method. In the current version of the model (v0.75), only one choice is available – "Constant", which corresponds to a constant trap surface density (its value must be entered in the nearby text box). If the selected interface traps coincide with interface traps defined in the adjacent layer (the "primary" traps), then the drop-down list "Surface density of the traps" is replaced with two static text fields containing the names of the adjacent layer and of the "primary" interface traps (see Fig. 7).
- The group "Parameters of charge carrier capture to selected traps" contains the controls that are used to specify names and cross-sections of charge carrier capture to current interface traps. A capture process can be added or removed using the button "Add or remove a process". When defining a new capture process, the captured carriers must be selected in the drop-down list "Captured carriers", and the trap charge prior to capturing a carrier must be specified in the text box "Initial trap charge" (in units of the elementary charge).
- The drop-down list "Capture cross-section" is used to select the method that should be used to compute the cross-section of charge carrier capture into the interface traps. The capture cross-section σ appears in the expression of the capture rate $R_{s,n}$:

  $$R_{s,n} = \sigma \upsilon_{th} n p_s , \qquad (6.1)$$

  where υ_{th} is the average thermal velocity of the captured charge carriers (it is calculated according to (4.12)), n is their concentration, and p_s is the surface density of interface traps whose charge state corresponds to the charge value entered in the text box "Initial trap charge". $R_{s,n}$ is defined as the number of free charge carriers that are captured into the interface traps in the unit area per unit time. The factor $\sigma\upsilon_{th}$ is sometimes called "the capture coefficient". In the current version of the model (v0.75), two choices are available in the drop-down list "Capture cross-section": a constant cross-section ("Constant") and a constant capture coefficient ("Known capture coefficient").

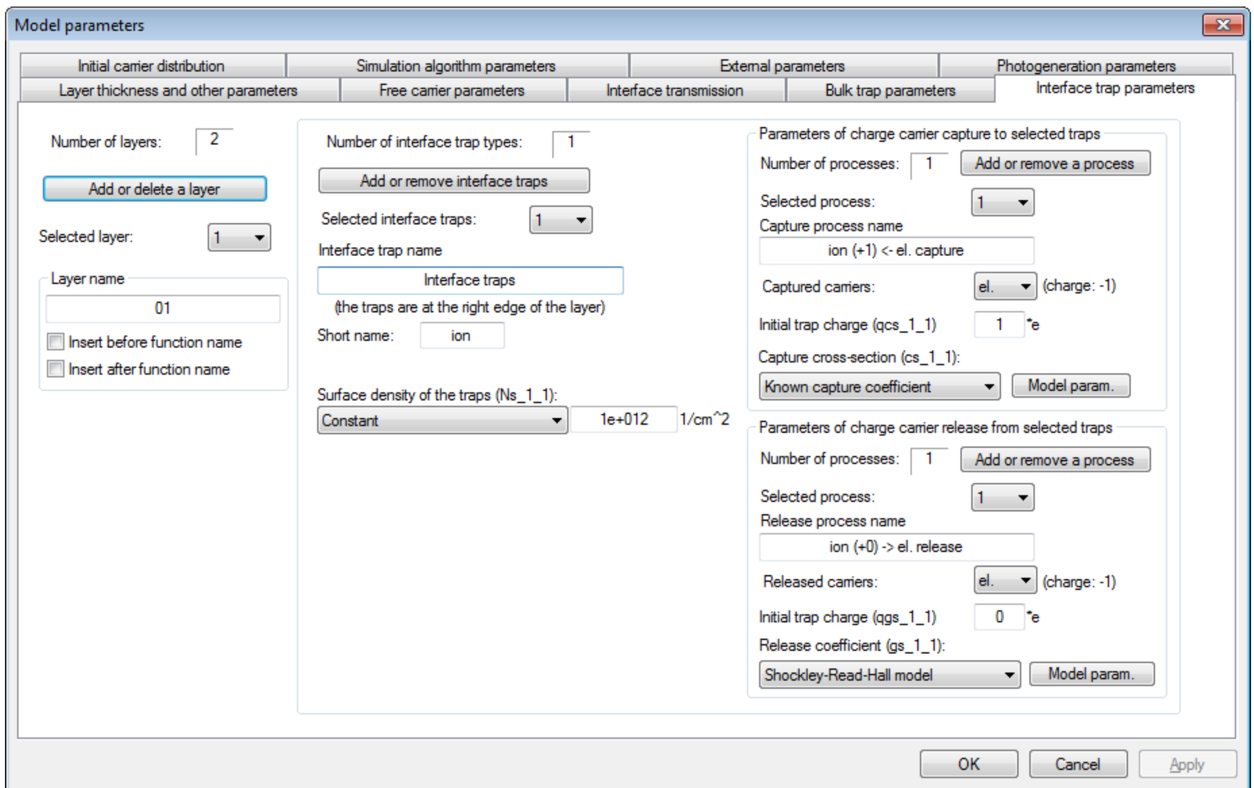


Fig. 6. An example of the parameter sheet "Interface trap parameters"

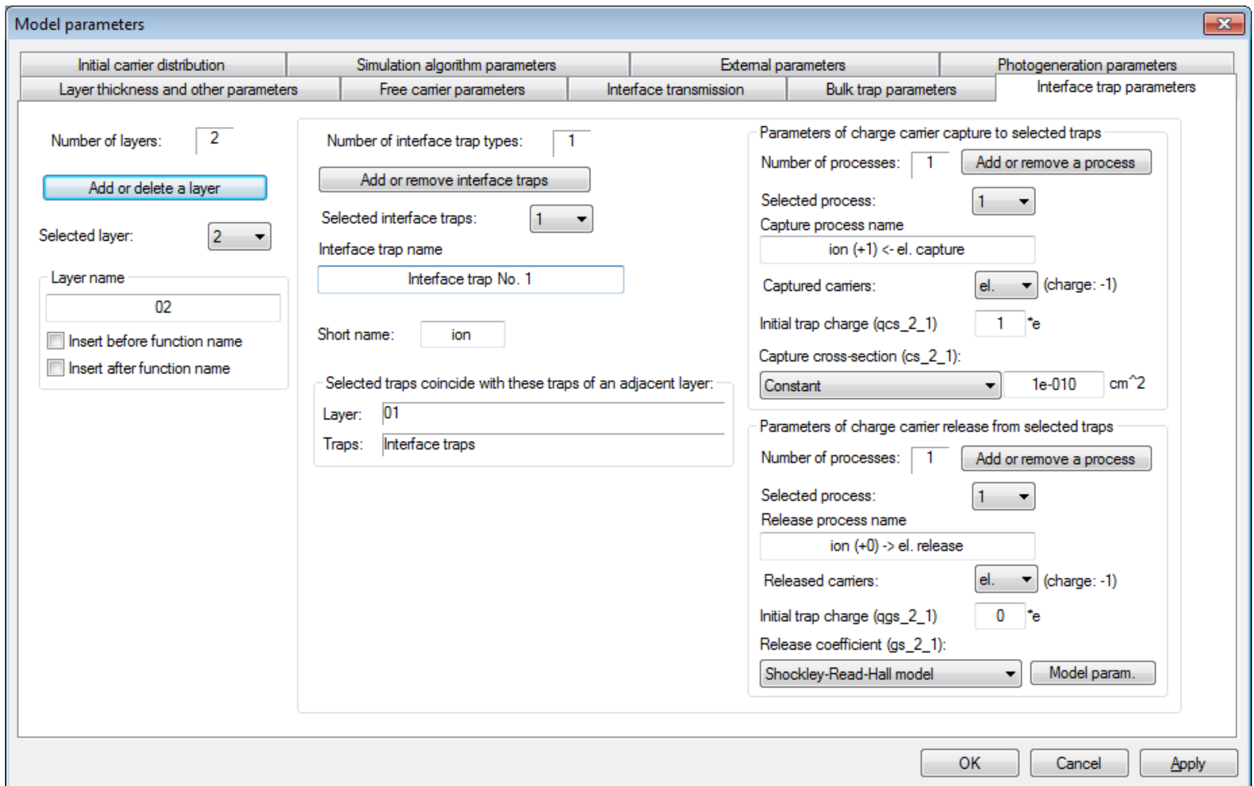


Fig. 7. An example of the parameter sheet "Interface trap parameters" when the selected interface traps "coincide" with interface traps that are defined in the adjacent layer

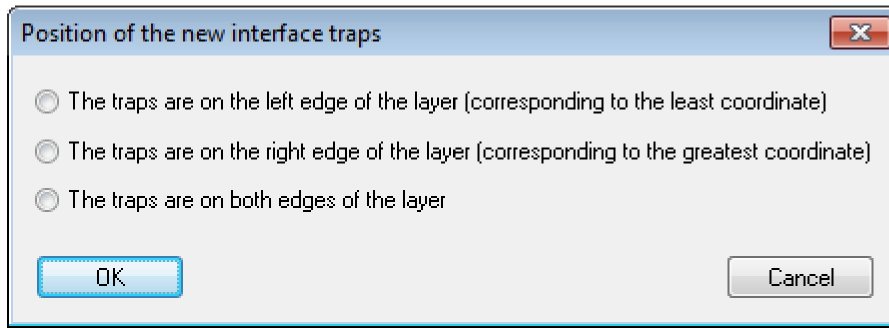


Fig. 8. The dialog window for specifying the position of new interface traps

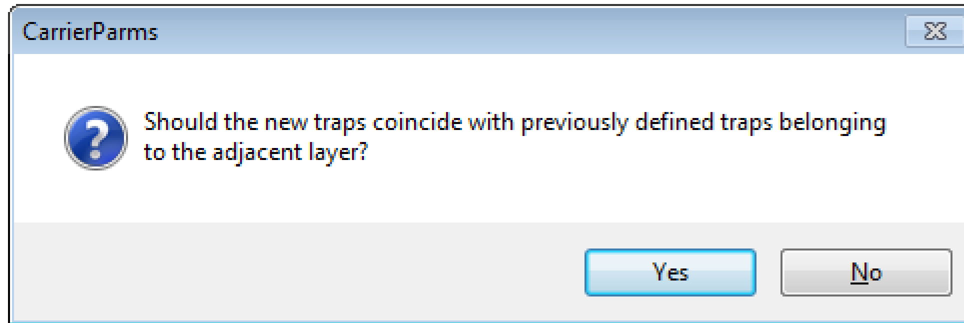


Fig. 9. The message box that pops up when new interface traps are being created and the adjacent layer already has interface traps defined

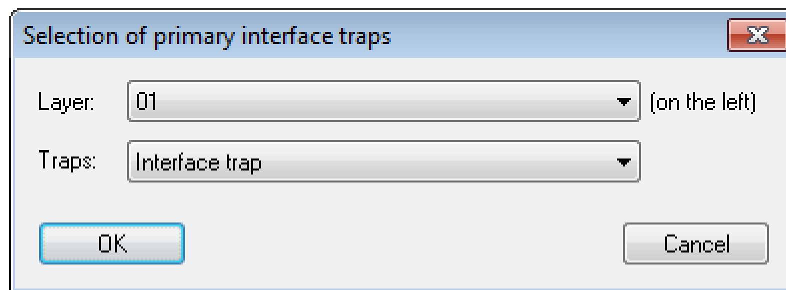


Fig. 10. An example of the dialog window for selecting the previously defined interface traps of the adjacent layer that should "coincide" with the new interface traps of the current layer

- The group of controls "Parameters of charge carrier release from selected traps" is used to specify names of release processes and parameters that define the release rates. A release process can be added or removed using the button "Add or remove a process". When defining a new release process, the released carriers must be selected in the drop-down list "Released carriers", and the trap charge prior to carrier release must be specified in the text box "Initial trap charge" (in units of the elementary charge).
- The drop-down list "Release coefficient" is used to select the method that should be used to compute the release coefficient. The release coefficient α appears in the expression of the release rate $G_{s,n}$:

$$G_{s,n} = \alpha n_s \,, \tag{6.2}$$

where n_s is the surface density of interface traps whose charge state corresponds to the charge value entered in the text box "Initial trap charge". $G_{s,n}$ is defined as the number of free charge carriers that are released from the interface traps in the unit area per unit time. Three choices are available in the drop-down list "Release coefficient":

1) A constant release coefficient;

2) The Shockley-Read-Hall model. According to this model, the release coefficient is proportional to the capture coefficient $\sigma \upsilon_{th}$ corresponding to the opposite process (charge carrier capture), where σ is the capture cross-section and υ_{th} is the average thermal velocity of the released charge carriers:

$$\alpha = \sigma \upsilon_{\rm th} N_c \exp\left(-\frac{E_{\rm a}}{kT}\right), \tag{6.3}$$

where N_c is the state density of free charge carriers, and $E_{\rm a}$ is the "energy depth" of the traps. The factor N_c in (6.3) is computed using the method specified in the parameter sheet "Free carrier parameters" (drop-down list "State density").

Thus, the Shockley-Read-Hall model may only be selected when the opposite process (capture) exists. If there is no corresponding capture process, then a warning appears after an attempt to start simulation.

3) The SRH model with modified state density is also defined by (6.3), but with an arbitrary state density N_c, whose value must be entered by the user. In this case, the value of N_c may be different from the state density defined in the parameter sheet "Free carrier parameters".

7. Photogeneration parameters

Examples of the photogeneration parameter sheet are shown in Fig. 11. Descriptions of all parameters of that sheet are given below:

- The parameter group “Parameters of spectral components” contains three parameters – the name of the light spectral component, the weight factor of its photon flux and the absorption coefficient in the selected layer (the layer selection drop-down list is on the left side of this parameter sheet). Spectral components can be added or removed by clicking the button “Add or remove a spectral component” (the maximum allowed number of spectral components is 100). Prior to starting the simulation, the program CarrierFunc.dll normalizes all weight factors to unity, i.e., it divides each weight factor by the sum of weight factors of all spectral components. The physical meaning of a normalized weight factor is the fraction of photons corresponding to the selected spectral component (the total photon flux density is defined in the parameter group “External illumination parameters”, which is described below). Consequently, only the ratios of the weight factors are important, but not their absolute values. For example, if there are three spectral components with weight factors 1, 2 and 3, then the same simulation results would be obtained using the weight factors 50, 100 and 150.
- The parameter group “Photogeneration process parameters” contains controls that make it possible to add, remove or modify photogeneration processes. A photogeneration process can be added or removed by clicking the button “Add or remove a process”. The photogenerated charge carriers are specified in the drop-down list boxes “Selected charge carriers” and “Carriers of opposite charge”. Photogeneration quantum yield is defined as the average number of charge carrier pairs (usually electron-hole pairs) corresponding to one absorbed photon. The drop-down list box “Photogeneration quantum yield” is used to select the method of specifying quantum yields for different spectral components of light. Two choices are available: “Constant” and “Specified for each component”:
  a) If “Constant” is selected, then quantum yields of all spectral components will be equal to the value entered in the nearby text box (see Fig. 11a). Besides, in this case it is possible to “turn off” some spectral components, i.e., to set their quantum yield equal to 0. This is done by clicking the button “Spectral components stimulating this process…”. Then a dialog window similar to the ones shown in Fig. 12 is opened. A spectral component can be “turned on” or “turned off” by left-clicking its name.
  b) After selecting “Specified for each component”, the mentioned text box is replaced by the button “Quantum yields…” (see Fig. 11b). By clicking that button, the dialog window with photogeneration quantum yields of all spectral components is opened (see Fig. 13a). A value of a quantum yield can be changed by left-clicking the corresponding line of this list and then clicking the button “Change the selected quantum yield”, or by right-clicking the line and then selecting the command “Change quantum yield…” in the context menu, or by double-clicking the line. In all cases, the dialog window “Quantum yield value…” is opened (see Fig. 13b).
- The parameter group “External illumination parameters” contains parameters that define the external illumination intensity and its time dependence. Two radio buttons that are in the group “Exposed edge of the system” are used to specify the position of the light source (either on the left of the system or on the right of it). The text box “Initial photon flux density” is used to specify the constant term in the expression of the external photon flux density (“photon flux density” is the number of photons incident upon one square centimeter of the layer per one second). The drop-down list “Time dependence of photon flux density” is used to select one of several standard time dependences. The selected time dependence is the deviation from the mentioned initial photon flux density. I.e., the instantaneous value of the total photon flux density is equal to the sum of the initial value and the selected time dependence. In the current version of the model (v0.75), one of four standard functions can be selected: “Constant illumination intensity”, “Periodic square pulse sequence”, “Periodic sequence of short pulses” and “Linear variation”. The other text boxes are used to enter the parameters of the selected time dependence (e.g., period, pulse height, etc.). If all parameters of the time dependence are zero, then the corresponding time dependence is also assumed to be zero. If at least one parameter is non-zero, then the parameter editor checks if the parameter values satisfy the restrictions that may exist in the context of the selected time dependence (for example, if the periodic square pulse sequence is selected, then pulse duration must be less than the period of the sequence). If a parameter value is outside those bounds, then a corresponding error message appears.

Note: If the line "Periodic sequence of short pulses" is selected, then the pulse duration will be assumed to be zero. I.e., in this case each pulse creates a certain concentration of charge carriers instantaneously. That concentration depends on the number of photons (per square centimeter) in one pulse. Consequently, in this case the number of photons per square centimeter must be specified instead of the photon flux density.

a)

b)

Fig. 11. Examples of the parameter sheet "Photogeneration parameters": a) photogeneration quantum yields of all spectral components are equal; b) quantum yield is specified for each spectral component separately.

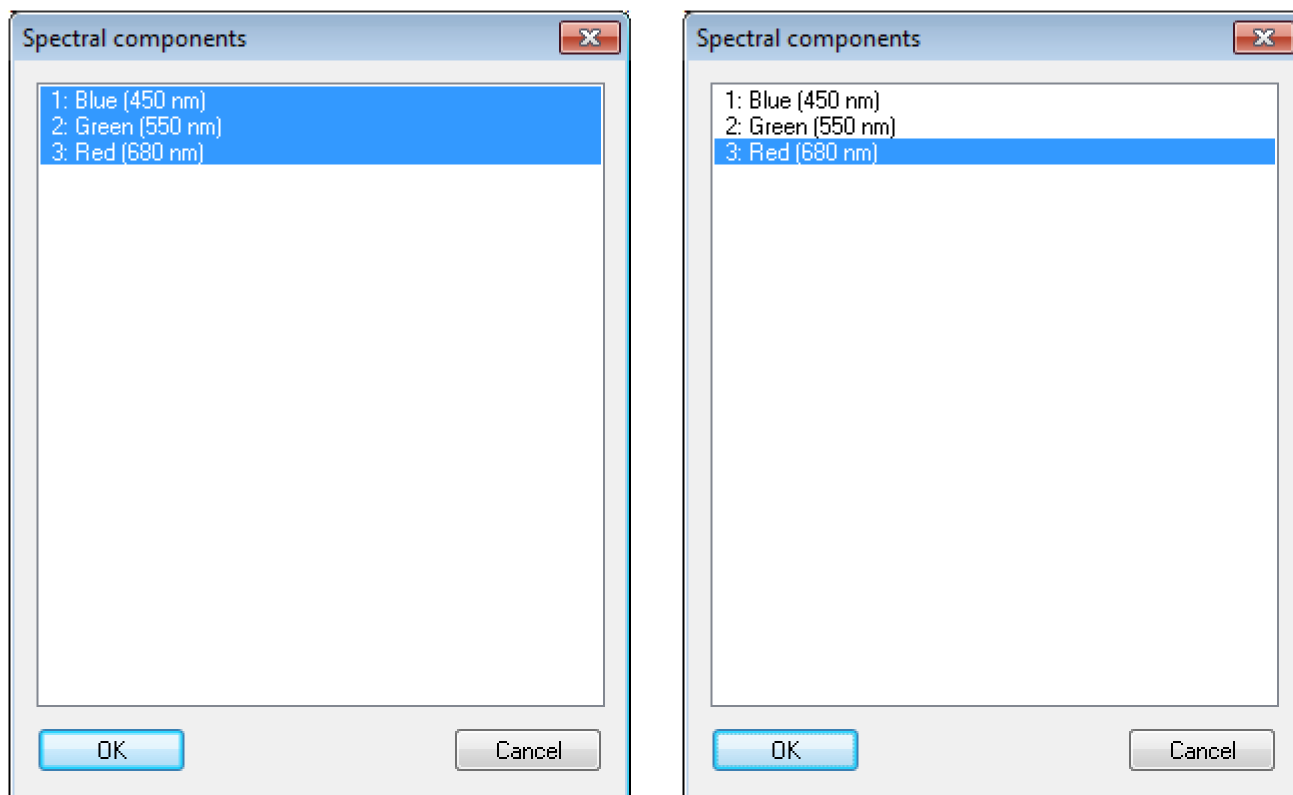


Fig. 12. Examples of the dialog window for selecting "active" spectral components of light when a constant photogeneration quantum yield is used. In the example on the left, all three spectral components are "turned on". In the example on the right, only the third spectral component is "turned on" (active), whereas the first two spectral components are "turned off" (inactive), i.e., their photogeneration quantum yields are zero

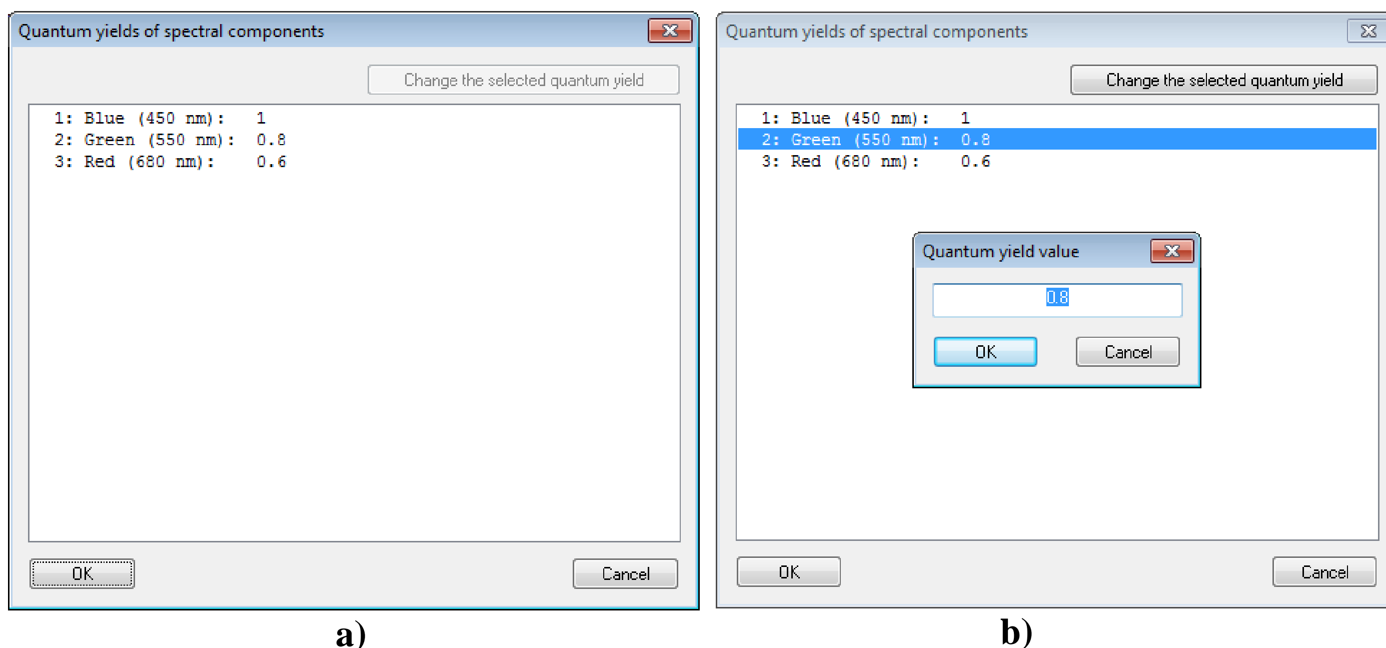


Fig. 13. An example of the dialog window for specifying quantum yields of individual spectral components: a) the initial view; b) the view after selecting a spectral component and opening the corresponding text box

8. Parameters of charge carrier transport through interfaces

The parameter sheet “Interface transmission” is used to define conditions of charge carrier transport through interfaces between the layers of the system. Those conditions are defined separately for each type of charge carriers. The charge carrier type is selected in the drop-down list “Selected charge carriers” (see Fig. 14). Mathematically, the mentioned conditions determine the boundary conditions of the solved system of differential equations. Four options are available (see Fig. 14):

- If the option “The interface blocks the selected charge carriers completely” is selected, then conduction current of the selected charge carriers on that interface will always be zero.
- If the option “The interface acts as an ohmic contact for the selected charge carriers” is selected, then the conduction current density of the selected charge carriers on that interface will be computed using the same expression as in the bulk of the layer (i.e., (1.2)), but with the concentration gradient $\partial n_i / \partial x$ computed as a “one-sided” derivative, rather than a “double-sided” derivative. The influence of this option on the charge distribution depends on presence or absence of an electrode on the other side of the interface. If that interface is a free surface of the system or if it separates two simulated layers of a multi-layer system, then the conduction current flowing through that interface will cause a variable surface charge. In this case, the charge carriers do not cross the interface, but accumulate on it as surface charge (in the names of model functions, that charge is called the “free surface charge”). If the given interface separates a simulated layer and an electrode, then the current that flows through that interface does not create any surface charge.

  In addition, after selecting the option “The interface acts as an ohmic contact for the selected charge carriers”, it becomes possible to specify a constant value of the charge carrier concentration on that interface. This option may decrease simulation time, e.g., when simulating stationary current flowing through an ohmic contact between a metal and semiconductor (semiconductor charge carrier concentrations at such a contact are always equal to their values at thermodynamic equilibrium). During simulation, charge carrier concentration at the corresponding surface node is kept constant by “turning off” all charge carrier generation-recombination processes that influence concentration of the selected charge carriers. In addition, the values of the current density at the surface node and at the nearest bulk node of that layer, which are computed according to (1.2), are replaced by their arithmetic average (this ensures that the gradient of the current density at the surface node is zero).
- If the option “The interface is transparent to the selected charge carriers” is selected, then charge carrier concentrations on both sides of the interface are computed on the basis of the continuity condition for the conduction current density and its gradient. This option can only be selected after

Fig. 14. An example of the parameter sheet “Interface transmission”

specifying adjacent layer's charge carriers that correspond to the selected charge carriers of the current layer. The drop-down list for selecting charge carriers of the adjacent layer is not visible in Fig. 14, because it appears only when the simulated system consists of more than one layer and when the selected interface is not the edge of the system (i.e., when it separates two simulated layers). The just-mentioned drop-down list contains the names of charge carriers of the adjacent layer with charge equal or opposite to the charge of the selected charge carriers of the current layer. Thus, the charge carriers crossing a "transparent" interface may be replaced by charge carriers of the same charge (e.g., electrons of one layer become electrons of another layer), or by charge carriers of the opposite charge (e.g., electrons on one side of the interface, and holes on the other side). In order to ensure continuity of conduction current density and of its derivative with respect to coordinate, the values of the conduction current density at the interface nodes and at two nearest bulk nodes are replaced by linearly fitted values. Thus, four values of current are involved: the values of current of the selected charge carriers on the interface node of the selected layer and on the nearest bulk node of the same layer, and the values of current of the corresponding charge carriers on the interface node of the adjacent layer and on the nearest bulk node of the same layer. Those four values are replaced by values computed according to the equation of a straight line (two middle values are equal to each other, because interface nodes of adjacent layers coincide with each other).

- If the option "The interface acts as a potential barrier for the selected charge carriers" is selected, then an additional term appears in the expression of the conduction current (1.2). That term reflects the difference of two fluxes: one is due to charge carrier transfer over the potential barrier in the positive x direction, and the other one is due to charge carrier transfer over the potential barrier in the negative x direction. The method of computing those two fluxes must be specified in the two drop-down lists that are at the bottom of this parameter sheet (see Fig. 14). The first two choices in those drop-down lists are "Constant" and "Free particles, Maxwell distribution". If the selected layer is an electrode and "Constant" is selected, then the nearby text box must contain the absolute value of the injection current density from that electrode into the layer. If the selected layer is not an electrode (i.e., if it is one of simulated layers) and "Constant" is selected, then the nearby text box must contain the ratio of injection flux density and charge carrier concentration at the corresponding interface node of the selected layer (the measurement unit of that ratio is cm/s). In the latter case, having selected "Constant", the injection flux density of the selected charge carriers from the selected layer into the adjacent layer (or into the electrode) will be calculated by multiplying that constant by the concentration of those charge carriers at the interface node of the selected layer (the injection current density is equal to the product of the injection flux density and the carrier charge). When "Constant" is selected, the text box "Potential barrier height" is disabled, because in this case the potential barrier height is not used for calculating the injection current density. If "Free particles, Maxwell distribution" is selected, then the charge carrier injection flux density will be calculated under the assumption that charge carrier speeds are distributed according to the Maxwell distribution and that the following two conditions are sufficient for a charge carrier to cross the potential barrier: 1) kinetic energy of the charge carrier must exceed the potential barrier height; 2) the x component of the charge carrier velocity vector must be directed outside of the layer (i.e., towards the selected interface). In this case, the potential barrier height must be entered in the text box "Potential barrier height". Then the current density component corresponding to transport of the selected charge carriers through the interface will be calculated as follows:
$$j = \frac{qn}{\sqrt{2\pi kTm^*}}(\Phi_b + kT)\exp\left(-\frac{\Phi_b}{kT}\right), \tag{8.1}$$
where q is the carrier charge, n is their concentration at the interface, m^* is the carrier effective mass, Φ_b is the potential barrier height, k is the Boltzmann constant, T is the absolute temperature. If the selected layer is an electrode, then two more choices are available in the mentioned drop-down list: "Elementary Richardson equation" and "Richardson equation with an additional factor". If "Elementary Richardson equation" is selected, then the current density due to thermionic emission from the electrode will be calculated according to the Richardson equation
$$j = AT^2\exp\left(-\frac{\Phi_b}{kT}\right), \tag{8.2}$$
where A is the Richardson constant ($A = 1{,}20173 \cdot 10^6\ \mathrm{Am^{-2}K^{-2}}$). However, when simulating thermionic emission from a metal into a semiconductor or a dielectric, it is more appropriate to use the "effective" Richardson constant $A^* = (m_t / m_0) \cdot A$, where m_t is the charge carrier effective mass in the

semiconductor in the transverse direction to the interface (in the case of an isotropic semiconductor, m_t is equal to the density-of-states effective mass m^*). Then, "Richardson equation with an additional factor" must be selected and the value of the ratio m_t / m_0 must be entered as the additional factor.

When the selected layer is an electrode and the potential barrier height is non-zero, then the Schottky effect can be taken into account. The term "Schottky effect" refers to the decrease of the potential barrier height in the presence of external electric field that accelerates the emitted charge carriers away from the electrode. In order to take into account the Schottky effect, the checkbox "Schottky effect" must be checked. Then, the expressions of the thermionic injection current density (8.1) and (8.2) will be modified by replacing Φ_b with $\Phi_b - \Delta\Phi_b$, where $\Delta\Phi_b$ is the mentioned decrease of the potential barrier height:

$$\Delta\Phi_b = e\sqrt{\frac{|qE|}{4\pi\varepsilon_0\varepsilon}}, \tag{8.3}$$

where E is the electric field strength at the interface in the simulated layer (semiconductor or dielectric), ε is dielectric permittivity of that layer, e is the elementary charge, q is the carrier charge, and ε_0 is the electric constant.

The remaining part of the conduction current density (i.e., the drift and diffusion current) is set equal to the average of the expression (1.2) at the surface nodes of the two adjacent layers (the coordinate values of those two nodes are equal to each other, because they belong to the same interface). Thus, in this case the conduction current is continuous, but its derivative with respect to the coordinate may have a discontinuity at the interface, because the conduction current value at the surface node is computed without taking into account the value of the current at the nearest bulk node of the same layer.

9. External parameters

The external parameters are the ambient temperature, electrode configuration (two electrodes or one electrode), and in the case of two electrodes – time dependence of external voltage and parameters of the external circuit components (resistance and capacitance). The terms “external voltage” and “external circuit” are only applicable in the two-electrode configuration. If there is only one electrode, then its potential is always zero, and the total current (i.e., the sum of conduction and displacement currents) is also zero. Prior to descriptions of the parameters whose values can be entered in the parameter sheet “External parameters”, below are the expressions of potentials at various points of the circuit, as well as the expressions of the total current in terms of those potentials in the two-electrode configuration.

Depending on the electrode whose potential is varied (i.e., the right electrode or the left electrode), two schematic circuit diagrams are possible. They are shown in Fig. 15a and Fig. 15b. The following notations are used in them:

U_0 – potential of the left electrode of the simulated system,
U_1 – potential of the right electrode of the simulated system,
U_2 – potential of one pole of the external voltage source, which is connected via the resistor R to one of the electrodes (the one whose potential is varied),
R – external resistance,
C – external capacitance,
i – total current of the simulated system.

If the right electrode potential is varied (as in Fig. 15a), then its time dependence is described by the following differential equation:

$$\frac{\mathrm{d}U_1}{\mathrm{d}t} = \frac{U_2 - U_1}{RC} + \frac{i}{C}. \tag{9.1a}$$

If the left electrode potential is varied (as in Fig. 15b), then its time dependence is described by the following differential equation:

$$\frac{\mathrm{d}U_0}{\mathrm{d}t} = \frac{U_2 - U_0}{RC} - \frac{i}{C}. \tag{9.1b}$$

The total current i is defined as follows:

$$i = S(j + j_\mathrm{d}) = S\left(j + \varepsilon_0 \varepsilon \frac{\mathrm{d}E}{\mathrm{d}t} \right), \tag{9.2}$$

where S is the electrode area, j is the conduction current density (i.e., the sum of expressions of the type (1.2), corresponding to all free charge carriers at a given point), j_d is the displacement current density, ε_0 is the electric constant, ε is dielectric permittivity, and $\mathrm{d}E / \mathrm{d}t$ is the time derivative of the electric field strength (the values of ε and $\mathrm{d}E / \mathrm{d}t$ correspond to the same point of the system as the value of j). The total current i does not depend on coordinate, although its components (the conduction current and the displacement current) are, in general, coordinate-dependent. The total current (9.2) may only depend on time t. In order to derive the equation for U_1 or U_0, the total current i must be expressed in terms of the time derivative $\mathrm{d}U_1 / \mathrm{d}t$ or $\mathrm{d}U_0 / \mathrm{d}t$, respectively. That expression is given below:

if the right electrode potential is varied:

$$i = S\left(j_\mathrm{eff} - \frac{\varepsilon_0}{w_\mathrm{eff}} \frac{\mathrm{d}U_1}{\mathrm{d}t} \right), \tag{9.3a}$$

and if the left electrode potential is varied:

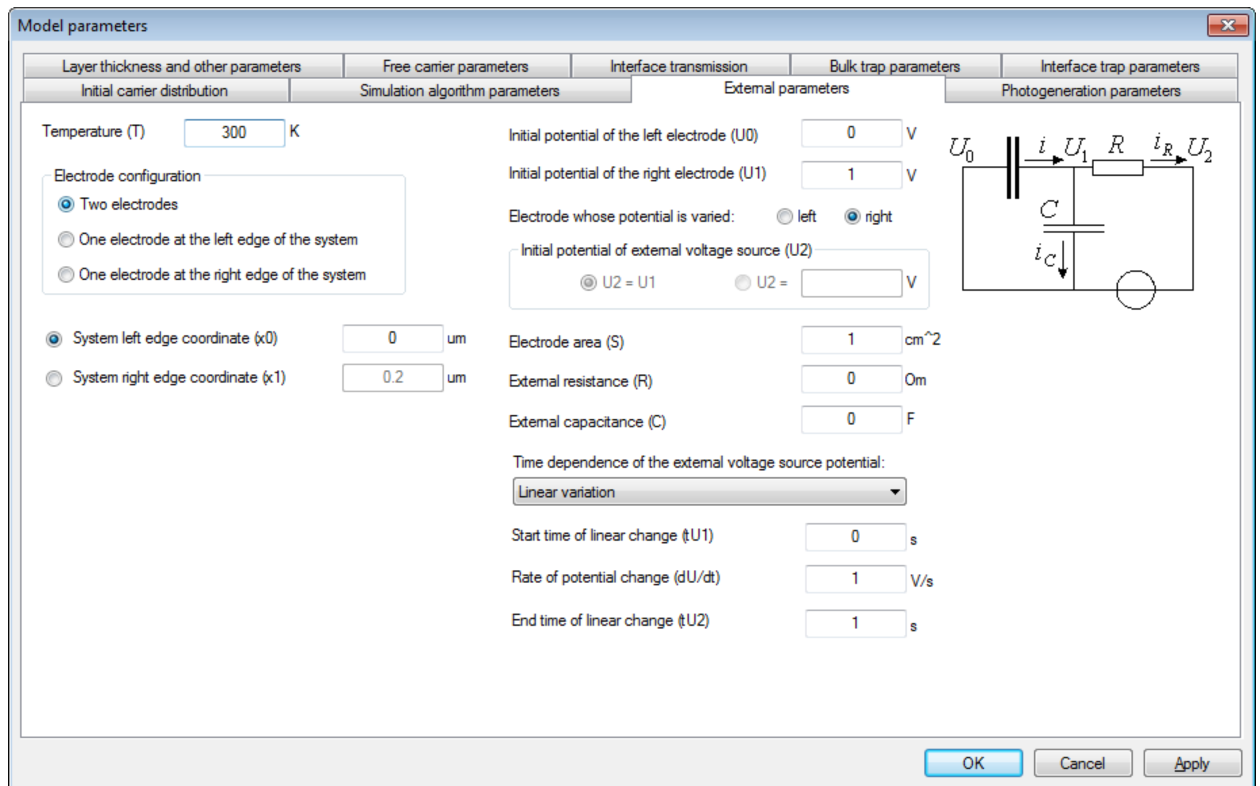
$$i = S\left(j_\mathrm{eff} + \frac{\varepsilon_0}{w_\mathrm{eff}} \frac{\mathrm{d}U_0}{\mathrm{d}t} \right), \tag{9.3b}$$

where w_eff is the “effective width of the system”, which is defined as

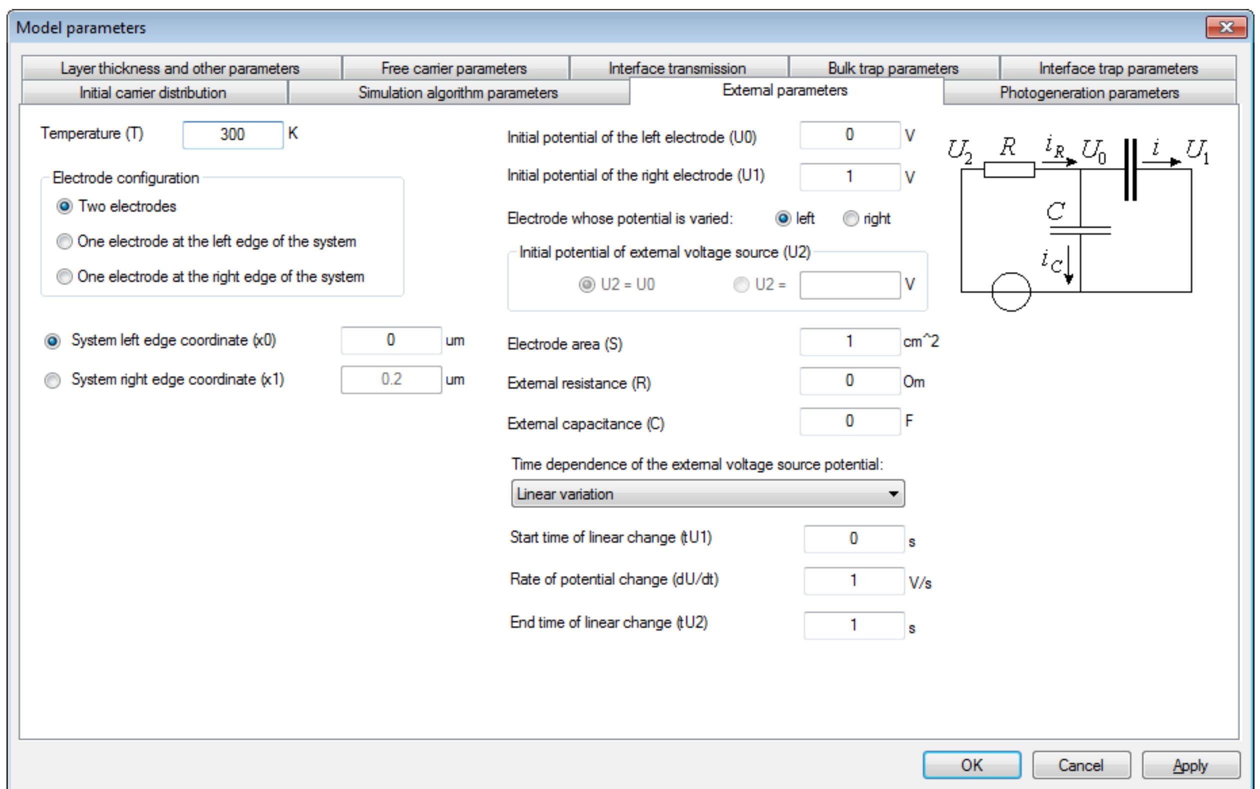
$$w_\mathrm{eff} \equiv \sum_{k=1}^{L} \frac{w_k}{\varepsilon_k}, \tag{9.4}$$

where L is the number of the layers in the system (excluding the electrodes), k is a layer number, w_k is thickness of the k-th layer, ε_k is dielectric permittivity of the k-th layer, and j_eff is the “effective conduction current density”, which is defined as

$$j_\mathrm{eff} \equiv \frac{1}{w_\mathrm{eff}} \sum_{k=1}^{L} \frac{1}{\varepsilon_k} \int_{x_{k-1}}^{x_k} j(x)\mathrm{d}x, \tag{9.5}$$



a)



b)

Fig. 15. Examples of the parameter sheet "External parameters": a) when the right electrode potential is varied; b) when the left electrode potential is varied

where x_k is the coordinate of the right edge of the k-th layer (x_0 corresponds to the left edge of the system). By inserting expressions (9.3a) and (9.3b) into equations (9.1a) and (9.1b), respectively, and expressing $\mathrm{d}U_1 / \mathrm{d}t$ and $\mathrm{d}U_0 / \mathrm{d}t$, the following two differential equations are obtained:

if the right electrode potential is varied:

$$\frac{\mathrm{d}U_1}{\mathrm{d}t} = \frac{1}{C + (\varepsilon_0 S / w_{\mathrm{eff}})} \left(\frac{U_2 - U_1}{R} + S j_{\mathrm{eff}} \right), \tag{9.6a}$$

and if the left electrode potential is varied:

$$\frac{\mathrm{d}U_0}{\mathrm{d}t} = \frac{1}{C + (\varepsilon_0 S / w_{\mathrm{eff}})} \left(\frac{U_2 - U_0}{R} - S j_{\mathrm{eff}} \right). \tag{9.6b}$$

Since at a given moment of time ($t = t_l$) all quantities on the right-hand side of equations (9.6a) and (9.6b) are known, the value of potential U_1 or U_0 at a later moment of time ($t_{l+1} = t_l + \Delta t$) can be computed in the same way as charge carrier concentrations, i.e., by applying the explicit algorithm (see formula (1.7)):

if the right electrode potential is varied:

$$U_1(t_{l+1}) = U_1(t_l) + \left. \frac{\mathrm{d}U_1}{\mathrm{d}t} \right|_{t_l} \Delta t \,, \tag{9.7a}$$

and if the left electrode potential is varied:

$$U_0(t_{l+1}) = U_0(t_l) + \left. \frac{\mathrm{d}U_0}{\mathrm{d}t} \right|_{t_l} \Delta t \,. \tag{9.7b}$$

Examples of the parameter sheet “External parameters” are shown in Fig. 15a and Fig. 15b. Below are descriptions of all parameters of that parameter sheet:

- The parameter “Temperature (T)” is the absolute ambient temperature (in kelvins).
- The three radio buttons that are in the group “Electrode configuration” are used to specify the number of electrodes (one or two), and if there is only one electrode, then its position is specified (either the left edge of the system, or the right edge).
- The text boxes “System left edge coordinate (x0)” and “System right edge coordinate (x1)” specify the position of the layer on the X axis. Since the width of the layer is specified in a different parameter sheet (“Layer thickness and other parameters”), the mentioned two coordinates are not independent (their difference must be equal to the width of the system). Consequently, the mentioned two text boxes can not be enabled simultaneously. The radio buttons that are beside them are used to specify which of those text boxes must be enabled. After changing a number in that text box and left-clicking any other control of this parameter sheet, the number in the other text box will be automatically updated so as to ensure that the difference of the two coordinates is equal to the width of the system.
- All remaining controls of this parameter sheet are used to specify the initial potentials of the electrodes and their time dependence. Those controls are enabled only in the two-electrode configuration. The two text boxes at the top are used to enter initial potentials of the left electrode and the right electrode (U_0 and U_1, respectively).
- The next two radio buttons are used to specify the electrode whose potential is varied during simulation (either the left electrode, or the right electrode). This option determines the schematic circuit diagram of the simulated system, which is shown at the top right corner of this parameter sheet (compare Fig. 15a and Fig. 15b).
- The two radio buttons and the text box that are in the group “Initial potential of external voltage source (U2)” are used to specify the initial potential of the external source pole, which is connected via the resistor R to the previously-specified electrode. If a non-zero value of R has been entered (see below), then that potential may be not equal to the potential of that electrode. The difference of those two potentials is equal to the voltage drop across the resistor R. In this case, the radio button “U2 =” must be clicked and the initial value of U_2 must be entered in the nearby text box. The radio button “U2 =” is only enabled when $R \neq 0$. The other pole of the external voltage source is directly connected to the other electrode, so that the potential of that pole is constant and equal to the potential of that electrode (which has been entered before). If the initial voltage drop across the resistor R is zero (i.e., either the initial current of the external voltage source is zero or $R = 0$), then the other radio button of this group must be clicked (when $R = 0$, this is the only option available). The text beside that radio button is either “U2 = U1” or “U2 = U0” (depending on which electrode’s potential is varied).

- The text box “Electrode area (S)” is used to enter the electrode area of the simulated layer. That area is used when calculating the total current $i = S\, j_{tot}$, where j_{tot} is the total current density.
- The text box “External resistance (R)” is used to enter the resistance of the mentioned resistor, which separates the external voltage source and the previously specified electrode of the system.
- The text box “External capacitance (C)” is used to enter capacitance of the external circuit (that capacitance is connected in parallel with the simulated system).
- The drop-down list “Time dependence of the external voltage source potential” is used to select one of four standard time dependences: “Constant voltage”, “Periodic square pulse sequence”, “Linear variation” and “Sine function”. The instantaneous value of potential U_2 of the external source pole, which is connected to the previously specified electrode of the system via the resistor R, is equal to the sum of the previously specified initial value and the selected time dependence.
- The remaining text boxes are used to enter parameters of the selected time dependence (e.g., period, pulse height, etc.). If all parameters of the time dependence are zero, then the corresponding time dependence is also assumed to be zero. If at least one parameter is non-zero, then the parameter editor checks if the parameter values satisfy the restrictions that may exist in the context of the selected time dependence (for example, if the periodic square pulse sequence is selected, then pulse duration must be less than the period of the sequence). If a parameter value is outside those bounds, then a corresponding error message appears.

10. Initial carrier distribution

The parameter sheet "Initial carrier distribution" is used to define the initial coordinate dependence of concentrations of free charge carriers as well as the initial charge state of bulk and interface traps. An example of this parameter sheet is shown in Fig. 16. Below are explanations of all controls of this parameter sheet:

- The group of controls "Initial concentration of free charge carriers" is used to specify initial coordinate dependence of concentrations of all free charge carriers of the current layer. After selecting a free carrier type in the drop-down list "Selected charge carriers", a method of calculating the mentioned dependence must be selected in the drop-down list "Initial carrier concentration". There are 2 choices:

  1) Constant concentration. In this case, the concentration value must be entered in the nearby text box.

  2) A concentration value proportional to concentration of one type of bulk traps belonging to the same layer (the "reference traps"). In this case, another drop down list appears on the right of the mentioned text box. That drop-down list contains the names of all bulk traps belonging to the same layer as the selected free charge carriers. The reference bulk traps must be selected in that drop-down list, and the proportionality factor must be entered in the mentioned text box (see Fig. 16).
- The group of controls "Initial filling of bulk traps" is used to specify the initial charge state of all bulk traps of the current layer. After selecting a bulk trap type in the drop-down list "Selected bulk traps", the initial charge state must be specified using the controls that are below. The two radio buttons make it possible to select either a single charge state for all traps of the selected type, or two possible charge states. In the latter case, the method of calculating the fraction of traps of each charge state must be selected in the drop-down list "Concentration of traps with specified charge". The selected method is only applied to one charge state (which is indicated by radio buttons that are under the two text fields where those charge values must be entered). Two choices are available: a constant concentration, or a constant fraction of the total concentration (which may be coordinate dependent, as explained in Section 5). That constant concentration, or the value of the mentioned fraction, must be entered in the text box that is to the right of the mentioned drop-down list. If this charge state is called the "first" one, then concentration of the "second" charge state will be calculated by subtracting concentration of the first charge state from the total trap concentration.
- The group of controls "Initial filling of interface traps" is used to specify the initial charge state of all interface traps of the current layer. Those controls are identical in function and appearance to controls of the group "Initial filling of bulk traps", which are described above (the only difference is that the bulk trap concentration is replaced by the surface density of interface traps).

Fig. 16. An example of the parameter sheet "Initial carrier distribution"

11. Layer thickness and other parameters

The parameter sheet "Layer thickness and other parameters" is used to specify thickness of each layer of the simulated multi-layer system as well as all parameters that do not belong to any of the previously mentioned categories. In the current version of the model (v0.75), that parameter sheet contains only two parameters: layer thickness and high-frequency dielectric permittivity of the layer (see Fig. 17).

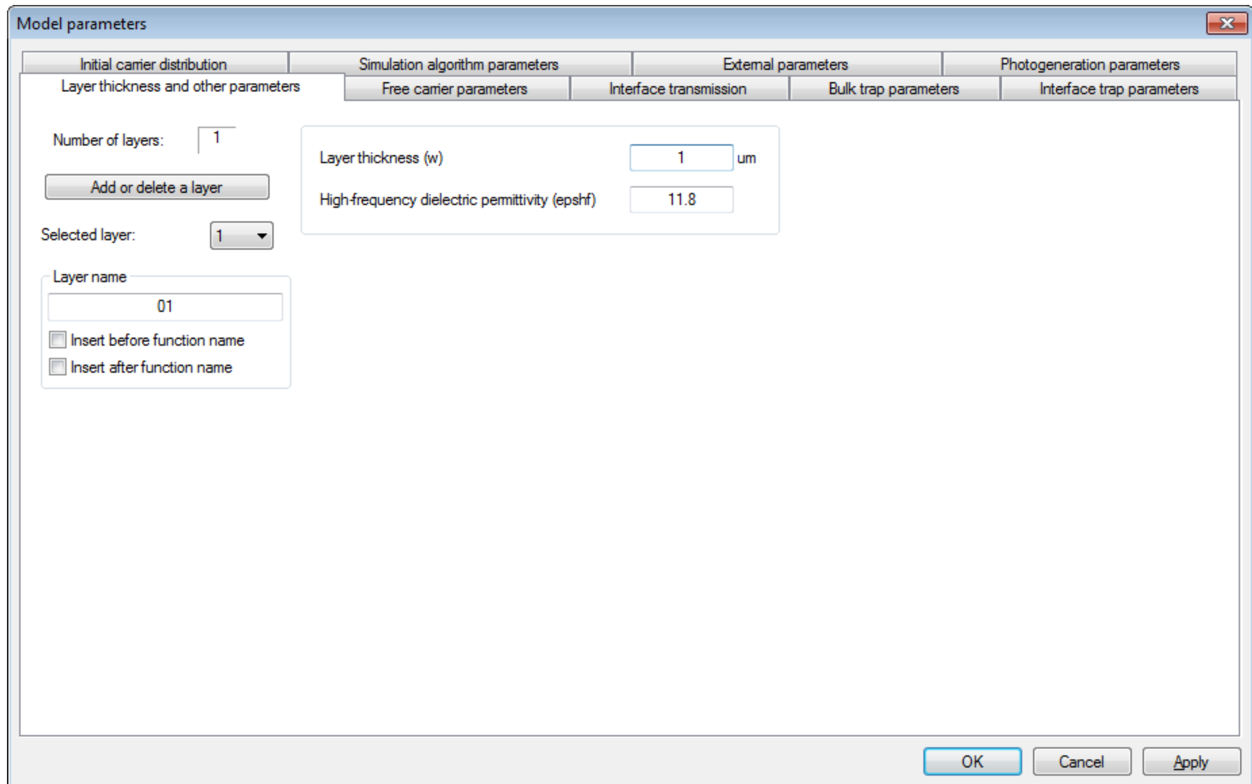


Fig. 17. An example of the parameter sheet "Layer thickness and other parameters"

12. Model functions

"Model functions" are the quantities that are computed by the simulator plug-in and stored in computer memory by the program GraphiXT. Most of those quantities characterize the state of the simulated system, but there are also several functions that characterize the computation procedure itself. The functions can be divided into two categories according to their arguments: $f(t)$ functions, whose only argument is time t, and $f(x, t)$ functions, which have two arguments – coordinate x and time t. Further on, $f(t)$ functions will be called "time functions", and $f(x, t)$ functions will be called "coordinate functions".

In addition, all model functions can be categorized according to a different criterion:

1) "global" functions, which are computed always, regardless of the details of the simulated system (the coordinate x values corresponding to stored values of the "global" coordinate functions coincide with node coordinates of all layers of the system);
2) "layer" functions, which are computed for each layer – even for empty layers (the coordinate x values corresponding to stored values of the "layer" coordinate functions coincide with node coordinates of the corresponding layer);
3) "object" functions, which are associated with specific parameter sets, e.g., with carriers of a particular type (since each "object" belongs to a particular layer, the coordinate x values corresponding to stored values of the "object" coordinate functions coincide with node coordinates of the same layer).

The default names of all functions are given below. Those names include the measurement units, which are written according to the same rules as model parameter units (see Section 2).

Note: The quote symbols ("…") that appear in some function names given in tables below are only for clarity (they do not appear in actual function names).

1) **Global functions:**

1a) Global coordinate functions:

Name	**Meaning**
Space charge density (e/cm^3)	Electric space charge density
Electric field (V/cm)	Electric field strength (a negative value means that the electric field vector is directed in the negative direction of the X axis)
Potential (V)	Electrostatic potential
Conduction current density (A/cm^2)	The sum of drift and diffusion current densities of all free charge carriers

1b) Global time functions:

Name	**Meaning**
Electric charge (e/cm^2)	The total electric charge of the system (the sum of the integral of space charge density over the width of the system and all surface charge densities, excluding electrode charges)
Total current density (A/cm^2)	The sum of conduction and displacement current densities
Total current (A)	The product of the total current density and the electrode area
External voltage source current (A)	The resistor R current i_R (see Fig. 15a and Fig. 15b)
External capacitor current (A)	The capacitor C current i_C (see Fig. 15a and Fig. 15b)
External photon flux density (1/cm^2/s)	Number of photons incident on unit area per unit time
Simulation time step (s)	The value of the last simulation time step Δt
Processing time of one time step of the simulation (s)	The processing time of the last simulation time step
Number of simulation threads	The number of active simulation threads
Total processing time (s)	The total processing time
Total number of simulation time steps	The total number of simulation time steps
Left electrode surface charge density (e/cm^2)	The left electrode surface charge density
Right electrode surface charge density (e/cm^2)	The right electrode surface charge density
External voltage source potential (V)	The potential U_2 (see Fig. 15a and Fig. 15b)
Voltage drop in the external resistor (V)	If the right electrode potential is varied, then the potential difference $U_1 - U_2$ (see Fig. 15a), and if the left electrode potential is varied, then $U_2 - U_0$ (see Fig. 15b)
Potential of the left edge of the system (V)	Potential of the point corresponding to the minimum value of the coordinate x (in Fig. 15a and Fig. 15b, it is denoted U_0)
Left edge surface charge density (e/cm^2)	The total surface charge density of the left edge of the system (it includes the charge of the interface traps and the "free surface charge", which was defined in Section 8)
Left edge free surface charge density (e/cm^2)	Free surface charge density of the left edge of the system

2) Layer functions:

2a) Layer coordinate functions:

Name	Meaning
Interval between nodes (um)	The distance between the node that is at a given point and the nearest node on the left (μm)

2b) Layer time functions:

Name	Meaning
Number of nodes in the layer	The number of nodes in the layer (the first and last nodes are on the opposite surfaces of the layer)
Right edge surface charge density (e/cm^2)	The total surface charge density of the right edge of the given layer (it includes the charge of the interface traps and the "free surface charge", which was defined in Section 8). If that edge is the interface between two simulated layers (i.e., if it is not the right edge of the entire system), then surface charges of both layers are taken into account. *Note*: This charge does not include the polarization surface charge caused by the difference of high-frequency dielectric permittivities of the layers.
Right edge free surface charge density (e/cm^2)	Free surface charge density of the right edge of the given layer. If that edge is the interface between two simulated layers (i.e., if it is not the right edge of the entire system), then free surface charges of both layers are taken into account.
Average space charge density (e/cm^3)	Average space charge density
Average electric field (V/cm)	Average electric field strength
Right edge potential (V)	Potential of the right edge of the given layer
Right- and left-edge potential difference (V)	Difference between potentials of the right edge and the left edge of the given layer
Average conduction current density (A/cm^2)	The average conduction current density, taking into account all free charge carriers of the given layer

3) Object functions:

3a) Object coordinate functions:

Functions corresponding to free charge carriers (in this table, "A" stands for the carrier name, which must be specified by the user):

Name	Meaning
"A" concentration (1/cm^3)	Concentration of charge carriers "A"
"A" current density (A/cm^2)	Conduction current density of charge carriers "A", i.e., the sum of drift and diffusion current densities, given by the formula (1.2)
"A" drift cur. dens. (A/cm^2)	Drift current density of charge carriers "A", i.e., the first term in the expression (1.2)
"A" dif. cur. dens. (A/cm^2)	Diffusion current density of charge carriers "A", i.e., the second term in the expression (1.2)
"A" mobility (cm^2/V/s)	Charge carrier "A" mobility
"A" conc. gradient (1/cm^4)	Derivative of charge carrier "A" concentration with respect to coordinate x

Functions corresponding to processes of bipolar recombination or generation of free charge carriers and charge carrier "transmutations" (i.e., processes that change the type of a free charge carrier, but do not change its charge). Those functions have the meaning of a process rate, i.e., the number of elementary events per unit volume and unit time. The default name of those functions is "P rate (1/s/cm^3)", where "P" stands for the name of the given process. The process name is specified by the user (also see Section 2 "Introduction to user interface"). The function names corresponding to the default process names are given in the table below (in this table, "A" and "B" stand for the short names of the primary and secondary charge carriers, which are specified by the user).

Name	Meaning
“A”-“B” recombination rate (1/s/cm^3)	Bipolar recombination rate
“A”-“B” generation rate (1/s/cm^3)	Bipolar generation rate
“A” -> “B” rate (1/s/cm^3)	The rate of charge carrier “A” transmutation into the charge carriers “B”
“A”-“B” photogeneration rate (1/s/cm^3)	Photogeneration rate

Functions corresponding to bulk traps (in the table below, “A” stands for the trap name, which is specified by the user):

Name	Meaning
“A” concentration (1/cm^3)	Concentration of bulk traps “A”
“A” charge density (e/cm^3)	Space charge density of bulk traps “A”, taking into account all charge states of those traps

Functions corresponding to charge states of bulk traps (in the table below, “A” stands for the trap name, which is specified by the user, and “Q” is an integer number indicating the charge state):

Name	Meaning
“A” (Q) concentration (1/cm^3)	Concentration of bulk traps “A”, whose charge is equal to *Q* elementary charges

Functions corresponding to processes of charge carrier capture into bulk traps and release from them. Those functions have the meaning of a process rate, i.e., the number of elementary events per unit volume and unit time. The default name of those functions is “P rate (1/s/cm^3)”, where “P” stands for the name of the given process. The process name is specified by the user (also see Section 2 “Introduction to user interface”). The function names corresponding to the default process names are given in the table below (in this table, “A” and “B” stand for the short names of bulk traps and free charge carriers, respectively, and “Q” is an integer number indicating the initial charge state of those traps):

Name	Meaning
“A” (Q) <- “B” capture rate (1/s/cm^3)	The rate of capture of charge carriers “B” into bulk traps “A”, whose charge is equal to *Q* elementary charges (this is the trap charge prior to capturing the charge carrier)
“A” (Q) -> “B” release rate (1/s/cm^3)	The rate of release of charge carriers “B” from bulk traps “A”, whose charge is equal to *Q* elementary charges (this is the trap charge prior to releasing the charge carrier)

3b) Object time functions:

Functions corresponding to interface traps (in the table below, “A” stands for the interface trap name, which is specified by the user):

Name	Meaning
“A” conc. (1/cm^2)	Surface density of interface traps “A”
“A” charge dens. (e/cm^2)	Surface charge density of interface traps “A”

Functions corresponding to charge states of interface traps (in the table below, “A” stands for the trap name, which is specified by the user, and “Q” is an integer number indicating the charge state):

Name	Meaning
“A (Q)” conc. (1/cm^2)	Surface density of interface traps “A”, whose charge is equal to *Q* elementary charges

Functions corresponding to processes of charge carrier capture into interface traps and release from them. Those functions have the meaning of a process rate, i.e., the number of elementary events per unit area and unit time. The default name of those functions is “P rate (1/s/cm^2)”, where “P” stands for the name of the given process. The process name is specified by the user (also see Section 2 “Introduction to user interface”). The function names corresponding to the default process names are given in the table below (in this table, “A” and “B” stand for the short names of interface traps and free charge carriers, respectively, and “Q” is an integer number indicating the initial charge state of those traps):

Name	Meaning
“A” (Q) <- “B” capture rate (1/s/cm^2)	The rate of capture of charge carriers “B” into interface traps “A”, whose charge is equal to *Q* elementary charges (this is the trap charge prior to capturing the charge carrier)
“A” (Q) -> “B” release rate (1/s/cm^2)	The rate of release of charge carriers “B” from interface traps “A”, whose charge is equal to *Q* elementary charges (this is the trap charge prior to releasing the charge carrier)

Note: If the given interface traps are at both edges of the layer, then each of the latter five functions is replaced by a pair of functions: one function for each edge of the layer. The name of the function corresponding to the left edge of the layer is obtained by adding the symbol “|< |” to the name defined above. The name of the function corresponding to the right edge of the layer is obtained by adding the symbol “| >|” to the name defined above.

In addition, for each “object” coordinate function there is a corresponding time function, which is equal to the average value of that coordinate function over the layer where it is defined. The name of that time function is obtained by inserting the abbreviation “avg.” into the coordinate function name (e.g., “Electron avg. concentration (1/cm^3)”).

It is possible to insert the layer name into the names of all “layer” and “object” functions defined in that layer. This is done using the checkboxes “Insert before function name” and “Insert after function name”, which are on the left side of some parameter sheets, under the text box with the layer name (see Fig. 1). This option may be useful if two or more layers of the system contain objects (i.e., carriers, traps, etc.) with identical names. For example, if there are two layers containing charge carriers of the type “Electron”, then, after selecting the GraphiXT menu command “Select f(x, t=const) functions…”, the function selection list will contain two functions with identical names “Electron concentration (1/cm^3)”. If the names of different layers are different, then such identical function names can be eliminated by inserting the layer name into them. Then it is easier to distinguish between functions corresponding to different layers. The default layer name is the layer number. The corresponding C format specifier is “%02d”. That format specifier corresponds to an integer number consisting of at least two digits, and if that number is less than 10, then the first digit is 0 (the format specifications are also mentioned in Section 2 “Introduction to user interface”). In the just-mentioned example, after checking the checkbox “Insert before function name”, the names of the mentioned two functions would become “01: Electron concentration (1/cm^3)” and “02: Electron concentration (1/cm^3)”. It is sufficient to check that checkbox in one parameter sheet only.

Note: After checking or un-checking the checkbox “Insert before function name” or “Insert after function name”, the names of all functions of the corresponding layer will become equal to default names. I.e., all changes of function names that were made in the program GraphXT.exe will be lost (only the changes made in the parameter editor will be retained).

After changing the name of a parameter set, the names of “object” functions corresponding to that parameter set also become equal to default names.

After changing the number or meaning of model functions (e.g., by inserting or removing a layer or a parameter set), the names of all “layer” functions become equal to default names.