List of changes in the GraphiXT plug-in for simulating charge carrier kinetics

Below is the list of changes for each version of the files CarrierFunc.dll and CarrierParms.exe that was available for download from www.graphixt.com , up to the current version, i.e.,

CarrierFunc.dll	v.0.75.19.4
CarrierParms.exe	v.0.75.15.4

Explanation of the version number format:

CarrierFunc:	XX.YY.ZZ.F
CarrierParms:	XX.YY.VV.P
GraphiXT:	AA.BB.F.P

The first two components (XX.YY) indicate the set of parameters and functions that define the simulation model. Thus, XX.YY can be called the "model version number". The numbers XX and YY only increase after adding or removing model parameters and functions or after changing the meanings of model parameters and functions. Those two numbers must be the same both for the function file and the parameter editor, because both those programs must correspond to the same set of model parameters and functions. The third component of the function file version number (ZZ) increases after improving the simulation algorithm or fixing simulation bugs. The third component of the parameter editor version number (VV) increases after improving the parameter editor user interface or fixing its bugs or revising the documentation of the simulator plug-in. After increase of any of the first two numbers (XX or YY), the third number (ZZ and VV) becomes equal to 10 or to a smaller value. The fourth components of the CarrierFunc.dll and CarrierParms.exe version numbers (F and P) indicate compatibility of those files with the program GraphiXT.exe. Thus, F and P can be called the "program interface version numbers" of the function file and the parameter editor, respectively. Those two numbers only change after a change in the rules of communication between GraphiXT.exe and the other two programs. In order to be able to load the files CarrierFunc.dll and CarrierParms.exe, the number F must coincide with the third component of the GraphiXT version number, and the number P must coincide with the fourth component of the GraphiXT version number.

All changes are grouped into three groups:

I. Changes of the number or meaning of model parameters and model functions (those changes are common to both mentioned programs; they are reflected by a change of the first two components of the version number).

II. Changes of the program CarrierFunc.dll that are related to improving the simulation algorithm and fixing the simulation bugs (those changes are reflected by a change of the third and fourth components of the CarrierFunc.dll version number).

III. Changes of the program CarrierParms.exe that are related to improvements of the parameter editor user interface, fixing its bugs and revising the documentation of the simulator plug-in (those changes are reflected by a change of the third and fourth components of the CarrierParms.exe version number).

In the following list of changes, the differences between the indicated version and the previous version are listed. Note: the changes given for the first entries (CarrierFunc.dll v.0.75.15.4 and CarrierParms.exe v.0.75.13.3) are the differences from the first English version (CarrierFunc.dll v.0.75.11.4 and CarrierParms.exe v.0.75.11.2), which was released in February, 2012.

I. Changes of the number or meaning of model parameters and functions

Currently – none.

II. Changes of the program CarrierFunc.dll related to optimizing the computation algorithm and fixing the simulation bugs

CarrierFunc.dll **0.75.15.4** (2012-07-06):

Multithreaded operation mode has been optimized (the percent decrease of the simulation time in comparison with the previous version is up to 10 %).

Detection of the stationary state has been improved.

In the current version, the CarrierFunc.dll build date is passed to the program GraphiXT.

A bug causing the absence of light absorptions coefficients and bulk trap region parameters from the GraphiXT nonlinear fitting dialog has been fixed.

CarrierFunc.dll **0.75.16.4** (2012-07-29):

A bug when computing charge carrier capture or release rate from interface traps belonging to an adjacent layer has been fixed.

CarrierFunc.dll **0.75.17.4** (2012-08-11):

A bug when calculating the processing time of one time step of the simulation has been fixed (because of that bug, the processing time of one time step was set to 1.#INF when a fixed number of simulation threads was used).

CarrierFunc.dll **0.75.18.4** (2012-08-31):

A bug causing a slight change of the next computed model time when the simulation is resumed after an interruption has been fixed.

CarrierFunc.dll **0.75.19.4** (2013-06-19):

If a single-layer system is being simulated, then no memory is assigned to x values corresponding to layer No. 0 (which is a "formal" layer, unlike the "true" layer No. 1, as explained in the "User Manual"), because in such a case layers No. 0 and No. 1 share the same set of node coordinates. If the number of "true" layers is greater than 1, or if an older version of GraphiXT is used (prior to v.1.17), then CarrierFunc.dll works as before, i.e., allocates memory for x values corresponding to layer No. 0. In the case of a multilayer system, the set of x values of layer No. 0 is the union of the sets of x values of all "true" layers of the system.

III. Changes of the program CarrierParms.exe related to improvements of the user interface and bug fixes

CarrierParms.exe **0.75.13.3** (2012-07-06):

It is no longer possible to enter zero charge of the free charge carriers.

After the user modifies the model parameters, the current version informs GraphiXT if the parameter change is major (i.e., the number or meaning of model parameters has changed), or if it is minor (i.e., only the values of existing parameters have changed)

In the current version, the CarrierParms.exe build date is passed to the program GraphiXT.

Minor changes in the dialog format (positions of various controls).

The simulator documentation (file "Charge carrier kinetics - _GraphiXT plugin_ - User Manual.pdf") has been revised. The introduction has been expanded, three sections have been added: "Interface trap parameters", "Initial carrier distribution", "Layer thickness and other parameters".

CarrierParms.exe **0.75.13.4** (2012-07-29):

If a dialog window with a list of model functions or with their properties is open in GraphiXT, then major modifications of model parameter values done in the parameter editor are not accepted until the user closes that dialog.

CarrierParms.exe **0.75.14.4** (2013-06-19):

The names of some controls in the parameter sheets have been changed.

CarrierParms.exe **0.75.15.4** (2013-10-20):

Photogeneration quantum yield is now allowed to be greater than 1. This is possible if the final number of free charge carriers includes not only charge carriers created in the initial interaction event, but also secondary charge carriers that are created later (for example, when free carriers created by incident photons have enough energy to ionize other atoms of the material, or when a single photon is incoherently scattered several times and releases an electron from an atom during each scattering event).