SiLENSe™

Simulator of Light Emitters based on Nitride Semiconductors

Release Notes

Version 5.2.1 & Version 5.2.1 Laser Edition

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1. Release Notes 5.2.1

This section describes new options in version 5.2.1 compared to version 5.2:

- Improved numerical algorithm to speed up computations with using quantum potential model.
- A minor error in computation of the conduction and valence band density of states (N_C and N_V) has been fixed. The results for version 5.2.1 are slightly differ from results for version 5.2 .

2. Release Notes 5.2

This section describes new options in version 5.2 compared to version 5.1:

- Custom inclination angle is supported to specify any semi-polar crystal orientations. To calculate the inclination angle one can use Eq. (2.8) of Physics Summary.

3. Release Notes 5.1

This section describes new options in version 5.1 compared to version 5.0:

- A model for effect of the composition fluctuations on the emission and gain spectra is implemented. In layer properties, a user needs to specify the characteristic energy of the reduced density of states similarly as for the DOS tails for the carriers. Please see Eqs. (8.7, 8.9, and 8.12) of Sec. 8.3 of Physics Summary for more details.
- The model for the effect of the composition fluctuations on the internal quantum efficiency was modified in such a way that now composition fluctuations effect only recombination at the dislocations; the lifetimes related to other defects (directly specified by the end-user) remains unchanged. Please see Sec. 6.2 of Physics Summary for more details.
- Power law for temperature dependence for the radiative recombination constant, as well as for the Auger recombination constants, can be directly specified by the user in "Global Parameters" tab. Default values used for new projects and for opening projects of older versions resemble the settings of version 5.0: $B \propto 1/T^{3/2}$, and no temperature dependence for Auger coefficients. It may be reasonable to set $B \propto 1/T$ assuming 2D carrier motion in the quantum wells.
- Improvements of the user interface:

- Current density converted into Shockley-Read-Hall recombination, current density converted into Auger recombination, and non-ideality factor are shown in the "List of Results" window in columns titled "J SRH", "J Auger", and "m", respectively. Then these values can be exported into the table using "Export -> IV characteristic" menu item or the respective button from the toolbar.
- Peak wavelength of the emission spectrum is available in the "List of Results" window by using "Run -> Update Peak Wavelength" menu item or the respective button from the toolbar. Then the peak wavelength can be exported into the table using "Export -> IV characteristic" menu item or the respective button from the toolbar.
- Export of all results (band diagram, Fermi levels, carrier concentrations, recombination rates, etc.) into a single text file is available in "List of Results" window by using "Export -> All Results in Single File" menu item or the respective button from the toolbar.

4. Release Notes 5.0

This section describes new options in version 5.0 compared to version 4.4:

- Quantum potential model is developed to account for quantum effects: tunneling current and quantum confinement of the carriers inside the quantum wells. Use of the quantum potential model allows more realistic prediction of the current-voltage characteristics of the p-n junction. Also, the carrier concentration in the quantum wells is predicted more accurately. One can switch on/off use of the quantum potential model in "Global parameters" tab.
- Recombination through the dislocation cores and through the point defects are combined into one Shockley-Read-Hall recombination channel. First, the overall carrier lifetimes are calculated as $\tau_{n,p}^{tot} = \left[\left(\tau_{n,p}^{dis}\right)^{-1} + \left(\tau_{n,p}^{def}\right)^{-1}\right]^{-1}$ and then the overall lifetimes are used to calculate the Shockley-Read-Hall recombination rate. The computations results remain generally the same, but minor differences compared to the previous versions may appear for the projects where dislocations and point defects are specified simultaneously.

5. Release Notes 4.4

This section describes new options in version 4.4 compared to version 4.2:

- Multiple periodic structures are supported. Periodic structures are specified exactly as in the previous versions.
- Automatic generation of data for SpeCLED. The user need once set a list of biases and a list of temperatures, and the program will automatically run simulations and store a set of *.sct files for input into SpeCLED. Optionally, intermediate SiLENSe project files with results are also stored.
- In *.sct files for SpeCLED, the information on the emission spectrum is reduced to the peak wavelength only. It is done to reduce the size of *.sct and *.dvx files. Users of SpeCLED are welcome to update the SpeCLED solver to support this change in the SiLENSe export data.
- Support of licensing system based on Senselock dongles (previous HASP dongles are also supported).

6. Release Notes 4.2

This section describes new options in version 4.2 compared to version 4.1:

- Material properties of zinc blende III-V compounds are updated. Particularly, AlGaInP and GaInAsP alloys lattice matched to GaAs are added, as well as respective simulation examples.
- After computation of the emission spectrum, detailed information about contribution of each subband of the valence band is available, as well as contribution of each particular transition. Use 'Window->Detailed Spectrum' menu item and enjoy complete info about emission spectrum!
- Carrier non-radiative lifetimes because of dislocations and point defects are available both in the internal visualization and in export ASCII files.

7. Release Notes 4.1

This section describes new options in version 4.1 compared to version 4.0:

- Material properties of InAlGaAs alloy and simulation example for AlGaAs laser diode are added.
- Material properties of CdMgZnO alloy and simulation examples for hybrid II-O/III-N heterostructures are updated.
- Computation of the band diagram, carrier energy levels and wave functions under reverse bias (see Sec. 11 of SiLENSe Physics Summary). **NB!** This option does not include prediction of the reverse current!

- Computation of the internal quantum efficiency taking into account only emission from the active region, and computation of the injection efficiency (see end of Sec. 7 of SiLENSe Physics Summary).

8. Release Notes 4.0

This section describes new options in version 4.0 compared to version 3.60:

- Simulation of nonpolar and semipolar orientations. The user can choose the orientation in the respective combo box in the 'Heterostructure' tab. To calculate the piezoelectric fields in semipolar structures, new material properties were introduced: lattice constant c, piezoelectric constant e_{15}, and stiffness constants C_{11}, C_{12}, and C_{44}.

NB! It is strongly recommended to add new material properties in the files created be earlier versions, use *'Material Properties->Import'* menu item and choosing default database supplied with the current version of the software.

- *'Substrate'* section is removed from the *'Heterostructure'* tab. Instead, the user should indicate if the first heterostructure layer is strained[1]. If yes, one should specify its lattice constants a and c. The option of input of the substrate lattice constant by composition is removed. By default, all files newly created or converted from older versions are assumed to have relaxed first layer. If you see a warning about the lattice constant specification during opening old project file, please check the input data in the 'Strain in the first layer' section in the center of the 'Heterostructure' tab.

- Changes in the user interface:
  - ✓ Export of plots to graphic files (`*.bmp`, `*.wmf`, and `*.emf`) is available by 'Export->Save current chart' menu item.
  - ✓ Visualization of the layer properties (doping, mobility, dislocation density, carrier lifetimes, etc) in the bottom chart of the '*Heterostructure'* window.
  - ✓ Two solver parameters are made read-only: '*Potential solver parameter'* and *'Fermi level solver parameter'*.

[1] First layer appearing in the heterostructure list is a thick n-type layer, usually made of GaN. Typically, it is not strained. The user need not input the nucleation and buffer layers in the heterostructure list.

9. Release Notes 3.60

This section describes new options in version 3.60 compared to version 3.42:

- Temperature dependence of the energy gap is described in terms of Varshni parameters a and b. However, SiLENSe project files (*.sls) of older versions will be converted as having temperature-independent energy gap (a=0, b=1), to provide backward compatibility of the results[2]. The user can update material properties by using 'Materials Properties -> Import' menu item.
- Model of Indium composition fluctuations on the IQE. SiLENSe project files (*.sls) of older versions will be converted as having no fluctuations (Un=Up=0) to provide backward compatibility of the results[2].
- Some improvements are made in the user interface. Particularly, we have added internal visualization of the following variables: unstrained and strained in-plane lattice constants, strain, spontaneous polarization, piezoelectric polarization, and total polarization.

10. Release Notes 3.42

This section describes new options in the version 3.42 compared to version 3.4:

- Computation, visualization, and export of the far field distribution (available in **Laser Edition** only).
- Support of network corporate/department HASP license.
- No limitation on the maximum number of the points in the quantum well in computation of the carrier wave functions. Instead, the maximum number of the energy levels is limited in order to prevent to long computations.
- Some improvements are made in the user interface.

11. Release Notes 3.4

This section describes new options in the version 3.4 compared to version 3.0:

- Computation of the gain spectrum.
- Visualization of the emission and gain spectra of individual quantum wells (the previous version shows the total spectrum only).
- Listing of the overlap integrals between each pair of electron and hole wave functions in the active region.

[2] It means that re-running simulations with new version will give the same results.

- A number of improvements in the user interface.

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:
  - ✓ Optical gain.
  - ✓ Optical losses caused by the free carrier absorption.
  - ✓ Threshold current and differential quantum efficiency.
- Updated database of materials properties to include optical characteristics of III-nitride materials.

- **NB:** To run laser computations for the project files of version 3.0 and older one should previously update the materials properties to add optical properties! Use the *Materials Properties I Import* menu item and select an appropriate file with materials properties. The default database is provided with the package, and the user can modify it via the **Properties Editor** tool.

12. Release Notes 3.0

This section describes new options in the version 3.0 compared to version 2.1:

- Non-radiative recombination through the point defects is calculated within the Shokley-Read-Hall model. The user can manually specify the electron and hole lifetimes in each layer of the heterostructure.
- Auger recombination. This option is included in order to enable the user to analyze conventional III-V heterostructures where Auger recombination is important channel of non-radiative recombination.
- Partial strain relaxation is included for accurate calculation of the piezoelectric charges at the boundaries of partially relaxed layers. The user can manually specify the degree of relaxation for each layer of the heterostructure.
- The user can specify different threading dislocation density for different layers.
- Export/import of material properties. The user can save the materials properties of the existing **SiLENSe** project (`*.sls`) in a separate material database file (`*.mats`) as well as load new material properties to the existing **SiLENSe** project from other database files or other **SiLENSe** projects.

- The project files of 2.1 version are converted as follows:
  - ✓ For each layer:
    - ❖ zero degree of relaxation
    - ❖ no additional recombination via point defects
    - ❖ dislocation density taken from the old file
  - ✓ Zero Auger coefficients are added to material properties of all materials listed in the project file.
  - ✓ In the saved results all the non-radiative recombination is suggested to come from the dislocations.
- Under these conditions re-running an old project file with version 3.0 will give the same result as for version 2.1.

13. Release Notes 2.1

This section describes new options in the version 2.1 compared to version 1.0:

- Boundary conditions for electrons are modified to account for their contribution to the current at the p-electrode. This effect has been found to control the current at a high forward bias. In version 2.1, an Ohmic contact is assumed for holes at the p-electrode, while the electron current at this boundary is calculated in terms of thermal emission. At a low bias, the model gives the results being in close agreement with those predicted by the former version of the code. At a high bias, the new approach provides more reasonable predictions.
- The package includes a module for setting/editing materials properties, which enables one to consider not only III-nitrides, but also a wide range of wurtzite semiconductor materials and alloys with user-defined properties. Version 2.1 includes data on properties of AlInGaN and ZnMgO alloys.
- The radiative recombination constant is considered as a temperature-dependent parameter.
- Advanced numerical algorithms are used providing more fast and stable code operation.
- New graphical user interface includes internal vizualizer providing an excellent representation of the simulation results.
- Export of simulation results to the software package **SpeCLED** (http://www.str-soft.com/products/SpeCLED) for further 3D analysis of current spreading and temperature distribution in the LED chip.

14. Support

Hot-line support is provided for customers. The support includes free of charge supply of updated versions released during the support period and technical consulting on **SiLENSe** operation.

15. More info

More detailed information about the **SiLENSe** package is available at the site of STR, Inc.: http://www.str-soft.com/products/SiLENSe. Evaluation package can be requested by the e-mail address simuled-support@str-soft.com .