SiLENSe™

Simulator of Light Emitters based on Nitride Semiconductors

User Manual

Version 5.2 & Version 5.2 Laser Edition

User Support: SimuLED-support@str-soft.com
Software Sales: STR-sales@str-soft.com
Phone: +7 812 320 4390 Fax: +7 812 326 6194
STR Group Ltd. www.str-soft.com
Engels av. 27, P.O. Box 89, 194156, St. Petersburg, Russia

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1 Overview

SiLENSe (**Si**mulator of **L**ight **E**mitters based on **N**itride **Se**miconductors) is a specialized software tool for modeling the characteristics of light emitting diodes (LEDs) made of wurtzite semiconductor materials. The software allows simulation of an LED band diagram as a function of bias, electron and hole transport inside the structure, radiative and non-radiative carrier recombination, light emission efficiency, electric field distribution, and emission spectra from the LED. The software implements a one-dimensional drift-diffusion model with account for specific features of the nitride materials – strong piezoeffect, existence of spontaneous electric polarization, low efficiency of acceptor activation, and high threading dislocation density in the structure. The software enables the analysis of graded-composition heterostructures, which is important for designing LED structures of a new generation on the basis of bandgap engineering principles.

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

Advanced numerical algorithms are employed in the solver in order to make the software more effective and robust. In particular, the mixed finite-elements method is implemented in the program to solve the nonlinear carrier transport equations coupled with the Poisson equation for the electric potential in a complex multilayer LED structure.

The code has an easy-to-learn graphical user interface (hereafter, referred to as the shell) assisting the user in preparation of the input data, carrying out simulations, and results visualization. All the results can also be exported in ASCII files and explored within an external visualizer like Microcal Origin®, Tecplot®, Golden Software Grapher®, etc.

1.1 SiLENSe Options

The current version of **SiLENSe** package provides the user with 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.

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 differential quantum efficiency.

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.

NB The software should have write permission for its home directory!

The software is supplied with license protection system based on dongle key (HASP) which is a small USB device. During installation, the user is prompted to install the dongle key driver.

2.2 Single node license

The user can install the program on several PCs (for example, on the desktop and notebook) and run the program on the PC where the dongle key is plugged in. The registration procedure is as follows:

- Plug in the dongle key module.
- Start the license manager (`License.exe`) located in the HASP folder of the **SiLENSe** home directory. One can also do it by Windows *Start* button.
- Choose the *Key config* tab and press the *Make Key* button. The key containing the information about the plugged in dongle key will be generated.
- Send the key generated to STR by e-mail simuled-support@str-soft.com .

- When the reply from STR is received, start the license manager and press *Accept Key* button.
- Insert the received key from the clipboard.
- Close the license manager.
- Run **SiLENSe**.

2.3 Corporate/department network license

Corporate/department license allows the user to run 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 computers running the software simultaneously is limited by a certain number, e.g. 10, specified in the particular license agreement (quotation, purchase order, etc.).

Hereafter, by the 'server' we will understand the computer where the USB dongle key (HASP) is plugged in. The user should install the dongle key driver on this PC. A special tool `server.exe` called below 'license server' to 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 PCs and the license server.

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

All the PCs running the **SiLENSe** software we will call 'workstations'. Running the software on the server computer is also allowed. Installation of the software on the workstations is described in Sec. 2.1. The user need not install the dongle key driver on workstations. On the contrary, one should run the `License.exe` file, choose *Server config* tab, and specify the IP address of the server PC and the port number. The *Store* button saves this information in the `Str_Config.cfg` file in the WINDOWS 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 workstation: (i) the dongle key to be plugged into the server PC, (ii) license server to be running on the server PC, and (iii) the workstation is able to communicate with the license server by the IP address and port number specified in the `Str_Config.cfg` file in the WINDOWS directory.

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

2.4 Limitations of Free Demo Version

A free demo version of the **SiLENSe** software is available at STR web site www.str-soft.com. The demo version enables the user to evaluate the software. Demo version does not allow the user to run simulation of the band diagram and carrier transport. The user can only learn the interface and work with sample project files supplied by STR. Some of them contain pre-computed results.

3 Getting Started

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

- LED heterostructure
- Global physical and solver parameters
- Properties of the materials used in the heterostructure
- Simulation results

Warning: The package 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** in the **SiLENSe** package for editing the materials properties. It provides a unified way to set up the material properties of binary semiconductor compounds and their alloys. The properties of the contact and insulating materials are also can be stored. The input data are saved in the special project file of the **Properties Editor**. All the computational modules of the **SiLENSe** package load material properties from these files. The detailed description of the **Properties Editor** is given in [1]. Below we give a short description of the **Properties Editor** in respect to the **SiLENSe**.

Generally, the materials in the **Properties Editor** are divided into two types:

- semiconductor alloys like AlInGaN, ZnMgO, AlGaAs, AlInGaP, etc.
- all other materials of fixed chemical composition and structural modification.

Below we will call them “non-alloy” materials. The default database of the material properties is supplied with the **SiLENSe** package, but the user can add new materials as well as modify the properties of the existing ones.

Creating a new **SiLENSe** project file, one should specify the **Properties Editor** project file from which the material properties will be loaded. The **SiLENSe** project file can include the layers made of the described materials and alloys. In the *Material properties* tab window, the loaded values are shown in the read-only mode. Justification of the choice of the materials constants used in the **SiLENSe** by default is given in [2].

3.2 Heterostructure

A LED heterostructure is described as a sequence of layers. The user should specify the composition, doping and thickness of each layer. The growth direction is assumed to go from the first layer to the last one. However, this assumption does not limit the software capability because the user can choose the appropriate crystal orientation in the *Heterostructure* tab window.

NB: The first layer appearing in the ‘Heterostructure’ list is thick n-type contact layer (usually GaN). The user need not input nucleation and buffer layers!

3.3 Global Parameters

In the *Global parameters* tab window, the user can specify some global physical parameters, such as LED operating 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 spectrum and I-V curve to be started from the *List of Results* window. One can open it by the *Window* | *List of Results* menu item or by the respective button in the toolbar.

3.4.1 Band Diagram and Carrier Fluxes

To start single calculation of the LED band diagram, use the *Single Calculation* menu item. The modal window appears where you will be prompted to enter the bias and start the computations. The *Calculation* 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 a *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 the temperature. List of biases is specified exactly as for series calculations, and the temperature list is specified in a similar way.

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 *List of 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 quant 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 *List of 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 [3].

3.4.4 Waveguide Modes

To compute the electric/magnetic filed distribution of the waveguide modes, use the *Run* | *Waveguide Modes* menu item. The modal window appears where you 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 compute the threshold characteristics, select the desired polarization (TE/TM) and the mode index in the *Laser parameters* tab window, and use the *Run* | *Laser Characteristics* menu item. The program will seek for the threshold performing calculation of the gain and loss for each bias (the details are given in [3], Sec. 'Laser Characteristics'). The user can see the computation progress in the progress bar and stop calculations by the *Stop* button.

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

The project file contains some simulation results related to the project. The *Window* | *List of Results* menu item or the respective button opens the *List of 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 string 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 in an ASCII file. The output formats are described in details in Sec.5.

3.5.1 Export Simulation Results to SpeCLED Module

The user can export simulation results to the **SpeCLED** module for further 3D analysis of current spreading and temperature distribution in the LED chip. One should check simulation results in the *List of Results* window and use the *Export to SpeCLED* menu item or the respective button. An *Export to SpeCLED* modal window appears with list of selected voltages. The user should start computation of emission spectrum by the *Run spectra* button. The status of spectra computation is displayed in the table. When spectrum computations are completed one can finish export by the *Export* button.

Warning: The data for **SpeCLED** module should cover the whole IV range. The voltage step should be not greater than 0.1 V for voltages higher than a turn-off voltage. For a minor current under low biases a larger step of ~0.5 V is acceptable.

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). The **SiLENSe** is provided with the interactive shell designed for easy-to-learn specifying the input data, such as thickness, composition, and doping of each layer of a LED heterostructure, and for setting the computation parameters. The shell also provides an interactive control of computations as well as visualization of the results. The start window of the **SiLENSe** shell contains *Menu*, *Toolbar* and the title of the software tool in the center of the window.

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 shell.

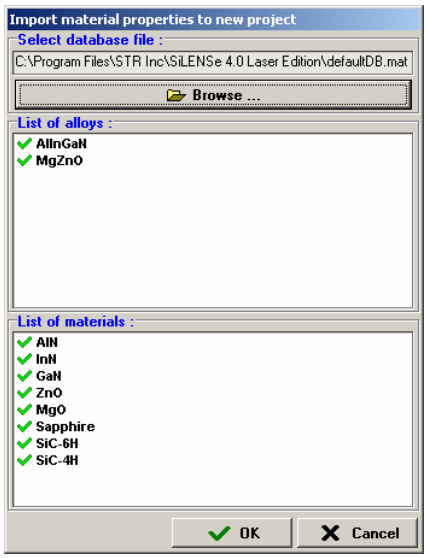


Fig. 1. Load material properties to the new project.

The menu item *New* is for creating new project. The modal window will appear where the user will be asked for the **Properties Editor** file with the material properties (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. All these actions are duplicated y 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 or overload the existent data from other **SiLENSe** project or material database file (import of the material properties).

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.

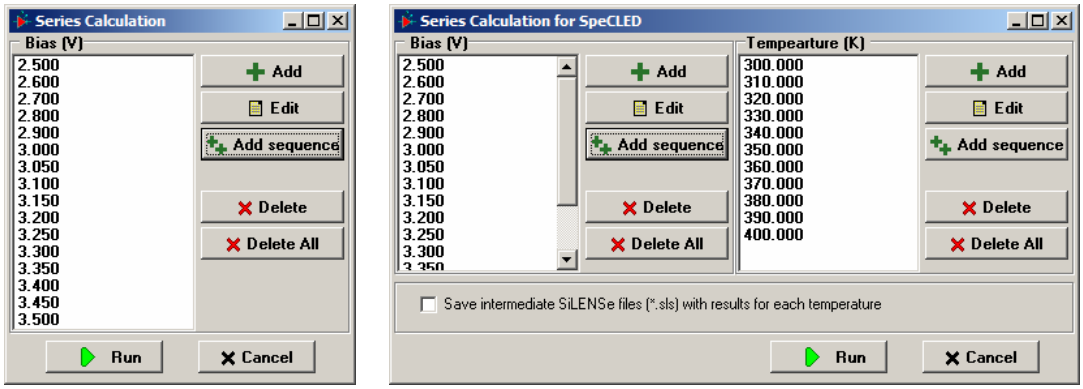


Fig. 2. Series calculations modal window (left) and series calculation for SpeCLED (right).

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 (*.sct files) 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* and *Laser Characteristics* items of the *Run* menu allow one to start the computation of the waveguide modes and laser characteristics, respectively.

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 form the *List of Results* window.

The *Export* menu enables one to save computed result to ACSII file. The band diagram for a certain bias or the I-V curve to be exported from the *List of 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 makes computations slower.

The *Window* menu is to open additional windows with solver log and auxiliary simulation results. The most important is the *List of 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 **SiLENSe**.

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.

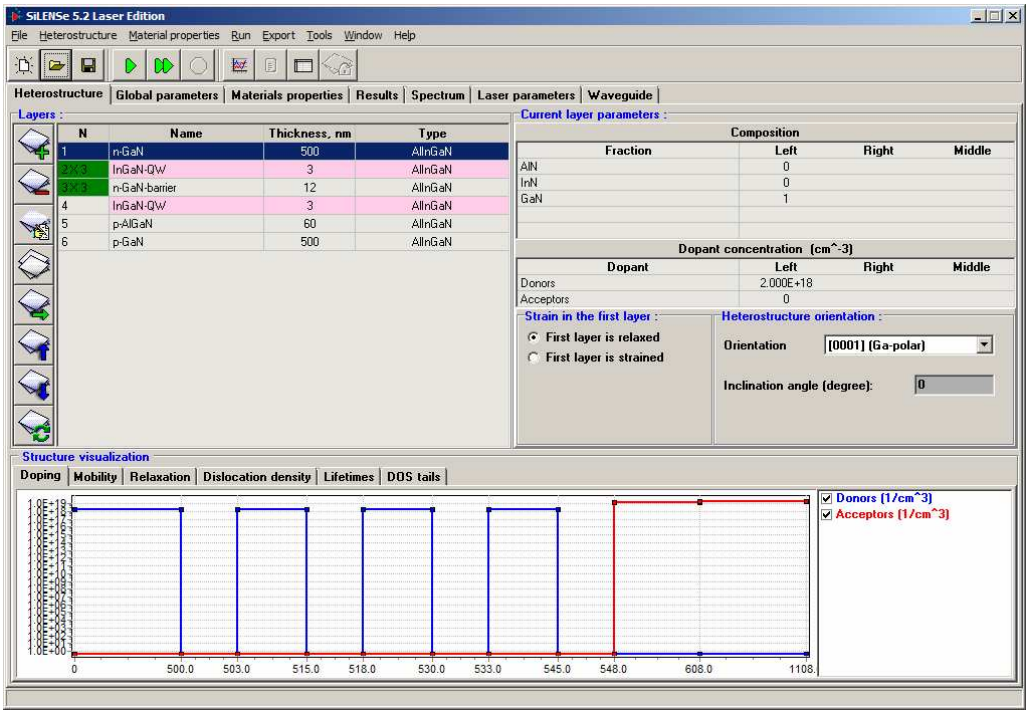


Fig. 3. Heterostructure tab window.

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, degree of the strain relaxation at the left interface of the layer, and dislocation density. Section *'Composition fluctuations'* allows the user to input parameters related to Indium composition fluctuations in InGaN material.

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.

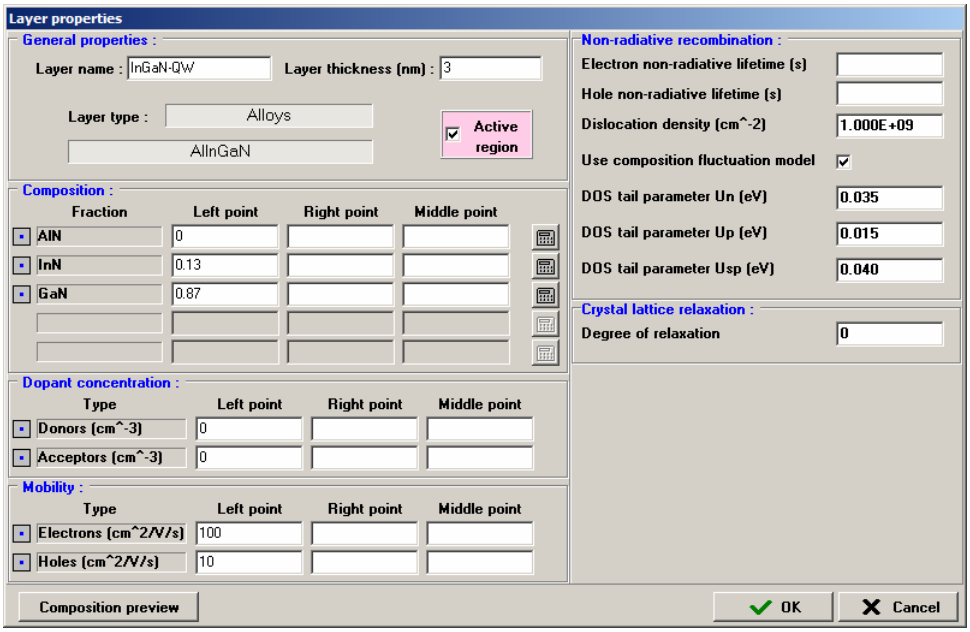


Fig. 4. *Layer properties* window.

One should mark quantum well layers by the checkbox *Active region* 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. Generally, it is recommended not to mark barriers as *Active region*. However, one can include them to see the coupling between the QWs. The details are described in [3] in the section related to the spectrum calculation.

NB: The *'Maximum number of levels in a QW'* parameter shows the maximum number of the wave functions calculated.

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 or 1 period. The heterostructure may 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. Along with conventional [0001] orientation, a number of nonpolar and semipolar orientations are supported in the software. 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.

To calculate the piezoelectric field, one need to know the strain in the heterostructure. Unstarined (natural) lattice constants for each layer are calculated from the Vegard law, while actual strained lattice constant is calculated as follows. By default, first heterostructure layer is assumed to be relaxed (*Relaxed first layer* option in the *Strain in the first layer* section), i.e. having its natural lattice constants. To specify strain in the first layer, one can choose ‘Strained first layer’ option and manually specify the lattice constant for the first layer. Then lattice constant in the next layers is calculated according to the ‘degree of relaxation’ property of the layer. Zero relaxation means that layer has the same lattice constant as underlying layer, unity relaxation means that layer has its natural unstrained lattice constant. For details, see respective section on [3].

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 Global Parameters

The Global parameters tab window (Fig. 5) represents the parameters applicable to the whole simulation and includes four subsections: *Physical parameters*, *Main solver parameters*, and *Spectrum solver parameters.*

Physical parameters are the temperature and 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. Temperature factors define the power law for temperature dependence of the radiative recombination constant and Auger recombination constants.

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

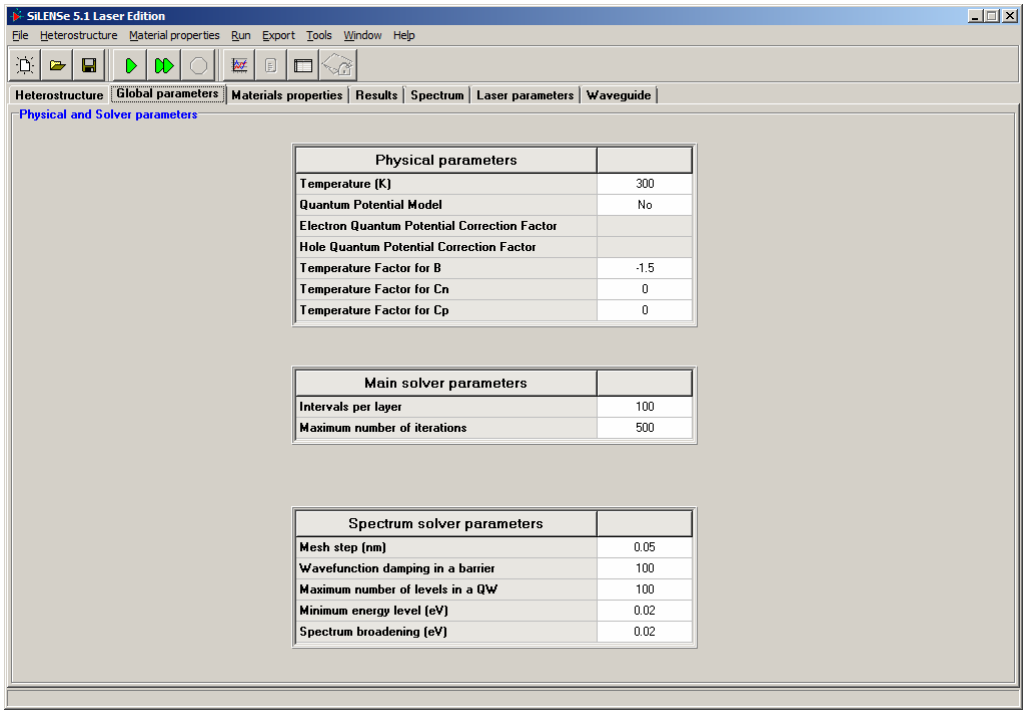
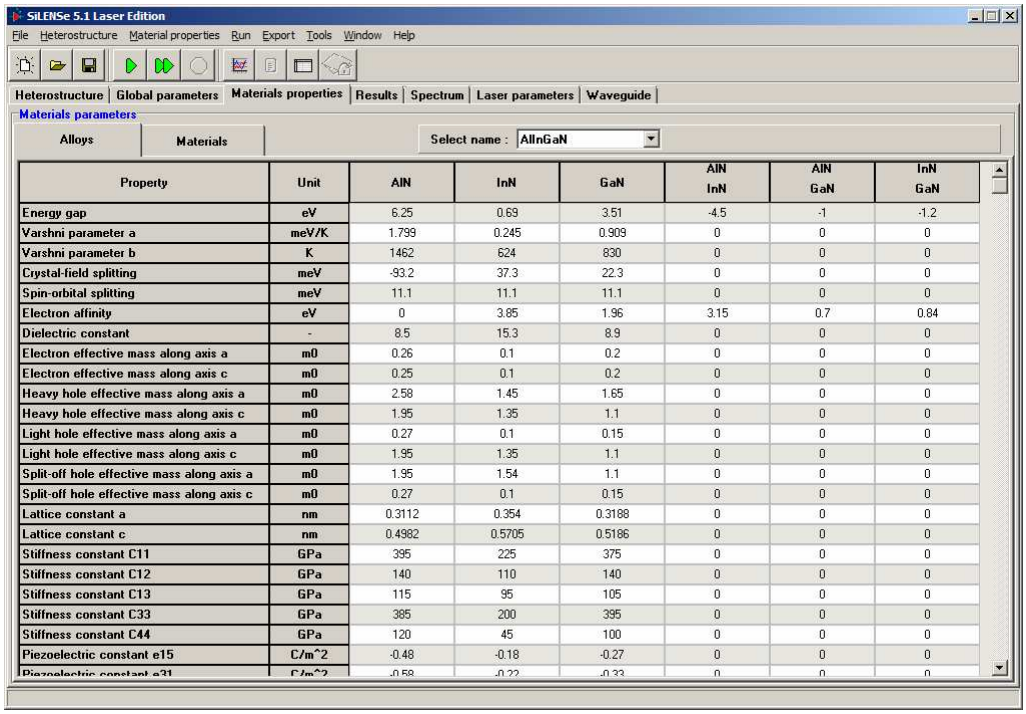


Fig. 5. Global parameters tab window.

4.2.3 Material Properties

The *Material properties* tab window 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	AlN InN	AlN GaN	InN GaN
Energy gap	eV	6.25	0.69	3.51	-4.5	-1	-1.2
Varshni parameter a	meV/K	1.799	0.245	0.909	0	0	0
Varshni parameter b	K	1462	624	830	0	0	0
Crystal-field splitting	meV	-93.2	37.3	22.3	0	0	0
Spin-orbital splitting	meV	11.1	11.1	11.1	0	0	0
Electron affinity	eV	0	3.85	1.96	3.15	0.7	0.84
Dielectric constant	-	8.5	15.3	8.9	0	0	0
Electron effective mass along axis a	m0	0.26	0.1	0.2	0	0	0
Electron effective mass along axis c	m0	0.25	0.1	0.2	0	0	0
Heavy hole effective mass along axis a	m0	2.58	1.45	1.65	0	0	0
Heavy hole effective mass along axis c	m0	1.95	1.35	1.1	0	0	0
Light hole effective mass along axis a	m0	0.27	0.1	0.15	0	0	0
Light hole effective mass along axis c	m0	1.95	1.35	1.1	0	0	0
Split-off hole effective mass along axis a	m0	1.95	1.54	1.1	0	0	0
Split-off hole effective mass along axis c	m0	0.27	0.1	0.15	0	0	0
Lattice constant a	nm	0.3112	0.354	0.3188	0	0	0
Lattice constant c	nm	0.4982	0.5705	0.5186	0	0	0
Stiffness constant C11	GPa	395	225	375	0	0	0
Stiffness constant C12	GPa	140	110	140	0	0	0
Stiffness constant C13	GPa	115	95	105	0	0	0
Stiffness constant C33	GPa	385	200	395	0	0	0
Stiffness constant C44	GPa	120	45	100	0	0	0
Piezoelectric constant e15	C/m^2	-0.48	-0.18	-0.27	0	0	0
Piezoelectric constant e31	C/m^2	-0.58	-0.22	-0.33	0	0	0

Fig. 6. Material properties tab window.

4.2.4 Results

The *Results* tab window includes six plots designed in order to clearly present the simulation results: *Band diagram*, *Potential & Electric field*, *Carrier concentration*, *Recombination*, and *Current*. Available manipulations with graphs are described in detail in Sec. 4.3.3.

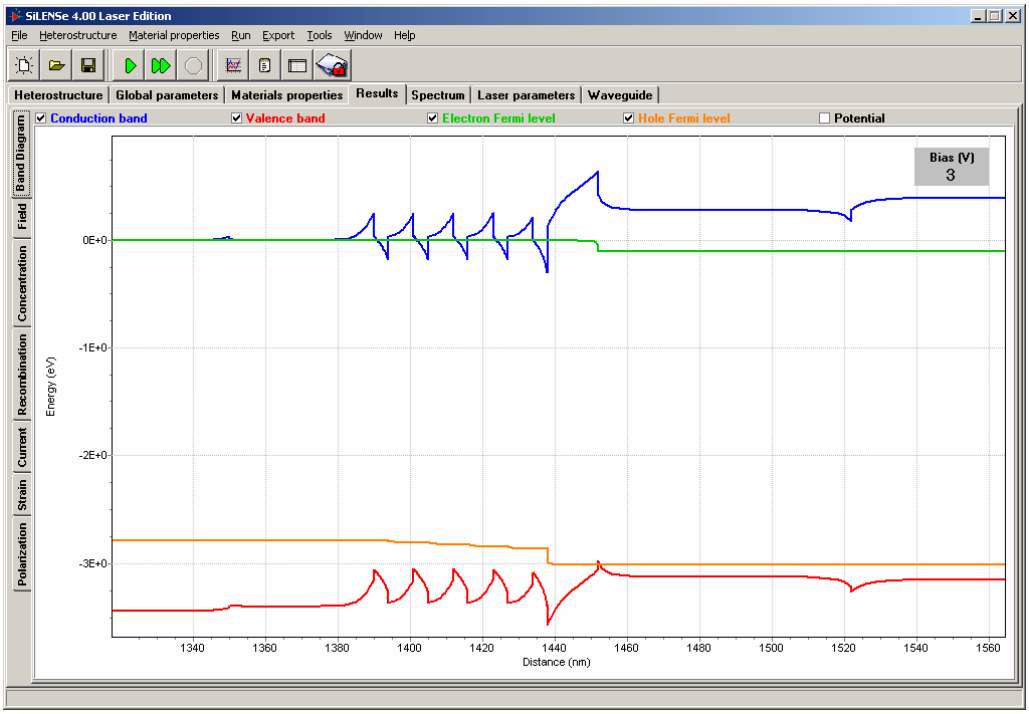


Fig. 7. Results tab window.

4.2.5 Spectrum

The *Spectrum* tab window is divided into two tabs: *Band diagram and wave functions* and *Spectrum*. The former tab contains a plot with the band diagram and carrier wave functions as well as a list of the quantum wells. The quantum wells are numbered subsequently and their indices are listed in the subsection. 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.

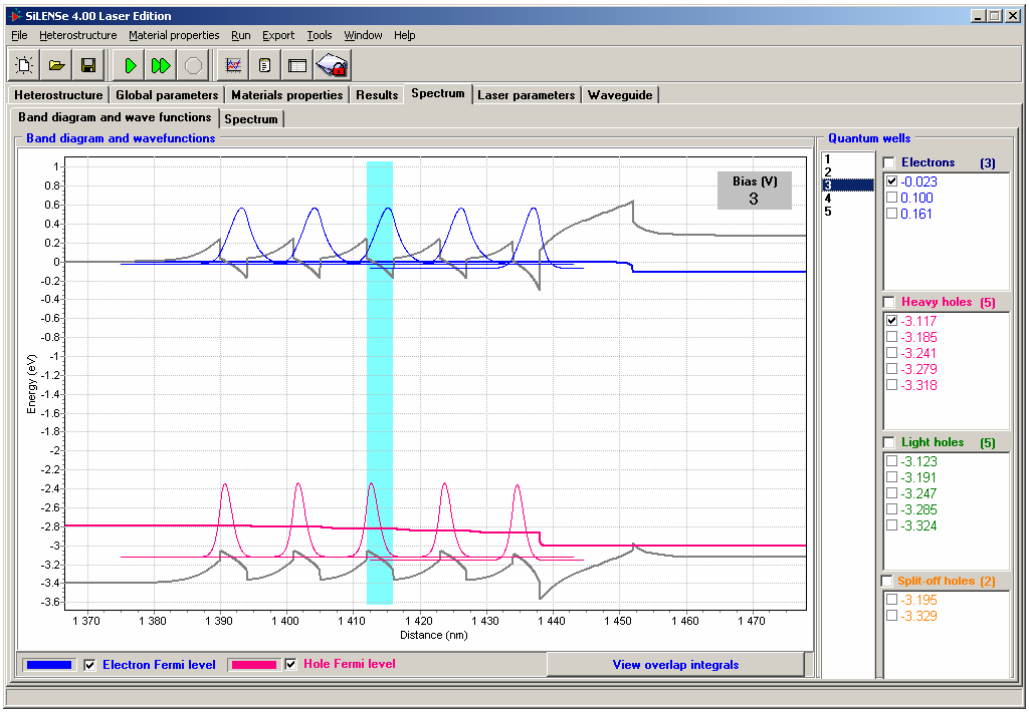


Fig. 8. Band diagram and wave functions tab window.

The *Spectrum* tab window 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 quant energy and the wavelength by the respective vertical tab.

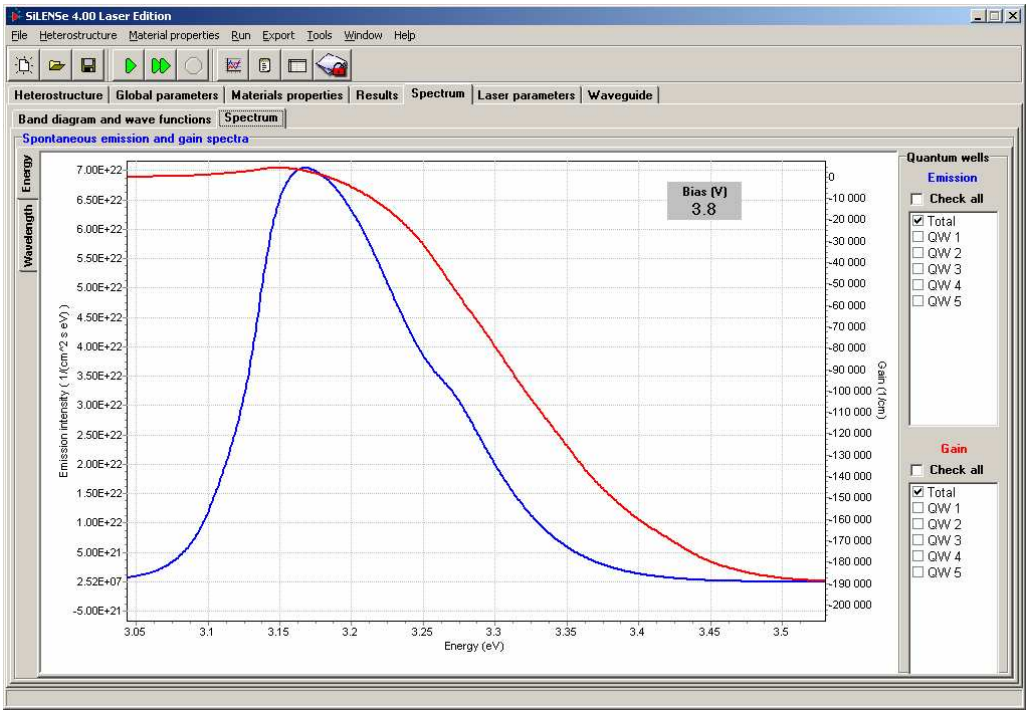


Fig. 9. Spectrum tab window.

4.2.6 Laser parameters tab window

The *Waveguide* tab window 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.

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.

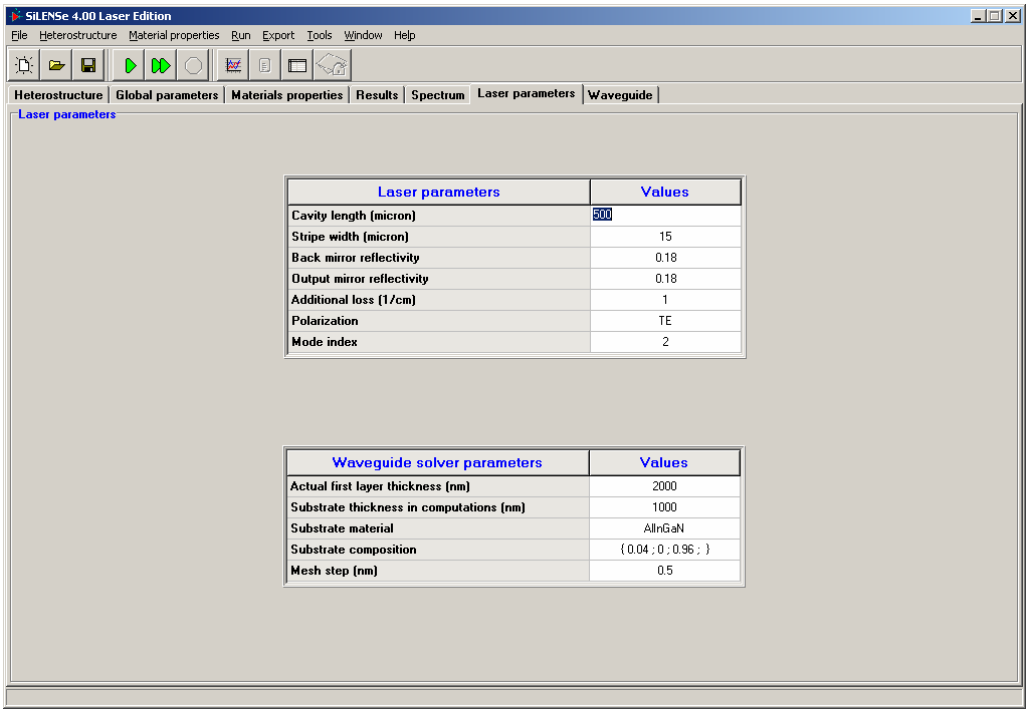


Fig. 10. Laser parameters tab window.

4.2.7 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. 11). 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 shows the distribution of the far field intensity.

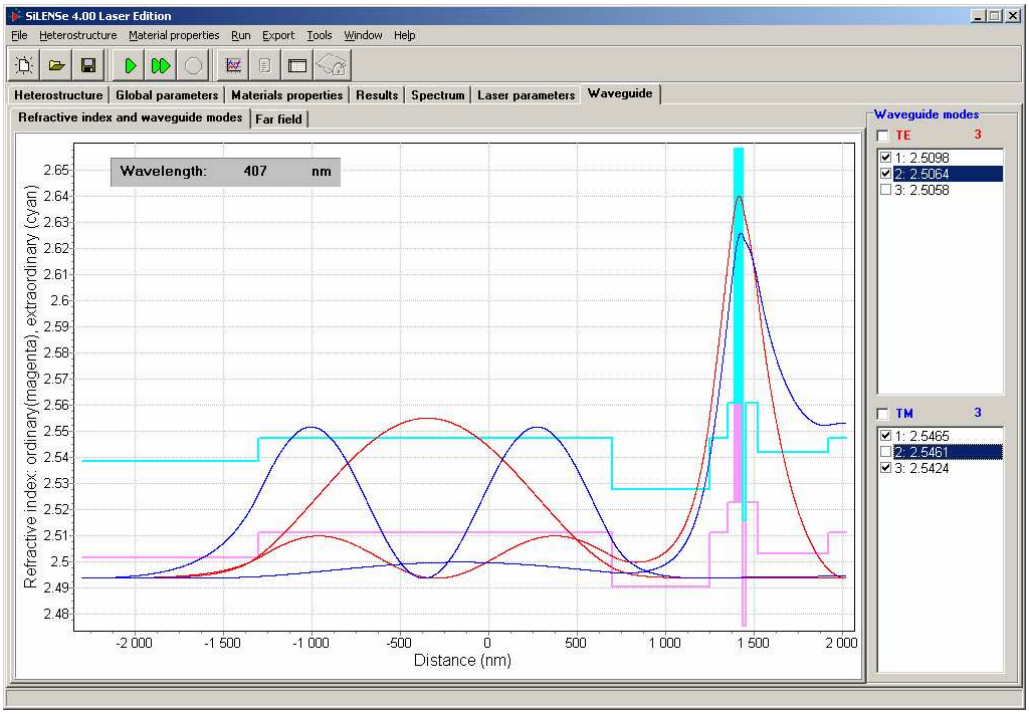


Fig. 11. *Refractive index waveguide modes* tab window.

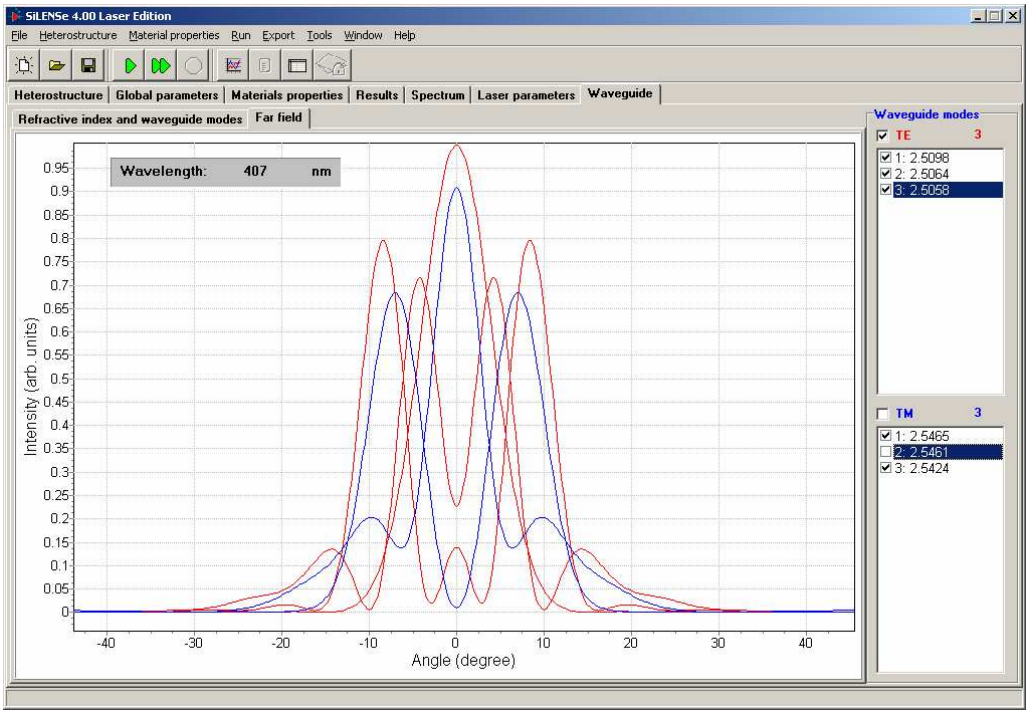


Fig. 12. *Far field* tab window.

4.3 Other Windows

4.3.1 List of Results

The *Window* | *List of Results* menu item opens the *List of 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, minority carrier current densities ($J_{n\ right}$ and $J_{p\ left}$), internal quantum efficiency (IQE), IQE computed taking into account only light generated in the active region (IQE QW), injection efficiency, non-ideality factor (m), and peak emission wavelength (Peak WL).

The menu bar of the *List of Results* window enables the user to manage the result computed. **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.

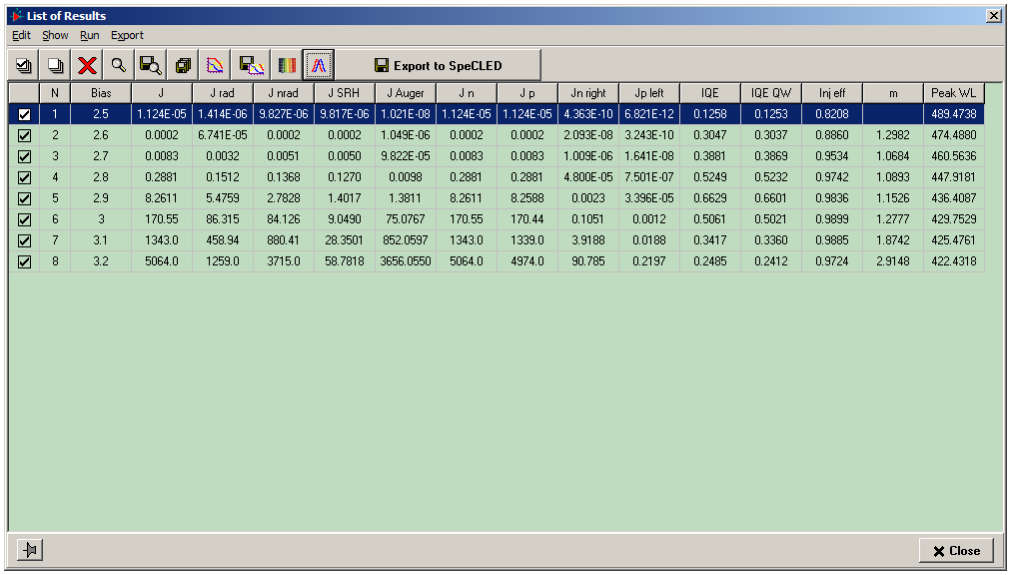


Fig. 13. List of Results window.

One can export simulation results to the **SpeCLED** module for further 3D analysis of current spreading and temperature distribution in the LED chip. One should check simulation results in the *List of Results* window and use the *Export* | *Export to SpeCLED* menu item. An *Export to SpeCLED* modal window appears with list of selected voltages. Prior to export one should start computation of emission spectrum by the *Run spectra* button. The status of spectra computation is displayed in the table. After the spectrum computation one can finish export by the *Export* button.

Warning: The data for **SpeCLED** module should cover the whole IV range. The voltage step should be not greater than 0.1 V for voltages higher than a turn-off voltage. For a minor current under low biases a larger step of ~0.5 V is acceptable.

4.3.2 I-V Characteristic

The *Show* | *I-V characteristic* menu item in the *List of 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 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 [3]. The plot is updated when one uses the *Apply* button.

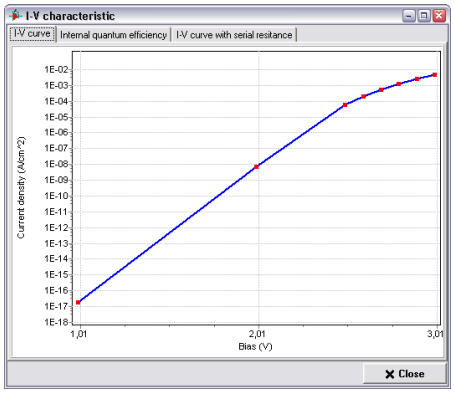
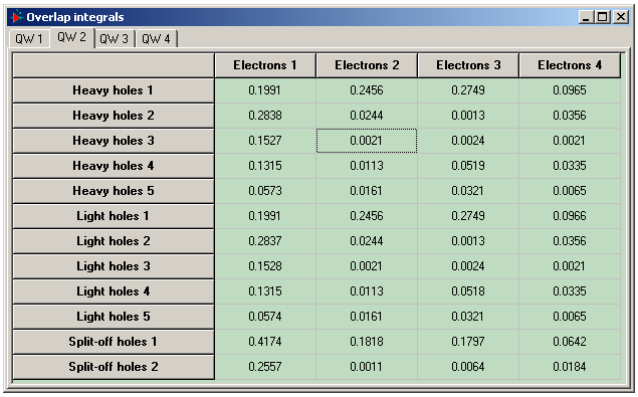


Fig. 14. I-V characteristics modal window.

4.3.3 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. 15. Overlap Integrals window.

4.3.4 Detailed Spectrum

This window allows inspect fine details of the emission spectrum. Tree in the left part of the window shows total emission spectra and total contribution of each of the valence band followed by contribution of individual QWs. Contribution of each QW is also divide into contribution 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 in ASCII format (the same effect has 'Export->Detailed Spectrum' menu item in the main window).

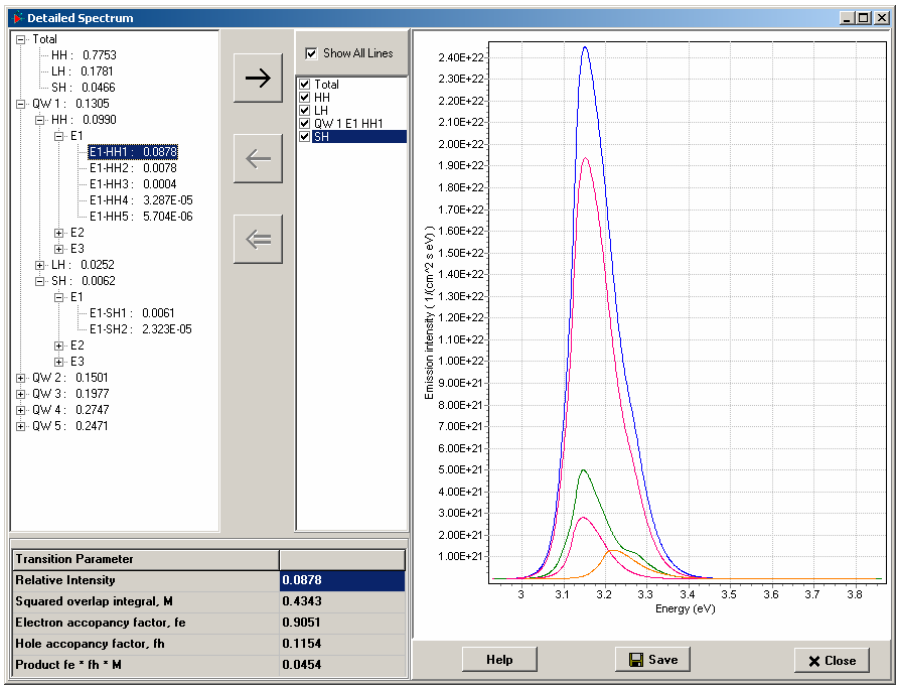


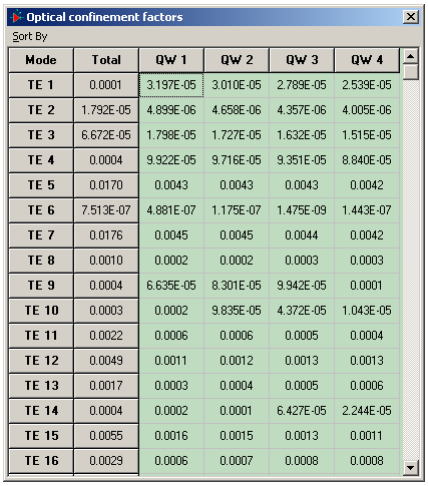
Fig. 16. Detailed Spectrum window.

4.3.5 *Optical Confinement Factors*

This window 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.



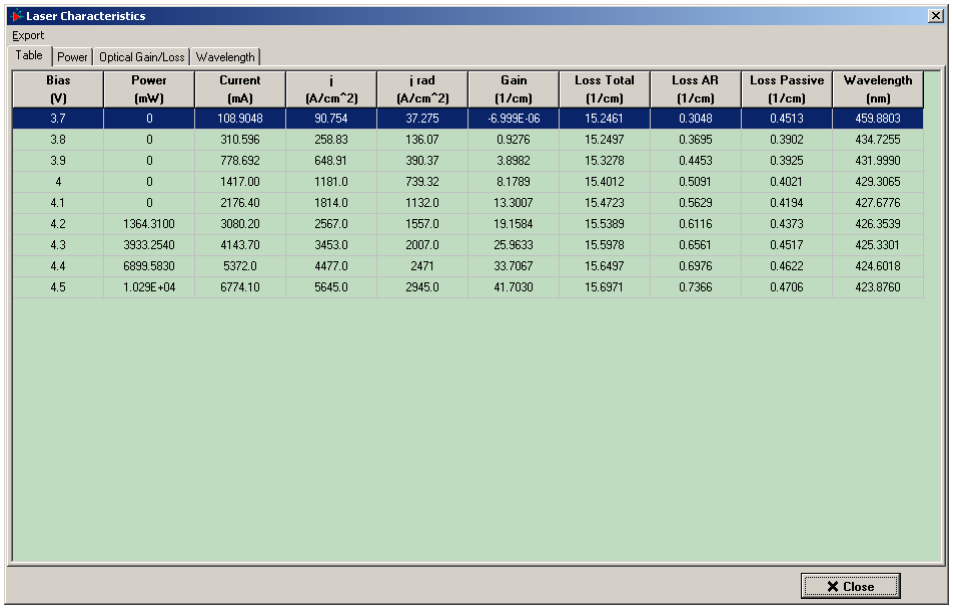
Mode	Total	QW 1	QW 2	QW 3	QW 4
TE 1	0.0001	3.197E-05	3.010E-05	2.789E-05	2.539E-05
TE 2	1.792E-05	4.899E-06	4.658E-06	4.357E-06	4.005E-06
TE 3	6.672E-05	1.798E-05	1.727E-05	1.632E-05	1.515E-05
TE 4	0.0004	9.922E-05	9.716E-05	9.351E-05	8.840E-05
TE 5	0.0170	0.0043	0.0043	0.0043	0.0042
TE 6	7.513E-07	4.881E-07	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. 17. Optical Confinement Factors window.

4.3.6 Laser Characteristics

The *Laser Characteristics* window presents the laser characteristics. The first tab 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)
- 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)	Gain (1/cm)	Loss Total (1/cm)	Loss AR (1/cm)	Loss Passive (1/cm)	Wavelength (nm)
3.7	0	108.9048	90.754	37.275	-6.999E-06	15.2461	0.3048	0.4513	459.8803
3.8	0	310.596	258.83	136.07	0.9276	15.2497	0.3695	0.3902	434.7255
3.9	0	778.692	648.91	390.37	3.8982	15.3278	0.4453	0.3925	431.9990
4	0	1417.00	1181.0	739.32	8.1789	15.4012	0.5091	0.4021	429.3065
4.1	0	2176.40	1814.0	1132.0	13.3007	15.4723	0.5629	0.4194	427.6776
4.2	1364.3100	3080.20	2567.0	1557.0	19.1584	15.5389	0.6116	0.4373	426.3539
4.3	3933.2540	4143.70	3453.0	2007.0	25.9633	15.5978	0.6561	0.4517	425.3301
4.4	6899.5830	5372.0	4477.0	2471	33.7067	15.6497	0.6976	0.4622	424.6018
4.5	1.029E+04	6774.10	5645.0	2945.0	41.7030	15.6971	0.7366	0.4706	423.8760

Fig. 18a. Laser Characteristics window : Table.

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

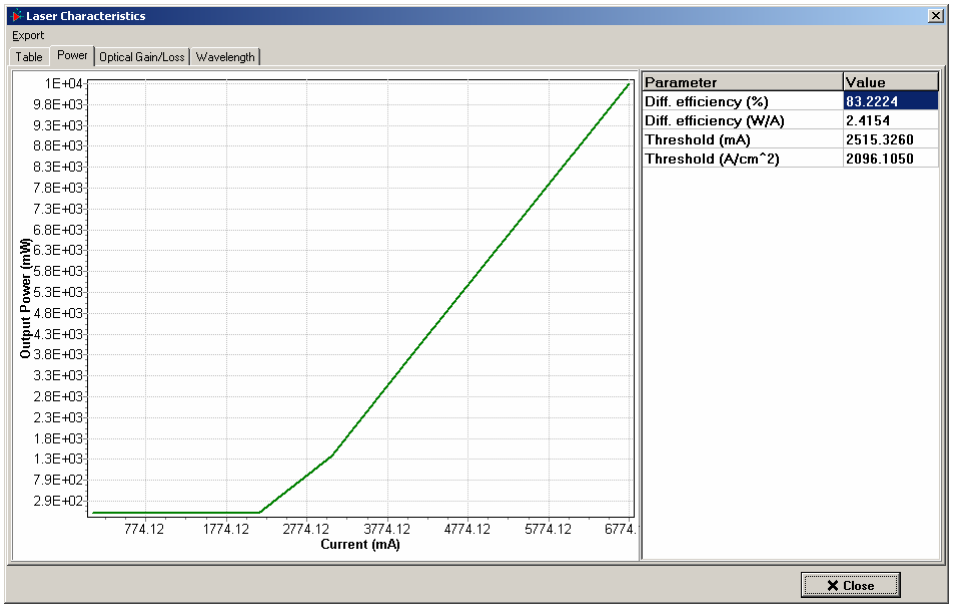


Fig. 18b. Laser Characteristics window : Power-Current characteristics.

The third tab shows variation of the optical gain and loss with the current density.

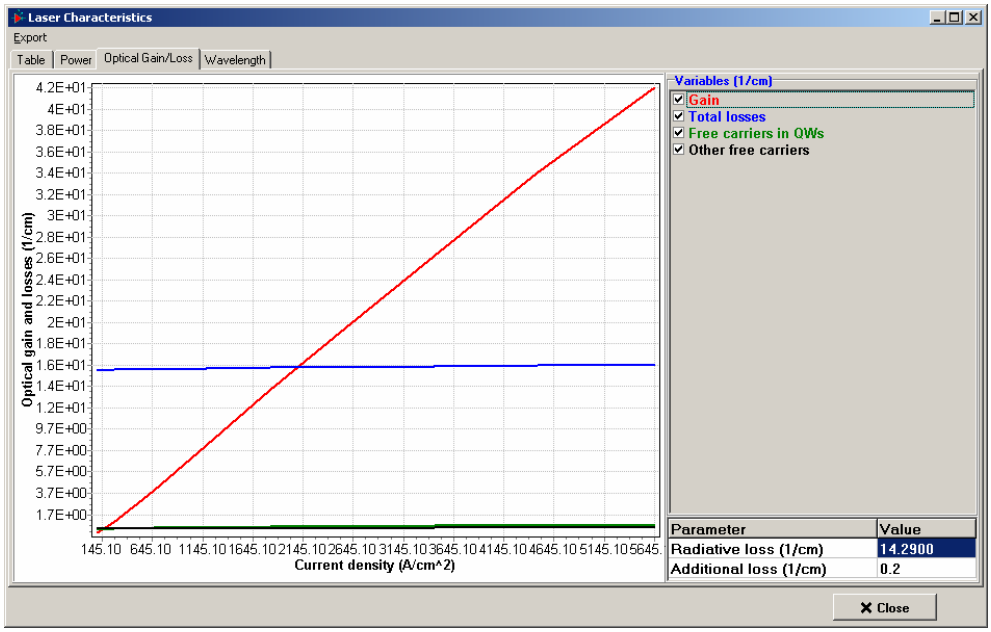


Fig. 18c. Laser Characteristics window : Optical Gain and Loss.

The fourth tab shows variation of the gain spectrum maximum with the current density.

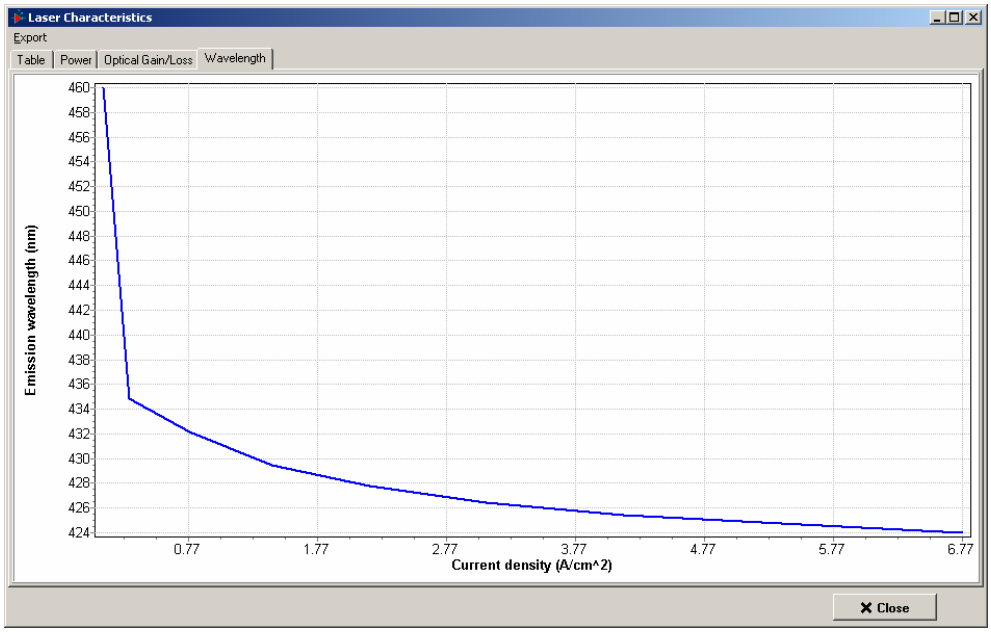


Fig. 18d. Laser Characteristics window : Wavelength.

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 either as plain text data files or as ASCII TecPlot® files (`*.plt`), which allows visualization within the graphic software package Tecplot®. Anyway, the data are stored in columns separated by tab and the difference is in the headers only.

5.1 Band Diagram, Carrier Concentrations, Recombination Rate etc.

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

- Position (nm)
- Conduction band, valence band, quantum potential for electrons and holes, electron Fermi level, hole Fermi level (eV)
- Electric potential (V) and electric field (MV/cm)
- Electron and hole current densities (A/cm^2)
- Concentration of electrons, holes, ionized donors and acceptors (cm^{-3})
- Radiative recombination, total non-radiative recombination, Shockley-Read-Hall recombination, and Auger recombination (cm^{-3} s^{-1})
- Spontaneous, piezoelectric, and total polarization (C/m^2)
- Four strain components: ε_{xx}, ε_{yy}, ε_{zz}, and ε_{yz}
- Non-radiative carrier lifetimes due to dislocations and point defects

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 *List of 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
- IQE computed taking into account recombination in QWs only
- Injection efficiency
- Peak emission wavelength (nm)
- Non-ideality factor
- Voltage (V)
- Current (A)
- 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)
- Injected electron current density (A/cm^2)
- Injected hole current density (A/cm^2)
- Electron current density at p-type boundary (A/cm^2)
- Hole current density at n-type boundary (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. 4.3.3).

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 [3].
- Refractive index for extraordinary wave modified
- Refractive index for extraordinary wave modified – see details in [3].
- 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. 4.3.6).

6 Solver Parameters

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

6.1 Main Solver Parameters

The grid is generated automatically using only the *Intervals per layer* parameter. First, the basic grid step *h* is calculated as *L* / *Intervals* , where *L* is the typical layer length. Then for all

layers the grid step in the central part of the layer equals to *h*. Near the layer boundaries, the step decreases down to 0.01 nm.

The computations are terminated if the iteration number exceeds the value of the *Maximum number of iterations* parameter.

The *Potential solver parameter* and *Fermi levels solver parameter* are used by developers to study the code performance and for further optimization. In regular version, they are shown in read-only mode.

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 [4] 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. 8.2 of [3]. 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. 8 of [3].

7 References

[1] Properties Editor User manual.

[2] Properties Editor Default Parameters.

[3] SiLENSe Physics Summary.

[4] 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.