SiLENSe™

Simulator of Light Emitters based on Nitride Semiconductors

User Manual

Version 6.5 & Version 6.5 Laser Edition

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1 Overview

SiLENSe software enables one-dimensional (1D) simulation of heterostructures used in light-emitting diodes (LEDs) and laser diodes (LDs). The structure can include tunnel junctions. The software simulates band diagram as a function of the applied bias, distribution of electron and hole concentrations, electron and hole current density, radiative and non-radiative recombination rates, carrier energy levels and wave functions in the quantum wells, emission and gain spectra, internal quantum efficiency (IQE), injection efficiency, etc. Mechanical strain due to lattice mismatch between epilayers is calculated and its effect on the band structure is included into the model.

Built-in database of material properties includes both zinc-blende (cubic) and wurtzite materials, such as AlInGaN, AlGaInAs, AlGaInP, and others. Specific features of III-nitride materials like strong piezoeffect, spontaneous electric polarization, low efficiency of acceptor activation, and high threading dislocation density inherent in III-nitride epitaxial layers are included into the model. The software enables the analysis of graded-index heterostructures, which is important for development of novel semiconductor devices by using the bandgap engineering principles.

Laser Edition of the package also enables computation of the waveguide modes and prediction of the threshold characteristics.

The software includes a graphical user interface for specification of the input data, starting and controlling computations, and built-in visualization of the results (they also can be exported in text format for import into any other visualization package). This document is aimed in detailed description of the user interface, while the physical model is described in "Physics Summary" document.

1.1 SiLENSe Options

The current version of **SiLENSe** package provides the following options:

- Calculation of the band diagram, current, internal quantum efficiency etc. for a given bias. One can also set up series computations to cover some range of the bias variation.
- Calculation of the carrier wave functions, and the emission and gain spectra from the known band diagram.

- Plot an integral characteristics of the LED operation for all the computed biases, such as I-V curves etc.
- Simulation of structure operation under external optical excitation (PL simulations).
- Simulation of characteristics of individual tunnel junctions includes into the structure.

The following options are available in **Laser Edition** only:

- Computation and visualization of the waveguide mode intensity distribution for both TE and TM polarizations with account for the birefringence in wurtzite crystals. Computation of the optical confinement factors.
- Analysis of the laser diode operation for selected waveguide mode:
    1. Optical gain.
    2. Optical losses caused by the free carrier absorption.
    3. Threshold current and laser output power.

2 Installation and Registration

2.1 Installation

To install the **SiLENSe** , run the installation executable file and follow the installer instructions. To uninstall the program, run the `unins000.exe` file in the program home directory or use the respective item in the *Programs* menu.

The software is supplied with license protection system based on dongle key which is a small USB device. During installation, the user is prompted to install the dongle key driver. Local administrator rights are required to install the dongle driver.

The software needs write permission for its home directory. During installation, the parameters of the home directory are changed accordingly.

2.2 Single node license

The user can install the software on several computers, for example, on a desktop and a notebook. The software will run only if a dongle key with a valid license is plugged into the computer. There is a limitation for maximum number of software copies running simultaneously (default is 4). The registration procedure is as follows:

- Plug in the dongle key module.
- Start the license manager (`License.exe`) located in the home directory. One can also do it by Windows *Start* button.

- Choose the *Key config* tab and press the *Make Key* button. The request file (*.req) containing the information about the dongle will be generated.
- Send the generated request file to STR by e-mail simuled-support@str-soft.com .
- When a reply from STR is received, plug in the dongle, start the license manager, press *Accept Key* button, and browse fro the license file (*.lic) received from STR.
- Now one can run **SiLENSe**.

2.3 Corporate/department network license

Corporate/department license allows users running the software on several computers within the local area network (LAN). The software may be installed on any computer of the network, but the maximum number of running copies of the software is limited by a certain number, e.g. 10, specified in the particular license agreement (quotation, purchase order, etc.).

Hereafter, by 'server' we will understand the computer where the USB dongle key is plugged in. The user should install the dongle key driver on this computer. A special tool `server.exe` called below 'license server' should be running on the server computer. After start, the respective icon appears in the system tray. The pop-up menu allows one to restore the window and inspect the event log or the license server. The *Change Port* button allows the user choose the port number for communication between the software running on other computers and the license server.

To obtain/update the license, on need run the `License.exe` file on the server computer. Further procedure is similar to that described in Sec. 2.2 .

All the computers running the **SiLENSe** software we will call 'client computers' (running the software on the server computer is also allowed). Installation of the software on the client computers is similar to Sec. 2.1, while there is no need to install the dongle key driver on client computers. Instead, one should run the `License.exe` file, choose *Server config* tab, and specify the IP address of the server computer and the port number. The *Store* button saves this information in the `Str_Config_SL.cfg` file in the software home directory. This file is used by the software to communicate with the license server. The *Remove* button clears the file. The *Test* button allows one to test the communication with the license server.

NB The following conditions to be fulfilled for running the software on a certain client computer: (i) the dongle key to be plugged into the server computer, (ii) the license server to be running on the server computer, and (iii) the software running on the client computer to

be able to communicate with the license server by the IP address and port number specified in the `Str_Config_SL.cfg` file in the software home directory.

NB Unplugging the dongle key from the server computer or stopping the license server will result in abnormal termination of all the running software copies!

3 Getting Started

SiLENSe project files have `*.sls` extension and store the following information:

- Heterostructure, i.e. sequence of layers, their composition, doping, etc.
- Global physical and solver parameters
- Material properties
- Simulation results

NB The software is designed in such a way that all the simulation results stored in the project file are always self-consistent with the input data. So the user can not modify the heterostructure and some global parameters like the temperature if there are some results stored (see description of the Tools->*Unlock Project* menu item).

3.1 Materials Properties

There is a special **Properties Editor** tool for editing the materials properties (see detailed description in Sec. 7). It provides a unified way to set up the material properties of binary semiconductor compounds and their alloys. The material properties are saved in the special project file of the **Properties Editor** (`*.matprop`). All the computational modules of **SiLENSe** load material properties from these files.

Generally, the materials are split into two types: (i) materials of fixed chemical composition, like GaN, GaAs, InP, etc. and (ii) alloys with variable composition, like $Al_xIn_yGa_{1-x-y}N$, $Al_xGa_{1-x}As$, etc.

The default database of the material properties is supplied with **SiLENSe**, but users can modify the material properties or add new materials and alloys.

Creating a new **SiLENSe** project file, one should specify the **Properties Editor** project file (or another **SiLENSe** project file) from which the material properties will be loaded. In the

Material properties tab window, the loaded values are shown in the read-only mode, but one can use *Material Properties -> Edit* menu item to change the data.

3.2 Heterostructure

A heterostructure is described as a sequence of layers. For each layer, one should specify the thickness, material composition, doping, and other parameters which can not be calculated from the composition.

NB The heterostructure layers can be listed from bottom to top or from top to bottom. User needs to choose the appropriate crystal orientation in the *Heterostructure* tab window and appropriate direction of current in *Global parameters* tab window.

NB As **SiLENSe** is aimed in simulation of the active region, only central part of the heterostructure can be specified, starting from n-type current spreading layer to p-type current spreading layer. Also, the thickness of the current spreading layers can be reduced down to ~500 nm in order to speed up the computations.

NB The simulations are 1D and the current is assumed to flow through the while structure. So for structures grown on insulating substrates, such as GaN on sapphire, the substrate and nucleation/buffer layer(s) should not be included into the simulation.

3.3 Global Parameters

In the *Global parameters* tab window, the user can specify some global physical parameters, such as the junction temperature and some internal solver parameters controlling the numerical computations. The parameters related to analysis of laser diodes are shown in the *Laser parameters* tab window. A default set of the parameters is loaded automatically in a new project. The solver parameters are discussed in details in Sec. 5.6.

3.4 Running the Calculations

Most of the calculations can be started from the *Run* menu. Some of the *Run* menu items are duplicated by the respective buttons in the toolbar and/or hot keys. The menu item ‘Stop’ allows the user to abort current calculation. The calculation of the emission and gain spectra can be started from the *LED Results* or *Laser results* or *PL Results* windows. One can open them by the respective items in *Window* menu or by the respective button in the toolbar.

3.4.1 Band Diagram and Carrier Fluxes

To start single calculation of the band diagram, use the *Single Calculation* menu item. The modal window appears where you will be prompted to enter the p-n junction bias and start

the computations. The solver window appears where the iterative solution process is described. The user can abort the computations by the *Stop* button. When the calculations are complete, the simulation results are shown in the *Results* tab window containing several plots. To switch between the plots, use the vertical tabs along the left side of the plots.

Series calculation menu item allows calculations for a number of bias values at once. The modal window appears with the list of biases which will be processed. The user can add a single bias by the *Add* button, while the *Add sequence* button enables one to add a sequence of biases varying from the *Start bias* to the *End bias* with a given *Number of intervals.* The entered biases can be edited or deleted by the buttons *Edit* and *Delete*, respectively. Use the button *Delete All* to clear the list.

Series calculation for SpeCLED menu item allows automatic computations for a given range of the p-n junction bias and temperature. List of biases is specified exactly as for series calculations, and the temperature list is specified in a similar way. When computations are completed, a .txt file with the name similar to the .sls name is generated. This file includes the tabulated dependence of the key parameters (current density, IQE, emission wavelength, etc.) on the applied bias and temperature. This file can be imported into **SpeCLED** software for 3D simulation of the current spreading and heat transfer in the LED chip.

NB The data for **SpeCLED** module should cover the whole range of the current density and temperature expected during 3D chip simulation. The recommended bias step is 0.01-0.05 V (it is OK not to run computations for the current density far below than that of interest). The recommended step for the temperature is 5-20 K.

3.4.2 Carrier Wave Functions, and Emission and Gain Spectra

The carrier wave functions, and the emission and gain spectra are calculated from the already known band diagram. To start the calculation, one should open the *LED/Laser/PL Results* window, select the desired bias, and use the *Run* | *Wave functions and spectrum* menu item or the respective button. The results are displayed in the *Spectrum* tab window containing two tabs with plots, *Band diagram and wave function* and *Spectrum*.

The list of individual quantum wells appears on the right of the former plot. An individual quantum well can be selected in the graph by the vertical cyan stripe initially located in the first quantum well. This stripe can be moved from one well to another either by choice of the

well number with the mouse in the quantum well list or by pressing the keys "→", "←", "↑", and "↓" on the keyboard.

The list of the localized state energies of the carrier in the selected quantum well is given in the mini-windows on the right of the quantum wells list. To show/hide the wave functions in the main graph, use the check boxes in the mini-windows *Electrons*, *Heavy holes*, *Light holes*, and *Split-off holes*, where the energies of the respective energy states are indicated.

The *Spectrum* plot shows the emission and gain spectra of individual quantum wells, as well as the total spectra. The user can switch the values of X-axis between the photon energy and the wavelength by the respective tab.

3.4.3 I-V Characteristic and Internal Quantum Efficiency

To get the I-V curve, one should open the *LED Results* window, select the desired biases, and use the *Show* | *I-V Characteristic* menu item or the respective button. The modal window appears with three plots. The former two plots represent the current density as a function of the bias and the internal quantum efficiency variation with the current density, respectively. The last plot is introduced to rely the calculated current density with experimentally observed I-V characteristics by qualitative accounting for the series and contact resistance. The user is prompted to specify the LED area, the series resistance, and the contact resistance for the n- and p-contacts. The current and voltage are calculated as described in Sec. 7 of [1].

3.4.4 Waveguide Modes

To compute the electric/magnetic filed distribution of the waveguide modes, one can use the *Run* | *Waveguide Modes* menu item. The modal window appears where one will be prompted to enter the light wavelength. When calculations are complete, the results are shown in the *Waveguide* tab window.

3.4.5 Laser Characteristics

To simulate operation of edge-emitting laser diodes, a number of additional parameters to be specified in the *Laser parameters* tab window: cavity dimensions, mirror reflectivity, polarization (TE/TM) and index of the mode (here one should choose the mode with highest optical confinement factor, which will reach the threshold first).

Run -> Single Calculation With Laser and *Run -> Series Calculation With Laser* menu items allows running simulations at specified bias (list of biases) with self-consistent account of stimulated recombination in the active region (the details are given in [1], Sec. 'Laser Characteristics'). Simulations will look similar to LED calculations, while results are stored into *Window -> Laser Results* and *Window -> Laser Characteristics* windows.

Run -> Laser Characteristics (Simplified Model) menu item allows to run a simplified laser model to compute the threshold current without self-consistent account of the stimulated recombination. The program will seek for the threshold performing calculation of the gain and loss for each bias and comparing them. The user can see the computation progress in the progress bar and stop calculations by the *Stop* button. Results are stored into *Window -> Laser Characteristics (Simplified Model)* window.

3.4.6 PL simulations

PL simulations be started by *Run* menu items *Run PL* and *Run PL Series*. User needs specify the excitation power density. PL simulations are stored in *Window -> PL Results* window and handled similar to simulations of the band diagram at the given bias. To get PL emission spectrum, one needs open list of PL results by using *Window -> PL Results* menu item, select the results for desired excitation power, and start simulation of the emission spectrum as described in Sec. 3.4.2.

3.4.7 Simulation of individual tunnel junction

One can start simulation of i-th tunnel junction by using *Run -> Run Tunnel Junction -> TJ#i* menu item or by selecting the tunnel junction in Heterostructure tab, using *Heterostructure -> Edit Tunnel Junction* menu item, and using *Run TJ button*. Then tunnel junction will be simulated for the specified range of bias and its j-V characteristic will be shown in the window with the tunnel junction parameters. If *Save TJ Results* checkbox is checked, the results (band diagram, carrier concentration, etc.) will be stored in the project file and can be inspected by using *Window -> Tunnel Junction Results -> TJ#i* menu item.

3.5 How to Load, Export, and Delete the Simulation Results

The project file contains some simulation results related to the project. The *Window* | *LED Results* menu item or the respective button opens the *LED Results* window with the table of the results which were stored in the project file or computed during the current session. The table includes an integral data like the bias, current, internal quantum efficiency etc. To load a result in the *Results* tab window, one should choose the result by single mouse click and use the *Show* | *Current result* menu item or the respective button. A double-click on the

respective row of the table has the same effect. One can use the *Edit* | *Delete selected* menu item or the respective button to delete results selected by the checkboxes in the left column.

The *Export* menu allows one to save the current result or the I-V curve as a text file. The output formats are described in details in Sec.5.

4 Graphical User Interface

The chapter describes the user's options available to control the data input, simulation of LED characteristics, and visualization of the simulation results within the Graphical User Interface (GUI).

4.1 Menu and Toolbar

The *Menu* contains the *File, Heterostructure, Material properties, Run, Export, Tools, Window,* and *Help* items. The *File* menu allows one to create new project, open an existing project, save changes in the current project file, and exit the program.

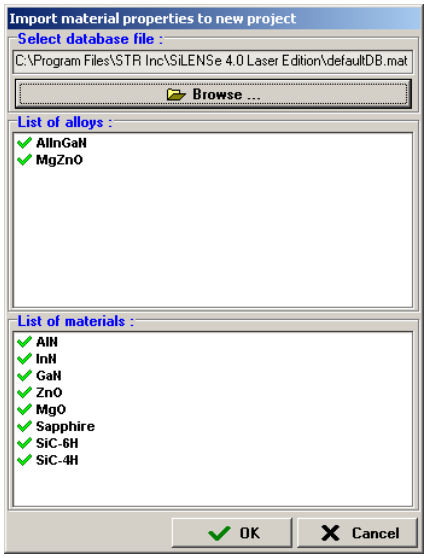


Fig. 1. Load material properties to the new project.

The menu item *New* is for creating new project. The modal window will appear where the user will be asked for the file with the material properties (see Sec. 3.1). The window also contains the lists of materials and alloys described in the selected file. The green tick and the red cross show if the respective item contains all the properties necessary for calculations.

The *Heterostructure* menu contains different operation with the heterostructure layers. Most of these actions are duplicated by the respective buttons in the *Heterostructure* tab window.

The *Material properties* menu allows the user to export the data from the current project to the separate material database file, overload the existent data from other **SiLENSe** project or material database file (import of the material properties), and open **Properties Editor** to edit the current dataset.

The *Run* | *Single computation* menu item starts single computation. The modal window appears where the user is prompted to input the bias. The *Run* | *Series computations* menu item allows one to perform a set of calculations for a number of bias values. The modal window appears with the list of biases which will be processed. The user can add a single bias by the *Add* button, while the *Add sequence* button enables one to add a sequence of biases varying from the *Start bias* to the *End bias* with a given *Number of intervals.* The entered biases can be edited or deleted by the buttons *Edit* and *Delete*, respectively. Use the button *Delete All* to clear the list.

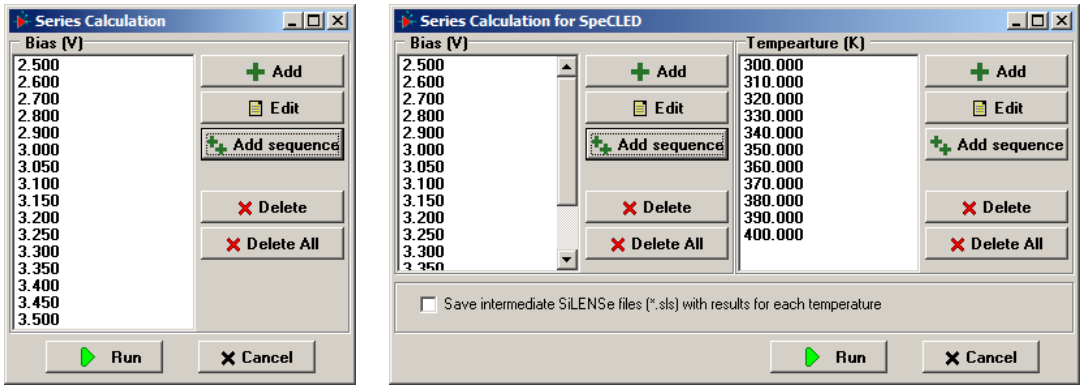


Fig. 2. Series calculations modal window (left) and series calculation for SpeCLED (right).

Series calculation for SpeCLED menu item allows automatic computations for a given range of the p-n junction bias and the temperature. List of biases is specified exactly as for series calculations, and the temperature list is specified in a similar way. Data for SpeCLED (a single *.txt file including key results for all temperatures) are generated automatically, and SiLENSe files (*.sls) with complete results are optionally saved for all temperatures.

During the computations, the bias values are indicated by colored rectangles. Grey color means that the calculation for the task has not been started, blue color marks the current task, successfully finished and failed tasks are shown by green and red colors, respectively.

The *Waveguide Modes* item of the *Run* menu allow one to start the computation of the waveguide modes.

The *Single Calculation With Laser* and *Series Calculation With Laser* items of the *Run* menu allow one to start simulation of the laser operation at the specified bias (or series of biases).

The *Run Tunnel Junction -> TJ#i* item of the *Run* menu allow one to start simulation of i-th tunnel junction according to the parameters specified for this tunnel junction. This menu item works similarly to the following sequence of actions: (i) select the tunnel junction in Heterostructure tab, (ii) use *Heterostructure -> Edit Tunnel Junction* menu item, and (iii) use *Run TJ button*.

The *Run PL* and *Run PL Series* items of the *Run* menu allow one to start simulation of PL experiment at the specified excitation power density (or for several powers).

The *Stop* item of the *Run* menu allows the user to abort current calculations.

Some of the *Run* menu items are duplicated by the respective buttons in the toolbar and/or hot keys.

NB The calculation of the emission spectrum and I-V curve to be started from the *LED Results* window.

The *Export* menu enables one to save computed results as a text file. The band diagram for a certain bias or the I-V curve to be exported from the *LED Results* window. *Save current chart* item allows the user to save current chart as a graphic file.

The *Tool* | *Unlock Project* menu item and the respective button in the toolbar are enabled only if there are some results computed during the current session or previously saved in the project file. Then the user can not modify the heterostructure and global physical parameters. This limitation is introduced to make sure that the input data and the simulation results are self-consistent. Use this item or the respective button to delete all the results and enable modification of the heterostructure and global physical parameters. The confirmation dialog appears with warning that all results will be deleted. To keep the results, the user

should (i) save the project to store the result obtained in the current session, (ii) save the project under a new name, and (iii) unlock the project and modify it.
The *Tool* | *View Iterations* menu item and the respective button in the toolbar allow one to inspect the iterative solution process. When this option is turned on, the plots in the *Results* tab window are updated after each iteration. However, it might make the computations slower.

The *Window* menu is to open other windows, such as solver window and different simulation results. The most important is the *LED Results* window containing a table of processed biases and some integral data like current density, internal quantum efficiency, etc.

The *Help* menu includes the *About* option providing the user with brief information on the version of the software and license.

The toolbar contains buttons for a quick access to the main options.

4.2 Tabs of the Main Window

4.2.1 Heterostructure

The *Heterostructure* tab window allows the user to specify the LED heterostructure considered to be a sequence of semiconductor layers (Fig. 3). To manage layers, one can use the *Heterostructure* menu items or buttons from the vertical toolbar in the left part of the tab. Use *Add Layer*, *Delete Layer*, *Edit Layer*, *Move Layer Up*, and *Move Layer Down* to create, delete, and move the layers. One can copy the selected layer into a buffer and insert the layer from the buffer after the selected layer by the buttons *Copy Layer* and *Insert Layer*, respectively.

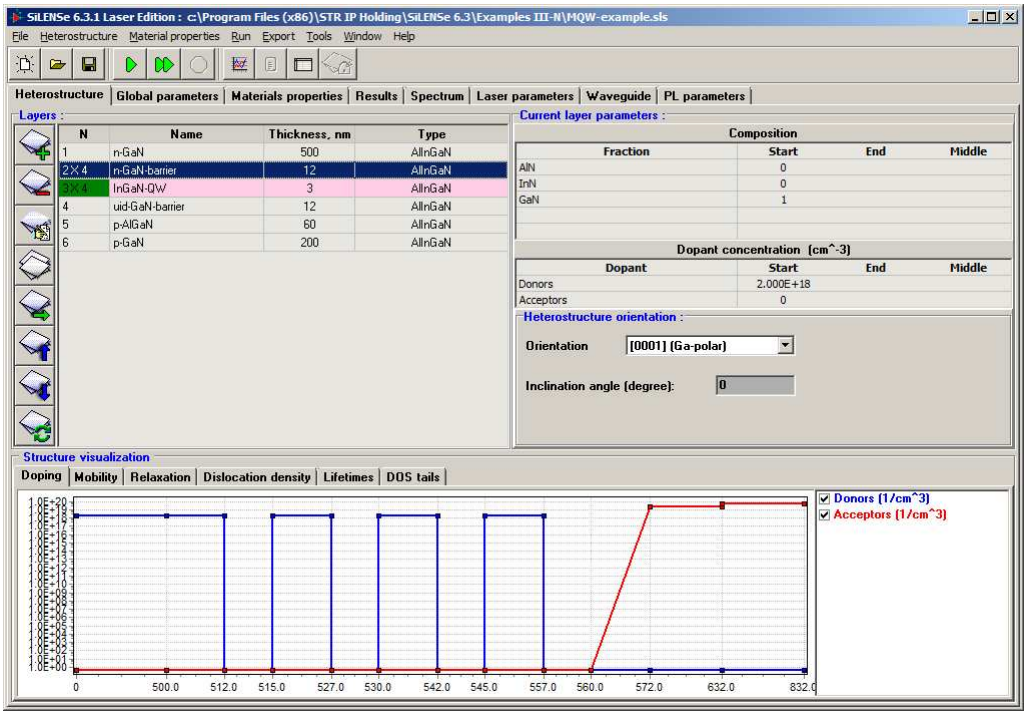


Fig. 3. Heterostructure tab window.

When the user clicks the *Add Layer* button, the pop-up menu appears where the material type should be chosen from the lists of available materials and alloys. The *Edit Layer* button allows one to edit the layer properties (Fig. 4). The *General properties* section contains the name[1], thickness, composition[2], doping, and mobilities of electrons and holes. One may view the specified composition profile by using the *Preview composition* button. The additional properties are the electron and hole lifetimes related to the point defects, relaxation parameters (degree of the strain relaxation at the left interface of the layer or the relaxed layer constant a), and dislocation density. Section *'Composition fluctuations'* allows the user to input parameters related to Indium composition fluctuations in InGaN material.

Layer composition and relaxed layer constant a may be specified by using a custom function, defined by user by a script or by a table which can be imported from a text file. To use function, one needs pick up the function name in the respective drop-down list. One can edit functions by using " Heterostructure->Functions" menu item.

1 The layer name is not used by the code and introduced just for convenience.

2 The composition is required only for layers made of alloys.

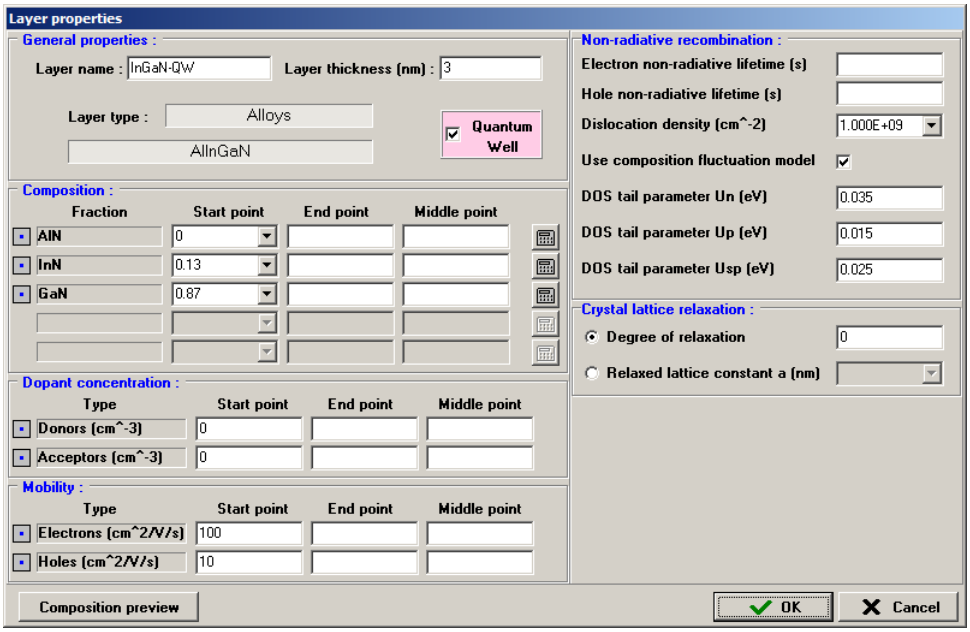


Fig. 4. *Layer properties* window.

One should mark quantum well (QW) layers by the checkbox *Quantum Well* in the *Layer properties* window. The marked quantum wells are indicated in the layer list by purple rows. Each “purple” region is treated as a separate QW.

Warning: The user is responsible for adequate selection of the quantum wells. If the QW consists of several layers (for example, triangular or trapezoidal QW) , all the layers should be marked as QW. It is recommended not to mark barriers as *Quantum Well* layers. In some special cases, one can mark barriers as QW layers to see the coupling between the QWs. The details are described in [1] in the section related to the spectrum calculation.

A *Periodic structure* button is introduced to simplify input of multiple quantum well structures. To create a periodic structure, one should select all layers in one period and use the *Periodic structure* button. The user is prompted to input a number of periods. When periodic structure is created, the number of periods is shown in the layer list, as seen in Fig. 3 for layers 5 and 6. To delete the periodic structure, one should use the *Periodic structure* button and input 0. The heterostructure can contain several periodic structures. Creating a new periodic structure overlapping with the existent ones will clear older periodic structures overlapping with a newly created one.

The *Orientation* combo box allows the user to specify the heterostructure orientation. For zinc-blende (cubic) materials, three orientations are supported: [001], [011], and [111]. For wurtzite III-nitride materials, along with conventional [0001] orientation, a number of nonpolar

and semipolar orientations are supported. Respective inclination angle is shown below the combo box. Choosing "Custom Inclination Angle" in the combo box allows one to specify a custom inclination angle in [0,180] range.

The bottom area of the *Heterostructure* window contains a plot representing variation of the following layer properties throughout the whole heterostructure: doping, mobility, degree of relaxation, dislocation density, lifetimes of recombination at point defects, and DOS tails. One can switch between the different variables by choosing the respective tabs.

4.2.2 Tunnel Junctions

Tunnel junction regions are highlighted in the table with heterostructure layers by grey color and index of the tunnel junction. Tunnel junction regions can not overlap with periodic structures or other tunnel junctions.

To create new tunnel junction region one needs select several adjacent layers in the table (similarly it is done for creating a periodic structure) and use *Heterostructure -> Create/Delete Tunnel Junction* menu item. If the selected range of layers overlaps with another tunnel junction or periodic structure, a dialog window will appear where user will be able to choose between three options:

- Delete old periodic structures and tunnel junctions and create a new tunnel junction in the selected range of layers
- Delete old periodic structures and tunnel junctions (this option enables deleting tunnel junctions)
- Cancel (quite dialog with no changes)

To delete tunnel junction one needs select a layer within the tunnel junction, use *Heterostructure -> Create/Delete Tunnel Junctio*n menu item, and choose *Delete old periodic structures and tunnel junctions* in the dialog.

To edit tunnel junction parameters, one needs select a layer within the tunnel junction and use *Heterostructure -> Edit Tunnel Junction* menu item. Then a window appears where one can set the parameters (Fig. 5). The button *Update Plot* plots the j-V curve of the tunnel junction. If *Simulation* type is chosen, it will cause simulation of the tunnel junction. J-V curve will be plotted in the same window. The band diagram, carrier concentrations, etc will be

saved in "*Results -> Tunnel Junctions -> TJ#i*" window if check box *Store TJ Results* is checked.

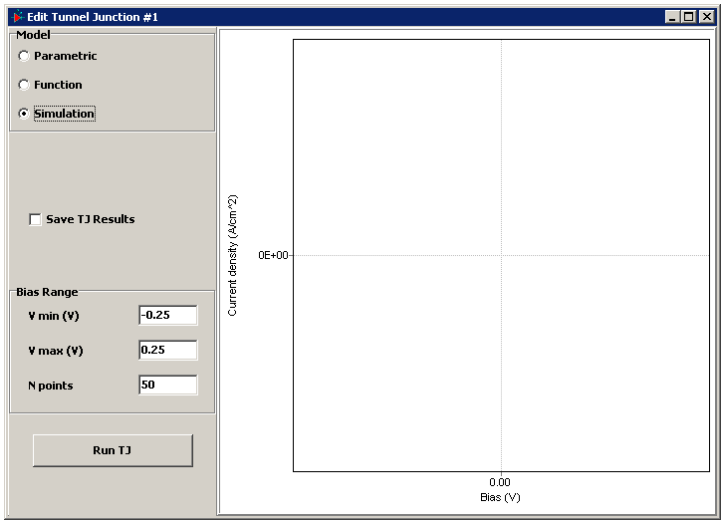


Fig. 5. Tunnel junction parameters window.

Briefly, tunnel junctions are included into simulations as following.

- First, the tunnel junction is simulated as a separate object, and dependence of the tunnel current on the local bias applied to the TJ is calculated. For each local bias, the band diagram of the tunnel junction region is calculated assuming Fermi levels to be constant and separated by the bias. Then the tunneling current is calculated in a conventional way. For each energy, the tunneling probability is calculated. The total tunneling current is calculated by integrating over the energy the product of the tunneling probability and factor describing presence of carriers at given energy. Alternatively, j-V characteristic of the tunnel junction can be specified by parametric approximation or user-defined function.
- Second, the whole heterostructure is simulated as usual, and the tunnel current is taken from the table generated at first step. Conventional drift-diffusion current in the tunnel junction region is also considered in the model.

NB When user starts simulation of the whole structure (LED, PL, laser), the simulation of all tunnel junctions included into the structure is started automatically. There is no need to start simulation of tunnel junctions manually prior to main simulation.

4.2.3 Import of the heterostructure from a STREEM output file

One can import the heterostructure from an output file of STR **STREEM InGaN** software by using *Heterostructure->Load Layers From STREEM file* menu item. Then the following procedure will be performs automatically:

- Old set of layers is deleted
- Old set of heterostructure functions is deleted
- According to the file, tabulated functions describing spatial variation of the layer composition and relaxed lattice constant ***a*** are created for each layer.
- New set of layers is created according to the layer specification in the file. For each layer, the material composition and relaxation are specified by using the respective functions. All other parameters contains default data and, generally, to be specified by the users.

NB After import of the heterostructure, user need specify all the parameters except to that imported from the file (composition and relaxation). Optionally, one can also add more layers, delete some layers, correct imported functions, or perform any other corrections of the input data.

4.2.4 Global Parameters

The *Global parameters* tab window (Fig. 6) represents the parameters applicable to the whole simulation and includes four subsections: *Physical parameters*, *Main solver parameters*, and *Spectrum solver parameters.*

Physical parameters are as following

- Temperature.
- Settings for the quantum potential model. One can switch it on/off, as well as specify correction factors. Zero correction factor provide the same results as without quantum potential model.
- Current direction to be specified to enable correct automatic setting of sign of bias and current density. The default setting is "negative", which corresponds to situation in version 6.4 and below (heterostructure is always specified from n-side to p-side, so z-axis is directed from n-side to p-side, and so forward current is directed opposite to z-axis).

- Algorithm to select the tunnel junction region in the computation of the whole structure. Several types are available, the recommended ones are "old" and "minmax".

Meaning of the solver parameters is described in detail in Sec. 5.6.

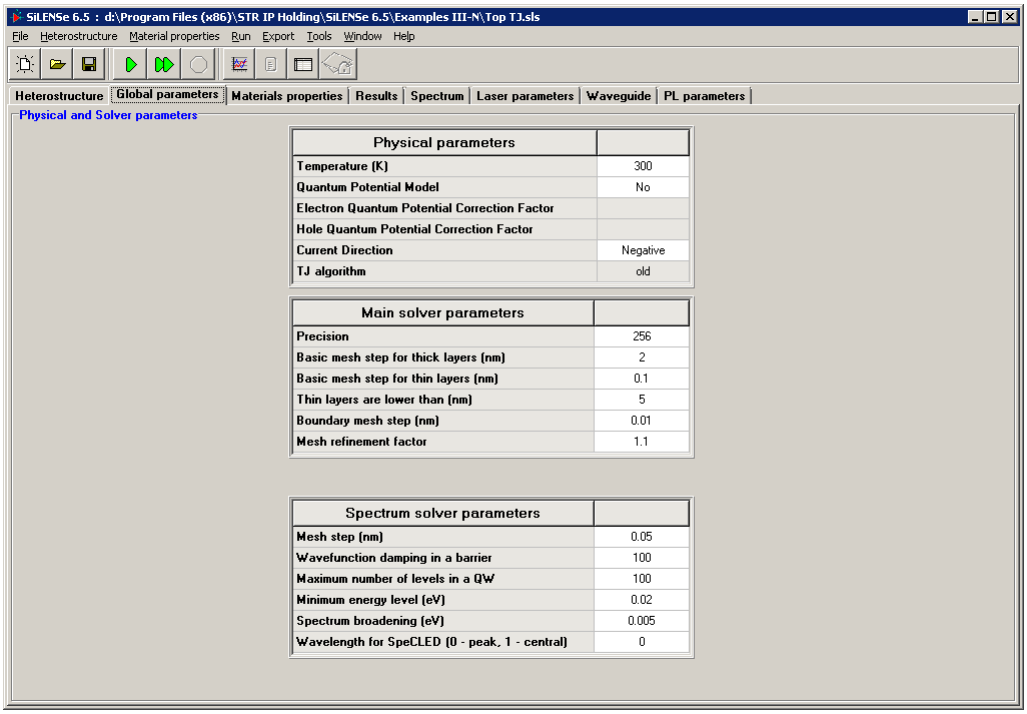
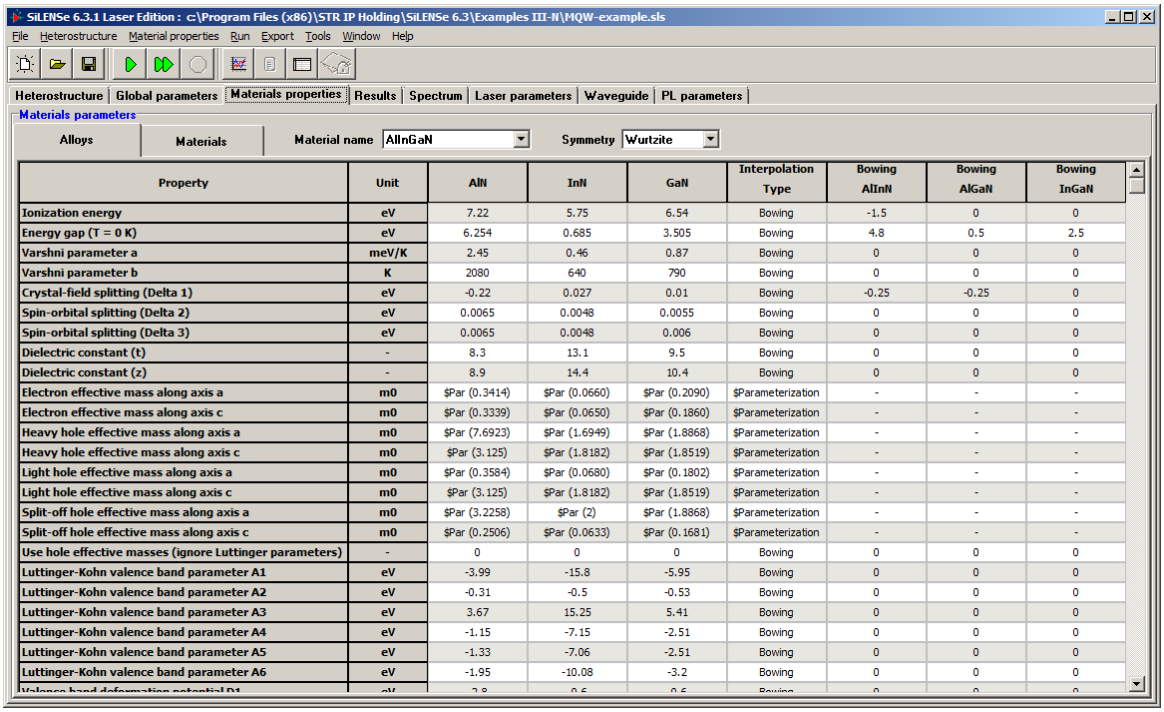


Fig. 6. Global parameters tab window.

4.2.5 Material Properties

The *Material properties* tab window (Fig. 7) shows the loaded materials properties in the read-only mode. The *Material properties* menu allows the user to export the data from the current project to the separate material database file or overload the existent data from other **SiLENSe** project or material database file (import of the material properties). The import can be done only if the new material database contains valid properties for all the materials used in the heterostructure.



Property	Unit	AlN	InN	GaN	Interpolation Type	Bowing AlInN	Bowing AlGaN	Bowing InGaN
Ionization energy	eV	7.22	5.75	6.54	Bowing	-1.5	0	0
Energy gap (T = 0 K)	eV	6.254	0.685	3.505	Bowing	4.8	0.5	2.5
Varshni parameter a	meV/K	2.45	0.46	0.87	Bowing	0	0	0
Varshni parameter b	K	2080	640	790	Bowing	0	0	0
Crystal-field splitting (Delta 1)	eV	-0.22	0.027	0.01	Bowing	-0.25	-0.25	0
Spin-orbital splitting (Delta 2)	eV	0.0065	0.0048	0.0055	Bowing	0	0	0
Spin-orbital splitting (Delta 3)	eV	0.0065	0.0048	0.006	Bowing	0	0	0
Dielectric constant (t)	-	8.3	13.1	9.5	Bowing	0	0	0
Dielectric constant (z)	-	8.9	14.4	10.4	Bowing	0	0	0
Electron effective mass along axis a	m0	$Par (0.3414)	$Par (0.0660)	$Par (0.2090)	$Parameterization	-	-	-
Electron effective mass along axis c	m0	$Par (0.3339)	$Par (0.0650)	$Par (0.1860)	$Parameterization	-	-	-
Heavy hole effective mass along axis a	m0	$Par (7.6923)	$Par (1.6949)	$Par (1.8868)	$Parameterization	-	-	-
Heavy hole effective mass along axis c	m0	$Par (3.125)	$Par (1.8182)	$Par (1.8519)	$Parameterization	-	-	-
Light hole effective mass along axis a	m0	$Par (0.3584)	$Par (0.0680)	$Par (0.1802)	$Parameterization	-	-	-
Light hole effective mass along axis c	m0	$Par (3.125)	$Par (1.8182)	$Par (1.8519)	$Parameterization	-	-	-
Split-off hole effective mass along axis a	m0	$Par (3.2258)	$Par (2)	$Par (1.8868)	$Parameterization	-	-	-
Split-off hole effective mass along axis c	m0	$Par (0.2506)	$Par (0.0633)	$Par (0.1681)	$Parameterization	-	-	-
Use hole effective masses (ignore Luttinger parameters)	-	0	0	0	Bowing	0	0	0
Luttinger-Kohn valence band parameter A1	eV	-3.99	-15.8	-5.95	Bowing	0	0	0
Luttinger-Kohn valence band parameter A2	eV	-0.31	-0.5	-0.53	Bowing	0	0	0
Luttinger-Kohn valence band parameter A3	eV	3.67	15.25	5.41	Bowing	0	0	0
Luttinger-Kohn valence band parameter A4	eV	-1.15	-7.15	-2.51	Bowing	0	0	0
Luttinger-Kohn valence band parameter A5	eV	-1.33	-7.06	-2.51	Bowing	0	0	0
Luttinger-Kohn valence band parameter A6	eV	-1.95	-10.08	-3.2	Bowing	0	0	0

Fig. 7. Material properties tab window.

4.2.6 Results

The *Results* tab window (Fig. 8) includes 8 plots presenting the simulation results: band diagram, electric potential and electric field, carrier concentrations, recombination rate, Shockley-Read-Hall lifetimes, current density of electrons and holes, strain components, and spontaneous and piezoelectric polarization. Available manipulations with graphs are described in detail in Sec. 4.3.4.

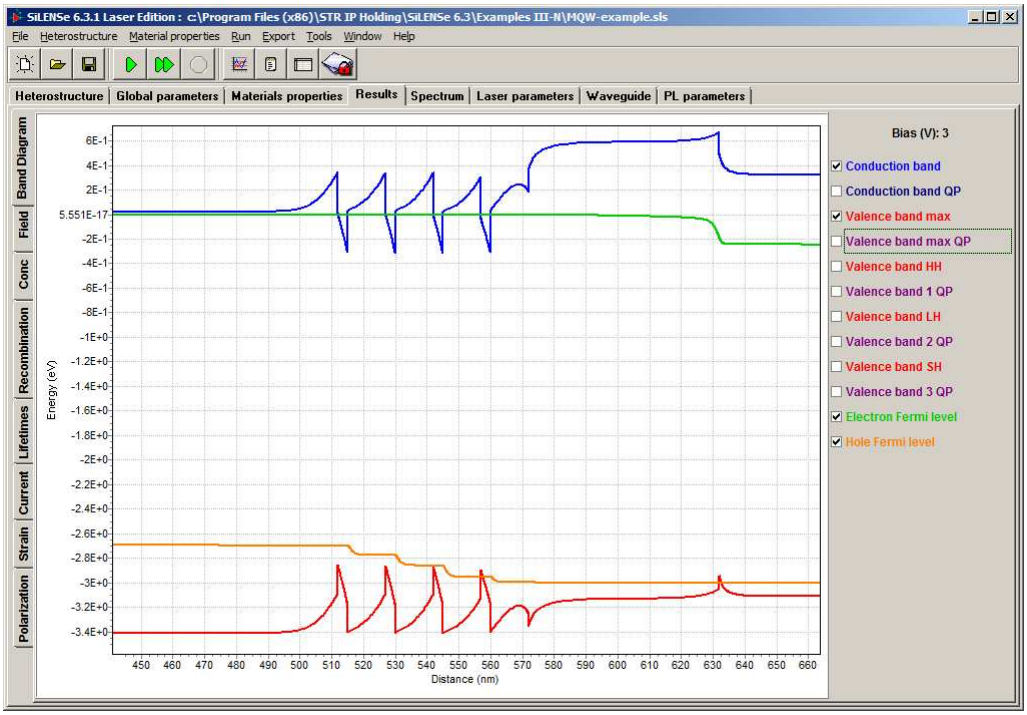


Fig. 8. Results tab window.

4.2.7 Spectrum

The *Spectrum* tab window is divided into two tabs: *Band diagram and wave functions* and *Spectrum*. The former tab (Fig. 9) contains a plot with the band diagram and carrier wave functions as well as a list of the quantum wells. The respective quantum well can be chosen by the mouse click and automatically marked by the cyan vertical stripe in the graph window. The movement from one well to another can be proceed either by direct choice of the well number by mouse or by the use of keyboard keys "→", "←", "↑", and "↓".

The energy levels in the chosen quantum well are listed in the right subsection. The user can turn on/off the wave functions in the selected quantum well by the checkboxes near the energy values. The total number of the energy levels in the selected quantum well is given in the brackets after the carrier type.

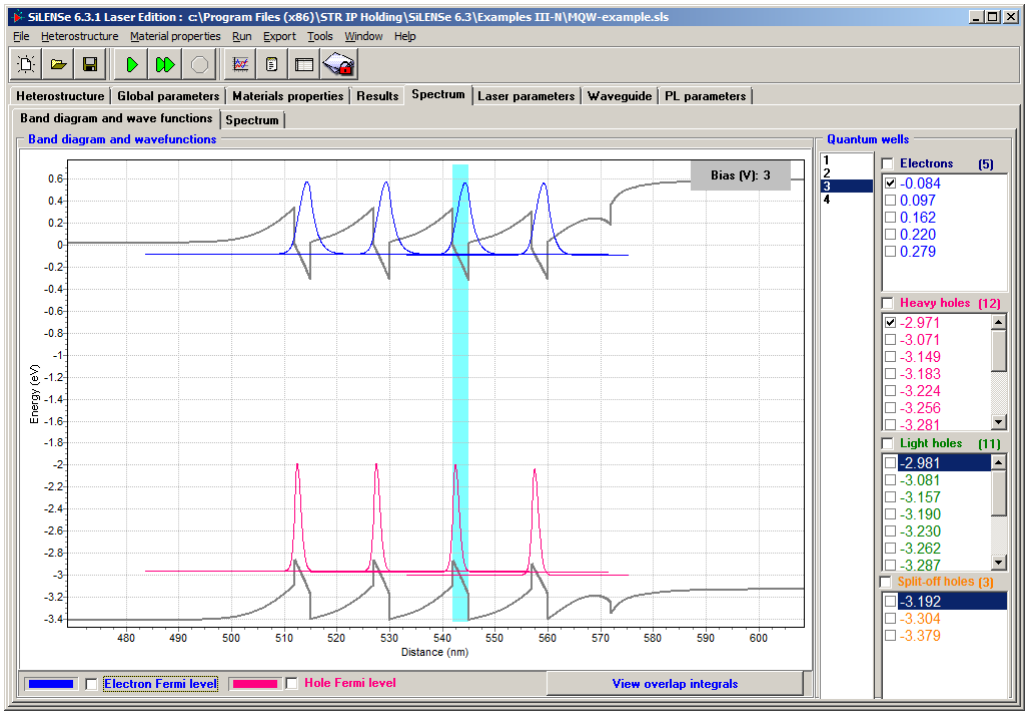


Fig. 9. Band diagram and wave functions tab window.

The *Spectrum* tab window (Fig. 10) shows the spontaneous emission and gain spectra of individual quantum wells, as well as the total spectra. The lines can be switched on/off by the respective checkboxes in the right part of the window. The user can switch between the photon energy and the wavelength by the respective vertical tab.

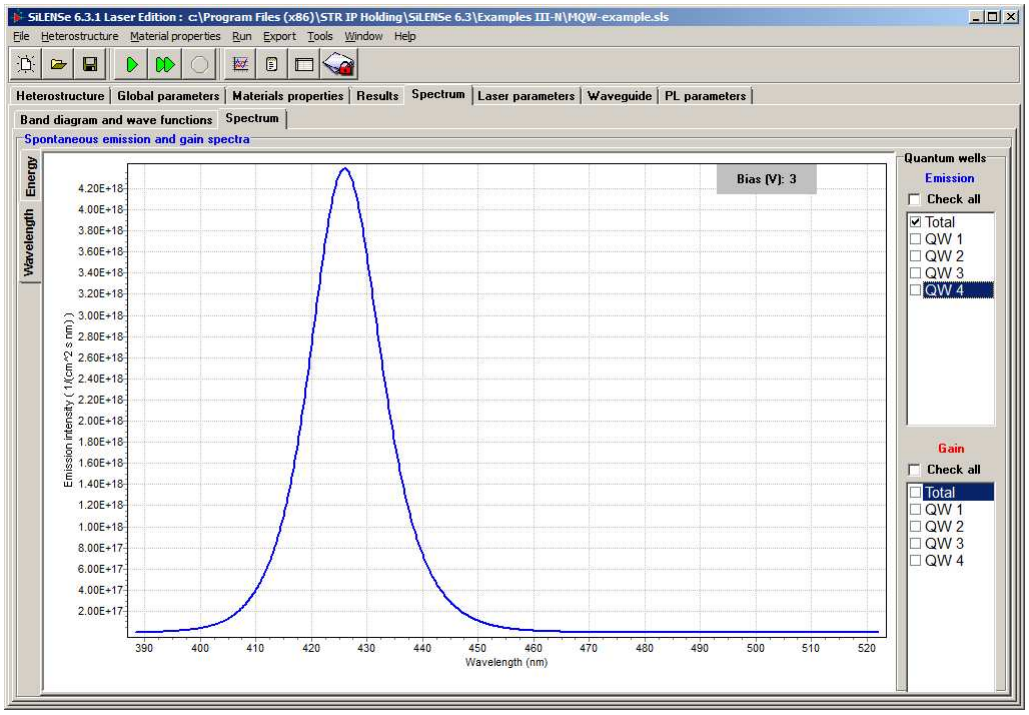


Fig. 10. Spectrum tab window.

4.2.8 Laser parameters tab window

The *Laser parameters* tab window (Fig. 11) contains global parameters related to the analysis of laser diodes. One group of parameters controls the calculation of the threshold characteristics. The user should specify the stripe geometry, reflectivity of the output and back mirrors, the polarization and index of the waveguide mode for which the analysis should be done. The *Additional loss* parameter allows one to specify an additional optical loss of any source. Next two parameters control the iterative adjustment of the current density converted into the stimulated recombination rate. The *Initial step* parameter means that the first initial guess will be the given fraction of the current density converted into the radiative recombination. The *Gain Fitting Accuracy* specifies the accuracy of fitting the condition that the total gain equals to the total losses. *Use Imported Gain Data* flag specifies whether user wants to replace calculation of the gain by a user-defined function. If this parameters is not "No", *Peak Gain vs Current Density Function* and *Peak Gain Wavelength vs Current Density Function* are the names of the functions for the maximum gain and respective wavelength. The button *Edit Gain Import Functions* enables editing these functions. *Use Absorption From Material Data* flag specifies whether the free-carrier absorption coefficient to be replaced by the absorption coefficient specified in the material properties data.

The other group of parameters controls computation of the waveguide modes. Since the electric/magnetic field distribution typically is much wider than the active region, for correct description of the waveguide one need to describe the thick n-contact layer and the substrate. The n-contact layer is assumed to be of the same composition as the first layer in the *Heterostructure* tab window, so one need only input its actual thickness. As for the substrate, the user should select the material from the drop-down list containing all the materials described in the project. The substrate composition field is enabled for alloy materials only. The *Substrate thickness in computations parameter* specifies the part of the substrate included in the waveguide computations. It should just provide an exponential decay of the field distribution. Do not input here the actual substrate thickness! The *Mesh step* parameter shows the mesh step used in waveguide computations.

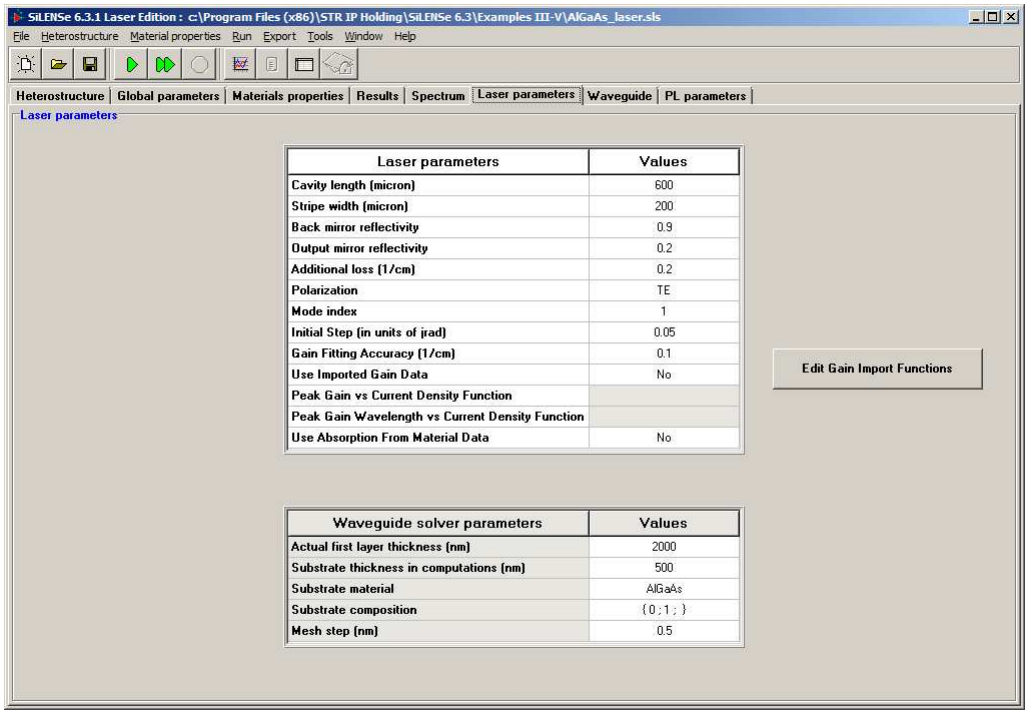


Fig. 11. Laser parameters tab window.

4.2.9 *Waveguide tab window*

The *Waveguide* tab window consists of two tabs: *Refractive index waveguide modes* and *Far field*. The former tab contains plot of the refractive index for ordinary (magenta line) and extraordinary (cyan line) waves (Fig. 12). The distribution of the electric and magnetic field intensity for TE and TM waveguide modes is shown by red and blue lines, respectively. The user can switch them on/off by the respective checkboxes in the right part of the window. The number appearing after the mode index is the effective refractive index β/k. The region of negative position represents the buffer layer and a part of the substrate.

The *Far field* tab (Fig. 13) shows the distribution of the far field intensity.

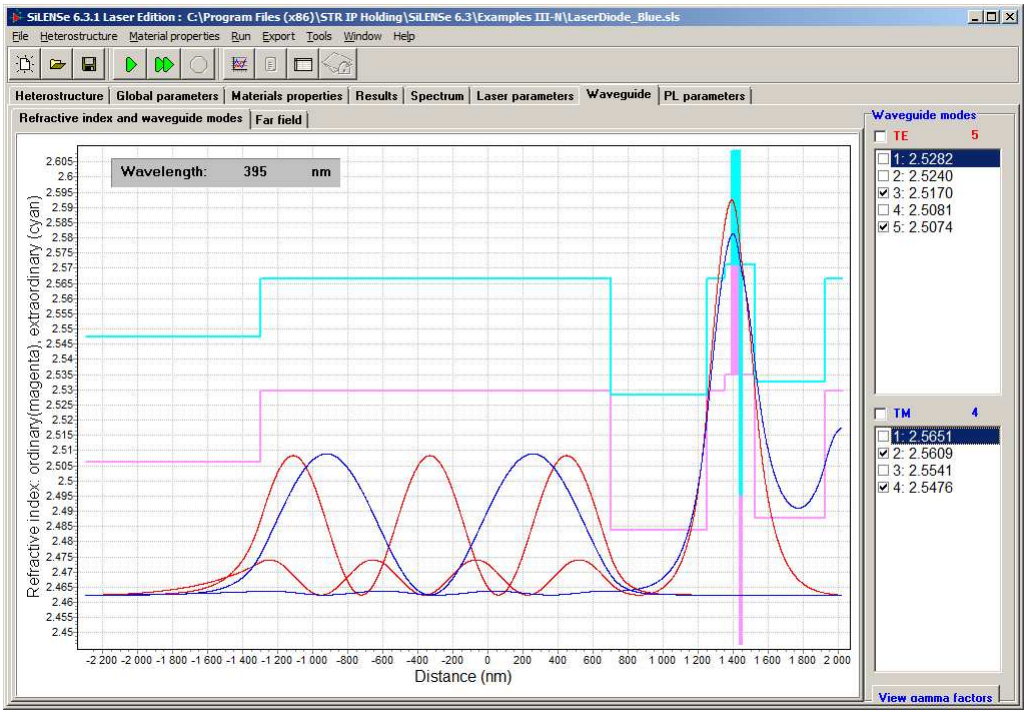


Fig. 12. *Refractive index waveguide modes* tab window.

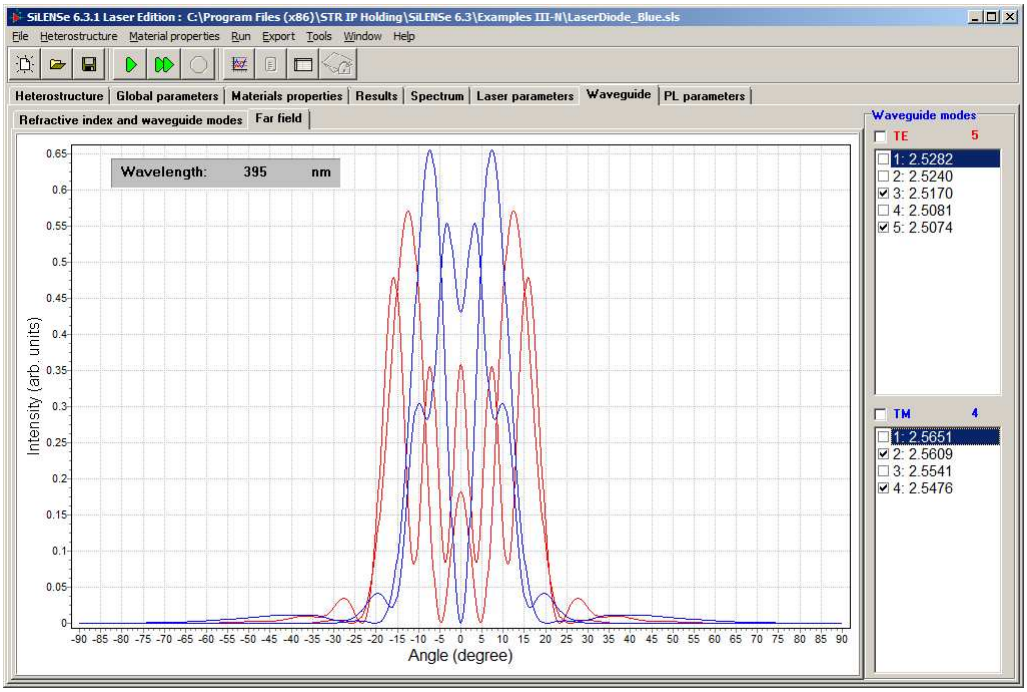


Fig. 13. *Far field* tab window.

4.2.10 PL parameters tab window

The PL parameters tab window contains global parameters related to PL excitation (Fig. 14), which includes the excitation wavelength, the excitation direction, reflectivity of the top and bottom boundaries of the structure, and p-n junction bias applied. The reflectivities can be

specified directly or calculated automatically by using refractive index of the top/bottom layers and of the immersion medium.

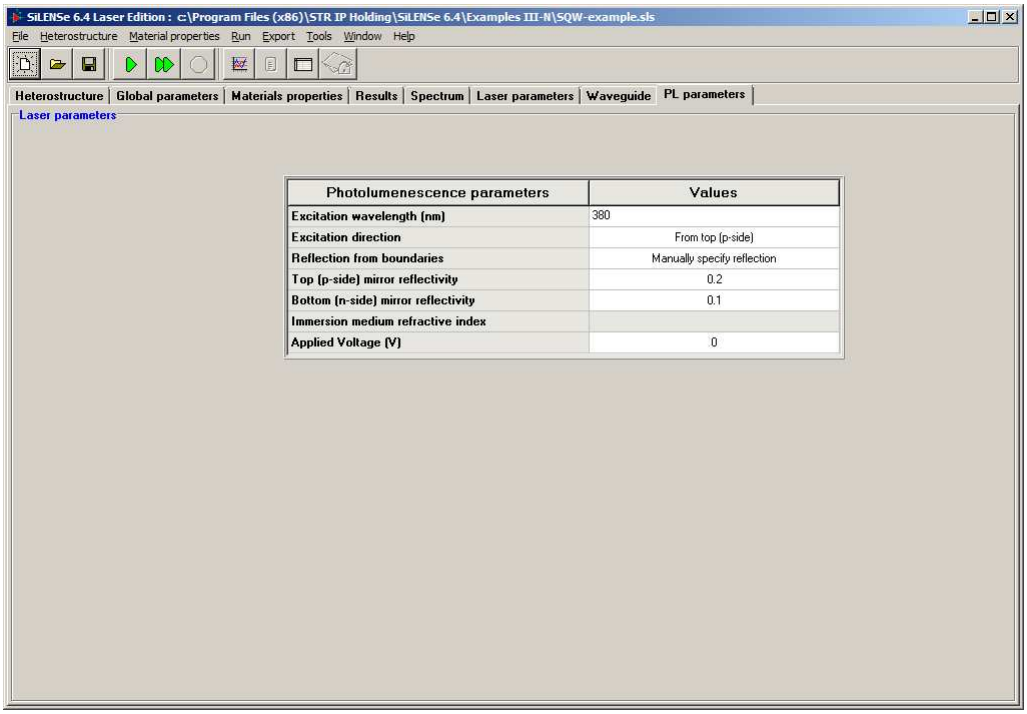


Fig. 14. PL parameters tab window.

4.3 Other Windows

4.3.1 LED Results

The *Window* | *LED Results* menu item opens the *LED Results* window with the table of the results which were stored in the project file or obtained during the current session. The table includes the following data: bias, current density (J), radiative (J_{rad}) , total non-radiative (J_{nrad}), Shockley-Read-Hall (J_{SRH}), and Auger (J_{Auger}) fractions of the current density, injected electron (J_n) and hole (J_p) current densities, leakage current densities of minority carriers ($J_{n\ right}$ and $J_{p\ left}$), internal quantum efficiency (IQE), injection efficiency, non-ideality factor (m), peak wavelength (Peak WL) and full-width at half-maximum (FWHM) of the emission spectrum, sheet carrier concentrations in the active region (n^{2D} and p^{2D}), and averaged differential lifetime in the active region.

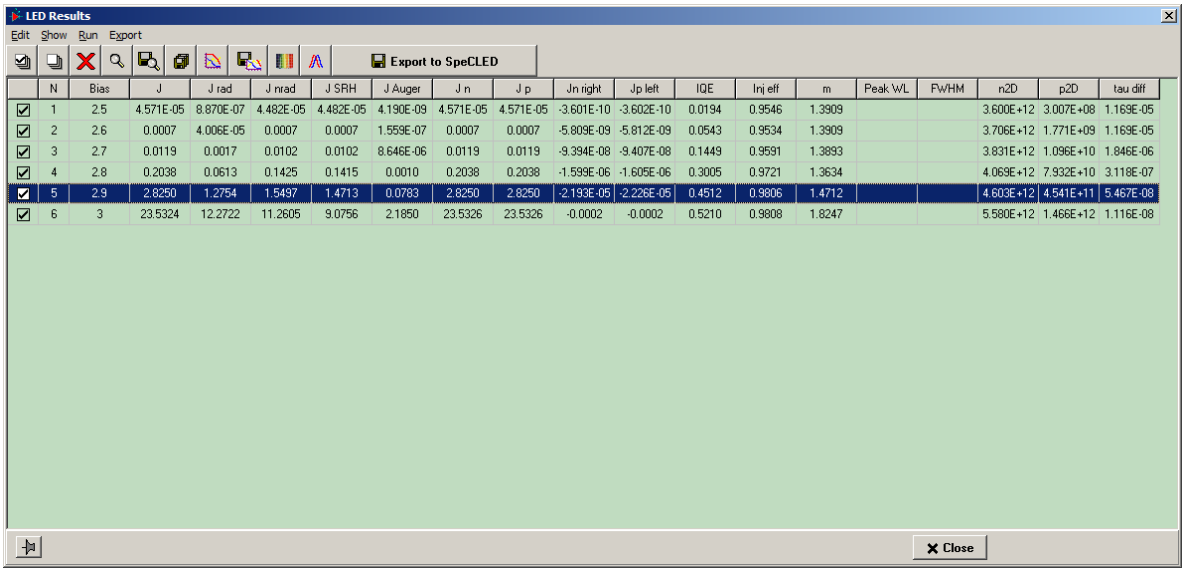
The menu bar of the *LED Results* window enables the user to work with the results.

NB All the menu items are duplicated by the respective buttons in the toolbar.

The *Edit* menu allows deleting selected results as well as select/unselect all the results. The user can load a result in the *Results* tab window by using *Show* | *Current result* menu item or just by double-click on the respective string in the table. To plot the current-voltage characteristics and internal quantum efficiency as a function of bias one should use the *Show* | *I-V characteristic* menu item. Only selected results will be evaluated.

The item *Run* | *Wave functions and spectrum* enables one to calculate the carrier wave functions and emission spectrum for the current result (marked by the gray color). To calculate the peak emission wavelength for all results, one can use *Run* | *Update Peak Wavelength* menu item.

The *Export* menu allows the user to export simulation result into a text file. First two items store the current result and I-V characteristic, respectively. *Export* | *All Results in Single File* menu item allows to export all the results for band diagrams, carrier concentration, and so on into a single text file for further analysis. The output formats are described in detail in Sec. 5.



N	Bias	J	J rad	J nrad	J SRH	J Auger	J n	J p	Jn right	Jp left	IQE	Inj eff	m	Peak WL	FWHM	n2D	p2D	tau diff
1	2.5	4.571E-05	8.870E-07	4.482E-05	4.482E-05	4.190E-09	4.571E-05	4.571E-05	-3.601E-10	-3.602E-10	0.0194	0.9546	1.3909			3.600E+12	3.007E+08	1.169E-05
2	2.6	0.0007	4.006E-05	0.0007	0.0007	1.559E-07	0.0007	0.0007	-5.809E-09	-5.812E-09	0.0543	0.9534	1.3909			3.706E+12	1.771E+09	1.169E-05
3	2.7	0.0119	0.0017	0.0102	0.0102	8.646E-06	0.0119	0.0119	-9.394E-08	-9.407E-08	0.1449	0.9591	1.3893			3.831E+12	1.096E+10	1.846E-06
4	2.8	0.2038	0.0613	0.1425	0.1415	0.0010	0.2038	0.2038	-1.599E-06	-1.605E-06	0.3005	0.9721	1.3634			4.069E+12	7.932E+10	3.118E-07
5	2.9	2.8250	1.2754	1.5497	1.4713	0.0783	2.8250	2.8250	-2.193E-05	-2.226E-05	0.4512	0.9806	1.4712			4.603E+12	4.541E+11	5.467E-08
6	3	23.5324	12.2722	11.2605	9.0756	2.1850	23.5326	23.5326	-0.0002	-0.0002	0.5210	0.9808	1.8247			5.580E+12	1.466E+12	1.116E-08

Fig. 15. LED Results window.

Export | *Export to SpeCLED* menu item allows one to export results for the **SpeCLED** module in old format. It is recommended to use *Run -> Series Calculations for SpeCLED* menu item of the main menu instead (see Sections 3.4.1 and 4.1 for details).

4.3.2 PL Results

The *Window->PL Results* menu item opens *PL Results* window (Fig. 16) representing a table with all completed PL simulations like *LED Results* window shows results for LED

mode. The most data shown in the table is similar to that of *LED Results* window. New columns are excitation power density (ExcPower, W/cm^2) and the respective current density (J gen, A/cm^2). The IQE for PL computations is defined as the ratio of the radiative current in QWs to J gen (not to J). All other functionality of *PL Results* window is similar to that of *LED Results* window.

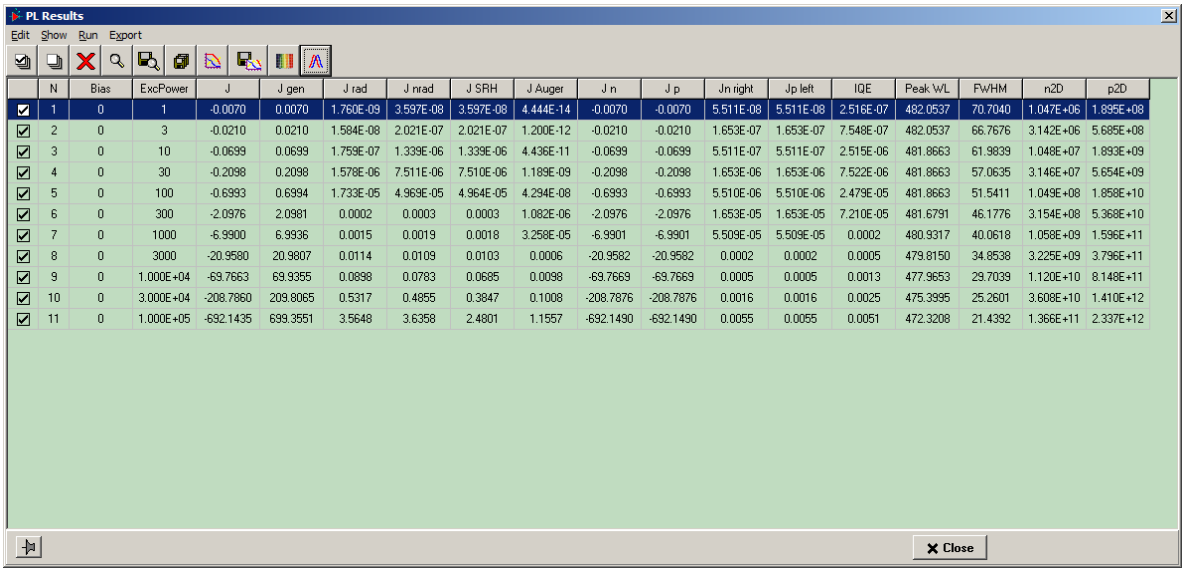


Fig. 16. PL Results window.

4.3.3 I-V Characteristic

The *Show* | *I-V characteristic* menu item in the *LED Results* window opens an *I-V characteristic* modal window with three plots. The former two plots represent the current density as a function of the bias (Fig. 17) and the internal quantum efficiency variation with the current density, respectively. The last plot is introduced to rely the calculated current density with experimentally observed I-V characteristics by qualitative accounting for the series and contact resistance. The user is prompted to specify the LED area and series resistance. The current and voltage are calculated as described in Sec. 9.2 of [1]. The plot is updated when one uses the *Apply* button.

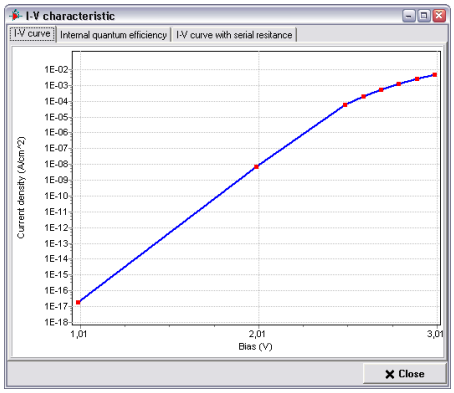
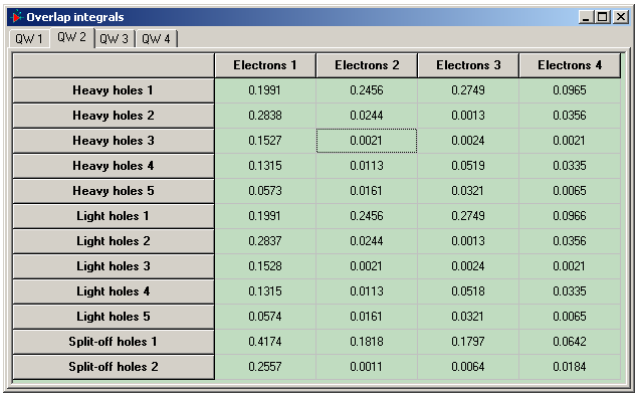


Fig. 17. I-V characteristics modal window.

4.3.4 Overlap Integrals

This window shows the squared overlap integrals between each pair of the electron and hole wave functions. The data for different quantum wells are shown in different tabs.



	Electrons 1	Electrons 2	Electrons 3	Electrons 4
Heavy holes 1	0.1991	0.2456	0.2749	0.0965
Heavy holes 2	0.2838	0.0244	0.0013	0.0356
Heavy holes 3	0.1527	0.0021	0.0024	0.0021
Heavy holes 4	0.1315	0.0113	0.0519	0.0335
Heavy holes 5	0.0573	0.0161	0.0321	0.0065
Light holes 1	0.1991	0.2456	0.2749	0.0966
Light holes 2	0.2837	0.0244	0.0013	0.0356
Light holes 3	0.1528	0.0021	0.0024	0.0021
Light holes 4	0.1315	0.0113	0.0518	0.0335
Light holes 5	0.0574	0.0161	0.0321	0.0065
Split-off holes 1	0.4174	0.1818	0.1797	0.0642
Split-off holes 2	0.2557	0.0011	0.0064	0.0184

Fig. 18. Overlap Integrals window.

4.3.5 Detailed Spectrum

The *Detailed Spectrum* window (Fig. 19) allows inspect fine details of the emission spectrum. Tree in the left part of the window shows the total emission spectra and total contribution of each subband of the valence band followed by contribution of individual QWs. Contribution of each QW is also split into contributions of three subbands and even individual transitions. Values after the colon indicate relative contribution of the item in the total emission spectrum. If the selected item represents parameters of an individual transition, the below table shows its following parameters: relative contribution to the total spectrum, squared overlap integral, occupancy factors of the electron and hole energy levels

(at zero energy of the lateral motion), and a product of the squared integral and occupancy factors.

One can visualize the emission spectrum of an item by using button with right arrow or double click on the item. Then the item will appear in the check list in the center of the window. Check boxes allow show and hide individual lines. To remove an item from the check list, use the button with left arrow. Button with double left arrow removes all items from the check list. Colors of lines resemble colors of the carrier wave functions. Blue lines show total emission spectrum and total contributions of an individual QWs (all subbands together), while red, green, and orange lines shows contributions of heavy, light, and split-off holes, respectively.

Save button allows to save these data as a text file (the same effect has 'Export->Detailed Spectrum' menu item in the main window).

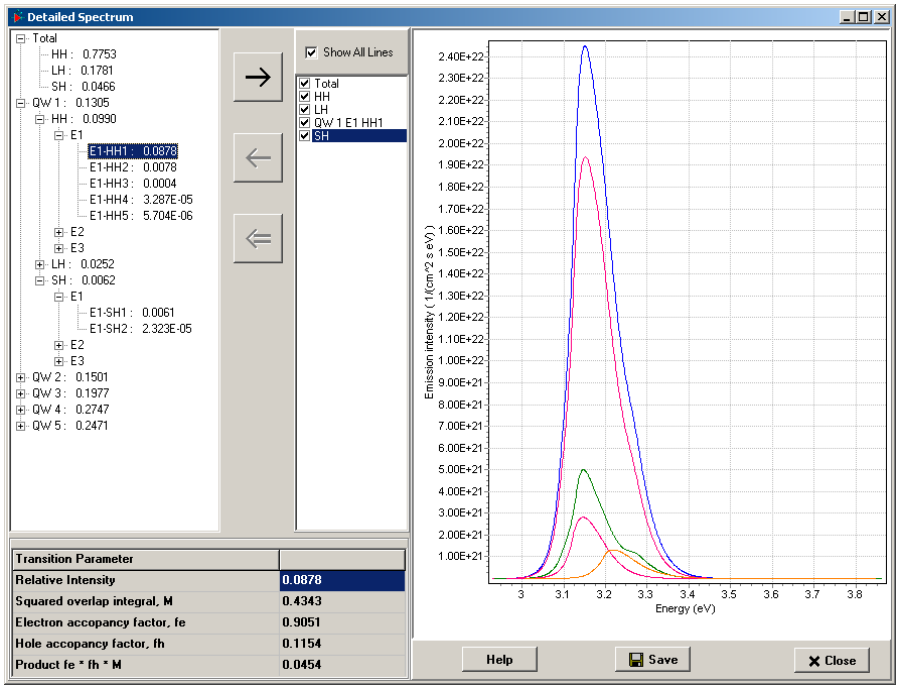


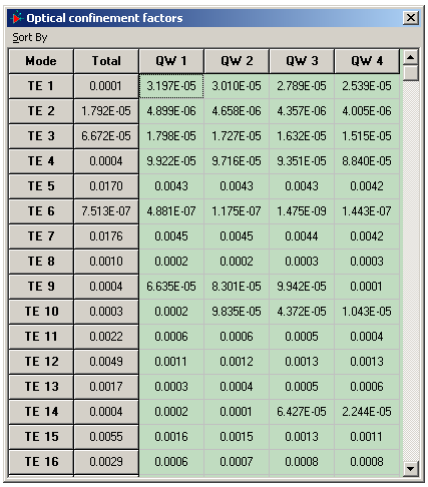
Fig. 19. Detailed Spectrum window.

4.3.6 Optical Confinement Factors

This *Optical Confinement Factors* window (Fig. 20) shows the optical confinement factors for each mode and each quantum well. The column *Total* shows the sum over the quantum wells. The user can sort modes using the following *Sort By* menu items:

- *Mode Index (First TE)* – modes are sorted by their index, TE modes go first.
- *Mode Index (First TM)* – modes are sorted by their index, TM modes go first.

- *Value* – the modes are sorted by the value of total optical confinement factor in the descending order. This option allows reveal the mode which is most favorable for laser generation, i.e. having larger optical gain and, therefore, lower threshold current.



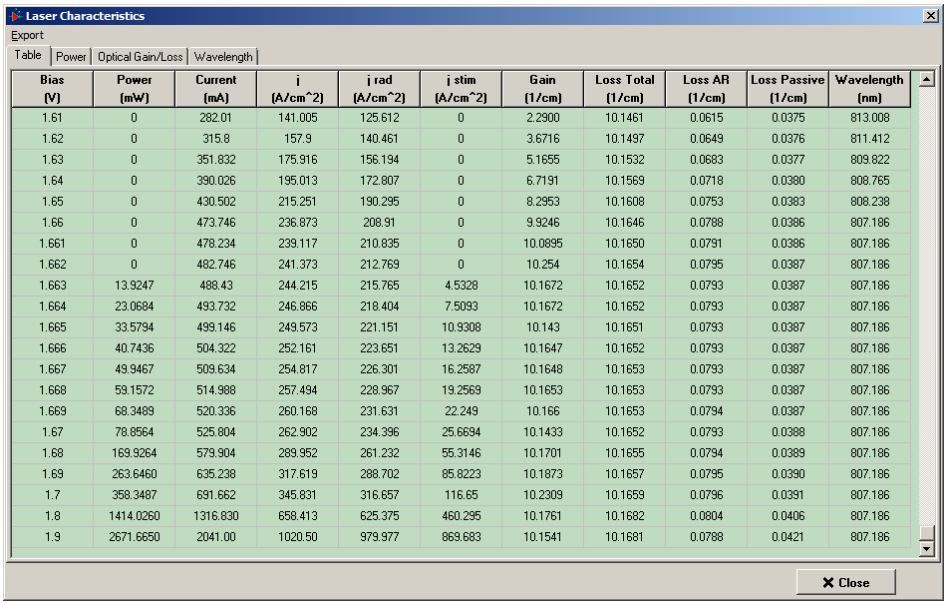
Mode	Total	QW 1	QW 2	QW 3	QW 4
TE 1	0.0001	3.197E-05	3.010E-05	2.789E-05	2.539E-05
TE 2	1.792E-05	4.899E-06	4.658E-06	4.357E-06	4.005E-06
TE 3	6.672E-05	1.798E-05	1.727E-05	1.632E-05	1.515E-05
TE 4	0.0004	9.922E-05	9.716E-05	9.351E-05	8.840E-05
TE 5	0.0170	0.0043	0.0043	0.0043	0.0042
TE 6	7.513E-07	4.881E-07	1.175E-07	1.475E-09	1.443E-07
TE 7	0.0176	0.0045	0.0045	0.0044	0.0042
TE 8	0.0010	0.0002	0.0002	0.0003	0.0003
TE 9	0.0004	6.635E-05	8.301E-05	9.942E-05	0.0001
TE 10	0.0003	0.0002	9.835E-05	4.372E-05	1.043E-05
TE 11	0.0022	0.0006	0.0006	0.0005	0.0004
TE 12	0.0049	0.0011	0.0012	0.0013	0.0013
TE 13	0.0017	0.0003	0.0004	0.0005	0.0006
TE 14	0.0004	0.0002	0.0001	6.427E-05	2.244E-05
TE 15	0.0055	0.0016	0.0015	0.0013	0.0011
TE 16	0.0029	0.0006	0.0007	0.0008	0.0008

Fig. 20. Optical Confinement Factors window.

4.3.7 Laser Characteristics

The *Laser Characteristics* window presents the laser characteristics. The first tab (Fig. 21) includes a table with the following columns:

- Bias (V)
- Output optical power (W)
- Current (A)
- Current density (A/cm^2)
- Radiative current density (A/cm^2)
- Stimulated current density (A/cm^2)
- Optical gain (1/cm)
- Total optical loss (1/cm)
- Optical loss because of the free carrier absorption in the quantum wells (1/cm)
- Optical loss because of the free carrier absorption outside the quantum wells (1/cm)
- Wavelength of the gain spectrum maximum (nm)



Bias (V)	Power (mW)	Current (mA)	j (A/cm^2)	j rad (A/cm^2)	j stim (A/cm^2)	Gain (1/cm)	Loss Total (1/cm)	Loss AR (1/cm)	Loss Passive (1/cm)	Wavelength (nm)
1.61	0	282.01	141.005	125.612	0	2.2900	10.1461	0.0615	0.0375	813.008
1.62	0	315.8	157.9	140.461	0	3.6716	10.1497	0.0649	0.0376	811.412
1.63	0	351.832	175.916	156.194	0	5.1655	10.1532	0.0683	0.0377	809.822
1.64	0	390.026	195.013	172.807	0	6.7191	10.1569	0.0718	0.0380	808.765
1.65	0	430.502	215.251	190.295	0	8.2953	10.1608	0.0753	0.0383	808.238
1.66	0	473.746	236.873	208.91	0	9.9246	10.1646	0.0788	0.0386	807.186
1.661	0	478.234	239.117	210.835	0	10.0895	10.1650	0.0791	0.0386	807.186
1.662	0	482.746	241.373	212.769	0	10.254	10.1654	0.0795	0.0387	807.186
1.663	13.9247	488.43	244.215	215.765	4.5328	10.1672	10.1652	0.0793	0.0387	807.186
1.664	23.0684	493.732	246.866	218.404	7.5093	10.1672	10.1652	0.0793	0.0387	807.186
1.665	33.5794	499.146	249.573	221.151	10.9308	10.143	10.1651	0.0793	0.0387	807.186
1.666	40.7436	504.322	252.161	223.651	13.2629	10.1647	10.1652	0.0793	0.0387	807.186
1.667	49.9467	509.634	254.817	226.301	16.2587	10.1648	10.1653	0.0793	0.0387	807.186
1.668	59.1572	514.988	257.494	228.967	19.2569	10.1653	10.1653	0.0793	0.0387	807.186
1.669	68.3489	520.336	260.168	231.631	22.249	10.166	10.1653	0.0794	0.0387	807.186
1.67	78.8564	525.804	262.902	234.396	25.6694	10.1433	10.1652	0.0793	0.0388	807.186
1.68	169.9264	579.904	289.952	261.232	55.3146	10.1701	10.1655	0.0794	0.0389	807.186
1.69	263.6460	635.238	317.619	288.702	85.8223	10.1873	10.1657	0.0795	0.0390	807.186
1.7	358.3487	691.662	345.831	316.657	116.65	10.2309	10.1659	0.0796	0.0391	807.186
1.8	1414.0260	1316.830	658.413	625.375	460.295	10.1761	10.1682	0.0804	0.0406	807.186
1.9	2671.6650	2041.00	1020.50	979.977	869.683	10.1541	10.1681	0.0788	0.0421	807.186

Fig. 21. Laser Characteristics window : Table.

The second tab (Fig. 22) shows the power-current characteristics as well as the threshold current and the differential quantum efficiency.

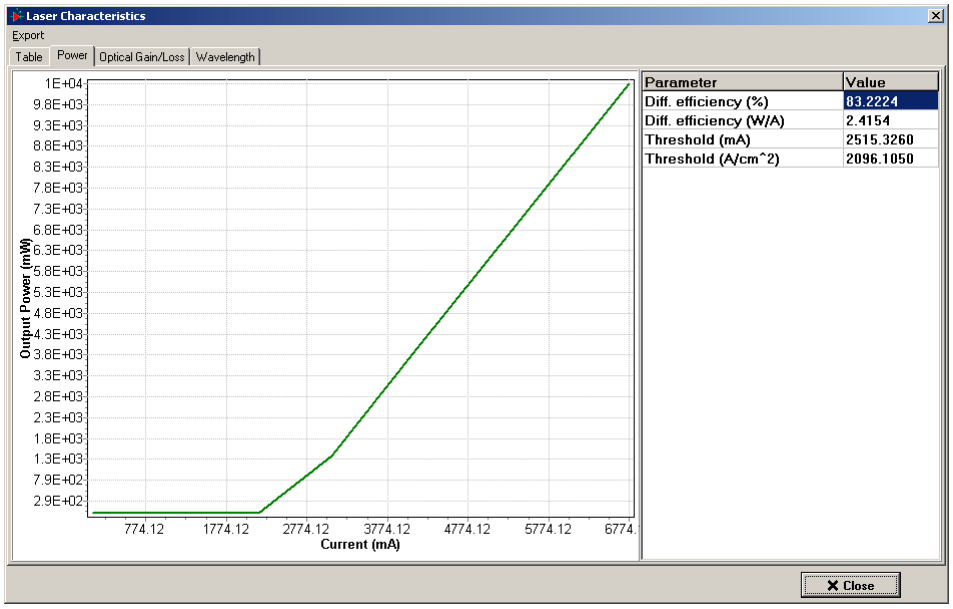


Fig. 22. Laser Characteristics window : Power-Current characteristics.

The third tab (Fig. 23) shows variation of the optical gain and loss with the current density.

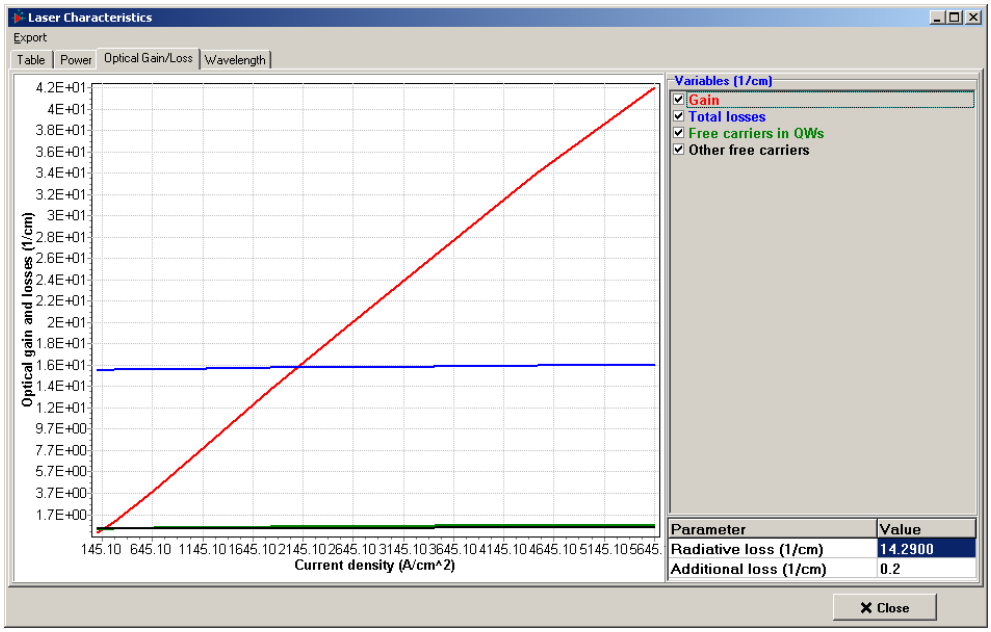


Fig. 23. Laser Characteristics window : Optical Gain and Loss.

The fourth tab (Fig. 24) shows variation of the gain spectrum maximum with the current density.

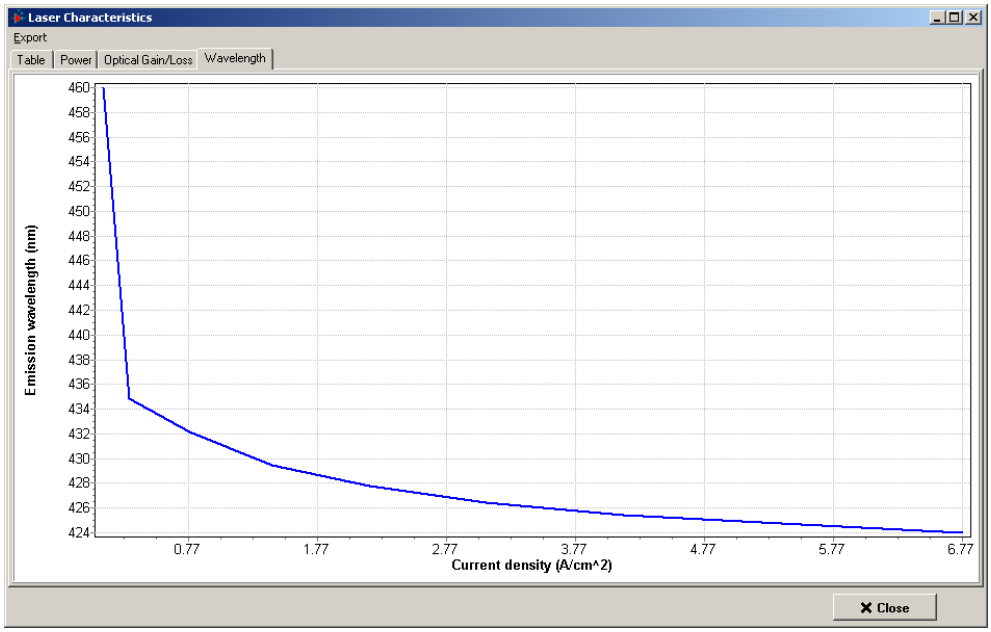


Fig. 24. Laser Characteristics window : Wavelength.

4.4 Exploring Plots

All the graphs in **SiLENSe** support the following operations:

- *Zoom in:* select the region of interest from the upper left to the right down keeping the left mouse button pressed. The zoomed region will appear in the plot window.

- *Zoom out:* select any region in the plot area from the right down to the left upper keeping the left mouse button pressed. This action returns a plot to the full-size mode.
- *Scrolling:* drug the plot inside the plot area keeping the right mouse button pressed. Then the adjacent region of the plot will be displayed.

NB *Save current chart* menu item allows the user to save current chart as a graphic file.

5 Output Files

The simulation results can be stored as plain text data files. Usually, these files start from a header with column names, then data are stored in columns separated by tab. In some cases, the structure of the file is more complicated.

5.1 Band Diagram, Carrier Concentrations, Recombination Rate etc.

The *Export* | *Current result* menu item in the *LED Results* window enables one to export the results of main drift-diffusion solver. The following variables are stored in columns separated by tab:

- Position and mesh step (nm)
- Three conduction bands (Γ, X, and L valleys) and minimum among them, three subbands of the valence band and maximum among them, and all these values with corrections due to the quantum potential model (eV)
- Electron Fermi level and hole Fermi level (eV)
- Electric potential (V) and electric field (MV/cm)
- Density of electron current, hole current, tunnel current, and total current (A/cm^2)
- Concentration of electrons in three valleys (Γ, X, and L) and total electron concentration (cm^{-3})
- Concentration of holes in three subbands of the valence band and total hole concentration (cm^{-3})
- Concentration of ionized donors and acceptors (cm^{-3})
- Concentration of states for three valleys of the conduction band and three subbands of the valence band (cm^{-3})
- Radiative recombination, total non-radiative recombination, Shockley-Read-Hall recombination, Auger recombination (cm^{-3} s^{-1}), and generation rate (for PL computations)

- Absorption coefficient (for PL computations)
- Spontaneous, piezoelectric, and total polarization (C/m^2)
- Four strain components in the coordinates related to the crystal lattice: u_{xx}, u_{yy}, u_{zz}, and u_{yz}
- Non-radiative carrier lifetimes due to dislocations and point defects
- Refractive index (ordinary and extraordinary)
- Field intensity for the waveguide mode selected in "Laser Parameters" tab
- Distribution of the free carrier absorption
- Product of the two above columns (field intensity and free carrier absorption)

The latter three columns are calculated for the wavelength of laser emission (i.e. peak of the gain spectrum for the selected result).

The *Export* | *All Results in Single File* menu item provides export of the same data for all the computed results. In this case, a column containing the p-n junction bias is inserted into first position.

5.2 I-V Characteristics

The *Export I-V characteristics* button in the *LED Results* window enables one to export the I-V characteristic and related values. The following variables are stored in columns separated by tab:

- Bias (V)
- Current density (A/cm^2)
- Internal quantum efficiency
- Injection efficiency
- Peak emission wavelength, central wavelength, and FWHM of the spectrum (nm)
- Non-ideality factor
- Total chip voltage (V) and chip current (A) - see Sec. 4.3.3
- Radiative current density (A/cm^2)
- Non-radiative current density (A/cm^2)
- Current density of Shockley-Read-Hall recombination (A/cm^2)
- Current density of Auger recombination (A/cm^2)
- Current density electrons and holes at external interfaces of the structures (A/cm^2)
- Sheet concentration of electrons and holes in the active region (cm^{-2})
- Averaged differential lifetime in the active region (s)
- Local bias and tunnel current density for each of the tunnel junctions (V, A/cm^2)

5.3 Carrier Wave Functions

The *Export* | *Carrier Wave Functions* menu item enables one to export the carrier wave functions. The output file contains the following variables stored in columns separated by tab:

- Position (nm)
- Conduction band, valence band, electron Fermi level, hole Fermi level (eV)
- QW indicator which equals to 1 if the point belongs to one of QWs and 0 otherwise
- Carrier wave functions ($nm^{1/2}$)

Wave functions are named as follows:

```
QW<QW index><carrier type><level index>,
```

where letters EE, HH, LH, and SH denotes electrons, heavy holes, light holes, and split-off holes, respectively.

5.4 Emission Spectra

The *Export* | *Emission Spectra* menu item enables one to export the emission spectra. The output file contains the following variables stored in columns separated by tab:

- Energy (eV)
- ETotal (cm^{-2} s^{-1} eV^{-1}) – total emission intensity
- EQW1 (cm^{-2} s^{-1} eV^{-1}) – emission intensity from the 1-st QW
- EQW2 (cm^{-2} s^{-1} eV^{-1}) – emission intensity from the 2-nd QW
- ……
- EQWN (cm^{-2} s^{-1} eV^{-1}) – emission intensity from the last QW

The following data are the same intensities normalized to the wavelength

- Wavelength (nm)
- WTotal (cm^{-2} s^{-1} nm^{-1}) – total emission intensity
- WQW1 (cm^{-2} s^{-1} nm^{-1}) – emission intensity from the 1-st QW
- WQW2 (cm^{-2} s^{-1} nm^{-1}) – emission intensity from the 2-nd QW
- …
- WQWN (cm^{-2} s^{-1} nm^{-1}) – emission intensity from the last QW

Warning: One should plot the data form the first group vs the energy, and from the second group vs the wavelength in order to keep the right normalization of the intensity to the total recombination rate!

5.5 Gain Spectra

The *Export* | *Gain Spectra* menu item enables one to export the gain spectra. The output file contains the following variables stored in columns separated by tab:

- Energy (eV)
- ETotal (cm^{-1}) – sum of the following columns
- EQW1 (cm^{-1}) – gain in the 1-st QW
- EQW2 (cm^{-2} s^{-1} eV^{-1}) – gain in the 2-nd QW
- ……
- EQWN (cm^{-2} s^{-1} eV^{-1}) – gain in the last QW
- Wavelength (nm)

5.6 Overlap Integrals

The *Export* | *Overlap integral* menu item enables one to export the overlap integrals. The output is a text file. The data are arranged similarly to their appearance in the *Overlap Integrals* window (Sec. 4.3.4).

5.7 Waveguide Modes

The *Export* | *Waveguide Modes* menu item enables one to export the gain spectra. The output file contains the following variables stored in columns separated by tab:

- Position (nm)
- Refractive index for ordinary wave
- Refractive index for ordinary wave modified – see details in [1].
- Refractive index for extraordinary wave modified
- Refractive index for extraordinary wave modified – see details in [1].
- FieldTE1 (cm^{-1}) – squared electric field for the 1-st TE mode
- FieldTE2 (cm^{-1}) – squared electric field for the 2-nd TE mode
- ……
- FieldTEN (cm^{-1}) – squared electric field for the last TE mode
- FieldTM1 (cm^{-1}) – squared electric field for the 1-st TM mode
- FieldTM2 (cm^{-1}) – squared electric field for the 2-nd TM mode
- ……

- FieldTMN (cm^{-1}) – squared electric field for the last TM mode

5.8 Laser Characteristics

The *Export* | *Laser Characteristics* menu item enables one to export the laser characteristics. The data are arranged similarly to their appearance in the *Table* tab of the *Laser Characteristics* window (Sec. 4.3.7).

6 Solver Parameters

The section describes the solver parameters in the *Global parameters* tab window.

6.1 Main Solver Parameters

Precision parameter allows to increase the accuracy of the floating-point numbers in bits during the core computations and improve convergence. It is recommended to increase precision up to 256 in case of any problems with convergence. Variants "double" and "64" are very similar, the difference is that "double" is realized with default compiler options and "64" with the library for extended precision.

The grid is generated automatically by the procedure described below. First, the basic mesh step is chosen for each layer, which is equal to *Basic mesh step for thick layers* and *Basic mesh step for thin layers*, for layers with thickness higher and lower than *Thin layers are lower than* parameter, respectively. The grid step in the central part of the layer equals to this basic mesh step. The mesh step adjacent to the layer boundaries equals to *Boundary mesh step*. Then the mesh step is increased by the factor of Mesh refinement factor until it reaches the basic mesh step.

Some parameters controlling the computations are shown in the solver window. One can update them even during the computation and see its effect on the convergence.

6.2 Spectrum Solver Parameters

The spectrum solver generates a separate uniform mesh for each quantum well to solve the Schrödinger equation. The user should specify the *Mesh step* in the respective text field. The recommended mesh step is about 0.05-0.2 nm. Effective LAPACK computational routines [2] are used to solve the eigenvalue problem.

The *Minimum energy level* and *Wavefunction damping in a barrier* parameters are used for determination of the computational domain boundaries for each quantum well, as described in Sec. 10.2 of [1]. They are rarely needed to be modified. Generally, quantum wells with the barrier heights smaller than the value of the former parameter are ignored in the spectrum calculation. The last parameter determines the minimum damping of the wave function at the domain boundaries. The higher this parameter, the wider barrier regions are included in the domain.

The *Maximum number of levels in a QW* parameter is introduced to limit the maximum amount of the heap memory and computation time needed for the solution of the Schrödinger equation. If there are more levels exists in the quantum well, only first several levels will be calculated according to the maximum number.

The *Spectrum broadening* parameter determines the width γ used to calculate the spectrum broadening as discussed in Sec. 10.6 of [1].

7 Editor of Material Parameters

The **Properties Editor** is an additional tool for editing input data for materials properties. It is supplied free of charge with STR programs requiring these data. The input data are saved in the special project files of the **Properties Editor**. Other STR programs load material properties from these files. The default database of the material properties is supplied with the package.

The user can modify the properties of the existing materials as well as add new materials by using **Properties Editor**. Database files are stored in ASCII XML format. Advanced users may directly edit it via text editor to change material properties..

Generally, the materials in the **Properties Editor** are divided into two types: (i) materials of fixed chemical composition, like GaN, GaAs, etc. and (ii) alloys with variable composition, like $Al_xIn_yGa_{1-x-y}N$, $Al_xGa_{1-x}As$, etc. Alloys are formed from existing materials (at least two materials are needed to make an alloy). In Sec. 7.3 we will consider different ways for specification of properties of materials and alloys.

All materials and alloys are divided by their crystal symmetry, which is shown in the drop-down list in the top part of the window. The current version supports two symmetry types: zinc blende and wurtzite.

7.1 Materials Tab Window

Left part of the *Materials* tab window contains list of existing materials and buttons to manipulate with them. The right part of the window represents properties of the selected material. Properties are divided into several groups: electronic, optical, lattice-related properties, properties of impurities, etc.

To create new material or delete existing material, use buttons *Add Material* or *Delete Material*, respectively. Buttons *Copy Material* and *Insert Material* allows one to copy selected material into a buffer and insert material from the buffer after selected material, respectively. One can arrange materials in the list by buttons *Move Material Up* and *Move Material Down*.

Material name is an arbitrary string specified by user which serves as a unique identifier of the material. As created, new material has all properties initialized with default value (mainly zero). For each material property, one can edit the specification type (green column) and the value.

7.2 Alloys Tab Window

Left part of the *Alloys* tab window contains list of existing alloys and buttons to manipulate with them. The right part of the window represents how the material properties of the selected alloy are interpolated for an arbitrary material composition. The list of properties is similar to the *Materials* tab window.

Use button *Add Alloy* to create new alloy. A modal window *Add Alloy* appears where you are prompted enter alloy name. The list of materials of the selected type will appear. Mark materials you want to include in the new alloy. At least two materials are necessary to form alloy. As created, new alloy has all properties initialized with default value (mainly it will be zero bowing parameters, i.e. assumption of linear dependence of the property on the alloy composition). The number of bowing parameters is n(n-1)/2 , where n is the number of materials in the alloy. For each material property, one can edit the specification type (green column) and the value(s).

7.3 Specification of Properties

There are three different ways for specification of the properties of a material (types of property):

- constant values for materials and bowing parameters for alloys (default);
- user-defined functional dependence
- pre-defined parameterization (available for some properties)

To change the property type one needs click the respective cell of the table and pick up new type from the drop-down list appeared.

7.3.1 Default

Most of the properties are specified by setting constant values for materials and bowing parameters for alloys. Then property f of alloy including n species is calculated as

$$f(x_1, x_2, ..., x_n) = \sum_{i=1}^{n} f_i x_i - \sum_{i=1}^{n} \sum_{k=i+1}^{n} f_{ik} x_i x_k$$

where x_i are the species concentrations following the relation $\sum_{i=1}^{n} x_i = 1$, f_i are the values of the property f for pure materials, and f_{ik} are the bowing parameters. One can use zero bowing parameters to describe linear variation of the property f with the alloy composition, so called Vegard law.

7.3.2 Functions

Functions can depend on the temperature and wavelength (the latter is useful for optical properties like refractive index). Functions used in properties of alloys can also depend on the alloy composition. Functions can be specified by writing a Pascal-like script or by providing a tabulated dependence of the property on one of the function arguments.

Functions are edited within a special *Functions Editor* window available by using *Functions* menu item.

To set a function for a property one needs change property type to function and then pick up the function name in the drop down list in *Value* column. For alloys, the function name is shown instead of value of the first bowing parameter.

NB: Note that using functions may lead to the situation when the property of a material may differ from the property of the alloy which is in fact 100% consists of this material. For instance, we have AlN, InN, and GaN materials and $Al_xIn_yGa_{1-x-y}N$ alloy made of these

materials. If some property of $Al_xIn_yGa_{1-x-y}N$ alloy is specified with a function, it may happen that its value for *x=y=0* (i.e. the case when alloy entirely consists of GaN) differs from the value of this property in GaN material. This situation may lead to confusion when simulation results depend on how GaN layers are specified - as GaN material or as $Al_xIn_yGa_{1-x-y}N$ alloy with *x=y=0* composition.

7.3.3 Parameterization

Some properties can be calculated form other properties by pre-defined equation (parameterization). All the pre-defined parameterization are discussed in details in [1].

One can use function (or, generally, even constant) instead of parameterization. To make property be calculated with the parameterization one needs change property type to parameterization. For alloys, the respective string is shown instead of value of the first bowing parameter

8 Frequently Asked Questions

8.1 Should I always start from n-type layers in 'Heterostructure' list?

Yes, the 'Heterostruture' list has a fixed direction, from n-side to p-side, no matter what is the actual growth direction. Besides, in all graphs representing the heterostructure (band diagram, waveguide modes, etc) direction from left to right corresponds to the direction from n-side to p-side.

8.2 What should be the first heterostructure layer?

If you are simulating an LED with planar current spreading, the first heterostructure layer to be thick n-type contact layer responsible for the lateral current spreading. You need not input nucleation buffer layers. For instance, your real structure looks as:

1. Sapphire substrate
2. Nucleation layer
3. Buffer layers
4. Undoped GaN
5. 3 um n-GaN
6. LED structure layer 1
7. LED structure layer 2
8. ….

Then your input in SiLENSe should be only

1. 200 nm n-GaN
2. LED structure layer 1
3. LED structure layer 2
4. ….

The reason is that SiLENSe assumes that the current flows through all the layers specified in 'Heterostructure' tab of SiLENSe. Also, you can reduce the thickness of the first layer down to 200-300 nm (far away from the active region the current is governed just by the Ohm law).

8.3 Some materials (sapphire, SiC) have a lack of properties

As for sapphire and SiC materials, they was included to database only for their optical properties, since they are important for computation of the waveguide modes in laser diodes (see substrate specification in the 'Laser parameters' tab). We do not expect their use in the 'Heterostructure' tab, so we do not care about their properties except to the refractive index and related parameters.

8.4 Non-radiative recombination parameters

The non-radiative recombination is calculated as a sum of contributions of dislocations, point defects, and Auger recombination (Eq. 6.1 of SiLENSe Physics Summary). Both dislocations and point defects are described within the Shockley-Read-Hall approach. We have developed a special model which relates the dislocation density to the carrier non-radiative lifetimes. Direct input of the lifetimes is also possible in respective text fields. Blank value for both electron and hole non-radiative lifetimes results in zero recombination. If one value is blank, while other is filled, the only filled field is taken into account. For instance, if tau_e =1ns and tau_h = "blank", R = n/tau_e .

Thus, the user can use the model and input dislocation density (with blank recombination lifetimes because of point defects) or input lifetimes directly with zero dislocation density. Use of both dislocation density and lifetimes is possible, but in this case the lifetimes must describe the contribution of the defects except to the dislocations.

Some people claim that Indium fluctuations may improve IQE by capturing carriers and preventing them to reach dislocations. We have developed a model to describe this effect. The model needs characteristic fluctuations in the energy of the conduction and valence bands. It is assumed that DOS decays exponentially inside the energy gap. Details are given in Sec. 6.2.1 of SiLENSe Physics Summary.

The sum U_n+U_p is suggested to be nearly equal to the characteristic decay energy of the low-energy (long wavelegths) wing of the emission spectrum. It was experimentally found to about ~50 meV for different structures. Then, we suggest that U_n/U_p ratio equal to the ratio between band offsets dEc/dEv = 7/3 . So, the default values are 35 and 15 meV for conduction and valence bands, respectively.

8.5 Degree of relaxation in layer properties

By default, SiLENSe assume that all layers are grown pseudomorphically. There is an idea that at high In content real QWs are partially relaxed. In SiLENSe, the user can specify a degree of strain relaxation for each layer. Please keep in mind that if you set some strain relaxation in QWs, you have to simultaneously set complete strain relaxation in the next barrier or electron blocking layer. Otherwise, next layer will inherit lattice constant from the underlying QW. Example of an SQW structure with 50% strain relaxation is supplied with the program. Section 2 of SiLENSe Physics Summary contains all details of computation of the strain and the piezoelectric field.

8.6 What is the Indium composition fluctuation model ?

Some researchers believe that Indium fluctuations may improve IQE by capturing carriers and preventing them to reach dislocations. We have developed a model to describe this effect assuming that density of states (DOS) decays exponentially inside the energy gap. The only input parameters for the model are characteristics energies for DOS decay for conduction and valence band, U_n and U_p, respectively.

The default parameters were estimated as follows. The sum of U_n and U_p is suggested to be nearly equal to the characteristic decay energy of the low-energy (long wavelength) wing of the emission spectrum. The latter was experimentally found to be about ~50 meV for different structures. Then, we suggest that U_n / U_p ratio equals to the ratio between the band offsets $\Delta E_C/\Delta E_V$ = 7/3 . So, the default values are 35 and 15 meV for conduction and valence bands, respectively. Details are given in Sec. 6.2.1 of SiLENSe Physics Summary.

8.7 Why SiLENSe does not compute the reverse current density?

The reason is that there is no good model for the carrier transport in III-nitride p-n junctions under reverse bias (and under a low positive bias, say below 2 V). The conventional drift-diffusion model considers the reverse p-n junction current as a current due to the thermal

carrier generation in the depletion region and its proximity (~ diffusion length). This approach predicts the reverse current density many orders of magnitude lower that the experimental one, because wide bandgap leads to very low thermal carrier generation.

On the other hand, in III-nitride LEDs the reverse current density (as well as that at low positive bias below) is governed by the carrier transport along the extended defects (dislocations, grain boundaries). At least, there are many experimental observations that the reverse current is suppressed by increasing the crystal quality.

Description of carrier transport through the defects is beyond the model of the carrier transport implemented in SiLENSe. Instead, we assume that Fermi levels for electrons and holes are constant. This approximation is quite realistic and allows calculation of the band diagram under reverse bias. Having the band diagram, we can compute the carrier energy levels and wave functions in the same way it is done at positive bias.

8.8 Why SiLENSe underestimates the current at low bias for III-nitride LEDs?

The reason is basically similar to the considerations in the above section titled "Why SiLENSe does not simulate reverse current". Under a low positive bias (say below 2 V) the current density due to the carrier leakage along the extended defects is much higher than conventional injection current density.

9 References

[1] SiLENSe Physics Summary.

[2] Anderson, E. and Bai, Z. and Bischof, C. and Blackford, S. and Demmel, J. and Dongarra, J. and Du Croz, J. and Greenbaum, A. and Hammarling, S. and McKenney, A. and Sorensen, D., LAPACK User's Guide, 3 ed., Society for Industrial and Applied Mathematics, PA, 1999.