



# SiLENSe™

Simulator of Light Emitters based on Nitride Semiconductors

## Release Notes

Version 6.5 & Version 6.5 Laser Edition



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## Table of contents

1.	Release Notes 6.5.....	3
2.	Release Notes 6.4.....	3
3.	Release Notes 6.3.....	4
4.	Release Notes 5.15.....	6
5.	Release Notes 5.14.....	7
6.	Release Notes 5.13.....	7
7.	Release Notes 5.12.....	7
8.	Release Notes 5.11.....	8
9.	Release Notes 5.10.....	10
10.	Release Notes 5.9.....	11
11.	Release Notes 5.8.....	11
12.	Release Notes 5.4.....	12
13.	Release Notes 5.2.1.....	13
14.	Release Notes 5.2.....	13
15.	Release Notes 5.1.....	14
16.	Release Notes 5.0.....	15
17.	Release Notes 4.4.....	15
18.	Release Notes 4.2.....	15
19.	Release Notes 4.1.....	16
20.	Release Notes 4.0.....	16
21.	Release Notes 3.60.....	17
22.	Release Notes 3.42.....	18
23.	Release Notes 3.4.....	18
24.	Release Notes 3.0.....	19
25.	Release Notes 2.1.....	19
26.	Support.....	20
27.	More info.....	20

## 1. Release Notes 6.5

In version 6.5, simulation of structures with tunnel junctions (TJs) is implemented. Tunnel junction regions can be specified in the heterostructure similarly to the periodic structures. One can use "Heterostructure -> Create/Delete Tunnel Junction" and "Heterostructure -> Edit Tunnel Junction" menu items. 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.

In addition, the following improvements has been implemented.

- An error is fixed in computation of differential efficiency and laser output power in laser computations with simplified laser model. Instead of injection efficiency into QW, the ratio of the recombination current over the whole structure to the total current was used. The error was important in case when carrier leakage is considerable and also there is a considerable recombination outside QWs.
- An error is fixed in conversion of projects of versions 5.14 and 5.15 into versions 6.x. The error was related to the layers made of the following III-V materials "Ga(0.51)InP\_G", "Ga(0.51)InP\_X", "Al(0.52)InP\_G", and "Al(0.52)InP\_X".

## 2. Release Notes 6.4

In version 6.4, simulation of photoluminescence (PL) is updated in such a way that carriers generated by PL excitation are included into the main drift-diffusion computations. As users can specify the p-n junction bias together with PL excitation, PL simulation can predict the



photocurrent and can be used for simulation of photodiodes and single-junction solar cells. The default dataset includes a simple model for the absorption coefficient for III-nitrides. Users are welcome to update these data, if necessary.

Also, a minor error is fixed in computation of the free-carrier absorption coefficient used in laser computations.

### 3. Release Notes 6.3

Version 6.3 is a major update of the software including advanced models for material properties and a new solver with improved speed and convergence. Listed below are the new options in version 6.3 as compared to version 5.15.

- In cubic III-V compounds, three valleys of the conduction band ( $\Gamma$ , X, and L valleys) are included into simulation. The electron concentration in each valley is calculated independently. So, smooth transition from direct gap to indirect gap alloys is handled automatically with no additional efforts on the user side.
- Bowing parameters now include the sign "-" because this way of specification is more common. In other words, in version 6.0 if the bowing parameter for an alloy (say, InGaAs) is positive, it means that the energy gap of the alloy is lower compared to linear interpolation (Vegard law). In versions 5.x (and earlier) positive sign of bowing parameter meant increase of the energy gap compared to the Vegard law.
- Concentration of three types of holes (heavy, light, and split-off) is calculated independently.
- Strain effect on the energy band of each type of electrons ( $\Gamma$ , X, and L valleys) and holes (heavy, light, and split-off) is included into the model.
- Effective masses of electrons and holes can be calculated from k-p model (default option) or specified directly (like in previous versions). In "Material Properties" tab, if a property for a binary material is specified with "Parameterization" type, the respective cell of the table appears as "\$Par (x.xx)" where x.xx is a calculated value of the property. This is not applicable to refractive index and absorption coefficient, as they also depend on wavelength. The user can see calculated values of carrier effective masses which are used in simulations.
- Quaternary alloys where atoms in both sublattices can be varied, like InGaAsP and GaInAsSb, are fully supported now. The energy gap is calculated through energy gap of 4 binary compounds and bowing parameters for 4 ternary alloys.

- In cubic III-V compounds, new options are added allowing the user to automatically calculate the radiative recombination constant  $B$  and Auger recombination constant  $C_n$  from band structure parameters and effective masses (default option) or specify them directly (like in the previous versions).
- In the current version, the default value for Auger recombination constant  $C_p$  is zero, because there are a lot of different applicable models depending on the energy gap, spin orbital splitting, and temperature. Users are welcome to modify  $C_p$  value for their particular structure.
- In cubic III-V compounds, piezoelectric polarization is included into the model in case of [111] growth direction.
- New model for spectral dependence of the refractive index is implemented. For III-nitride materials, the resulting refractive index is close to the old model. However, the index of lasing mode (i.e. the mode with the maximum optical confinement factor) can be changed. So after updating laser projects from previous version, please do waveguide simulation and correct the mode index parameter in laser parameters, if necessary.
- To specify the band offsets between different materials, the ionization energy (the distance between the vacuum level and valence band) is introduced instead of electron affinity (the distance between the vacuum level and conduction band). This approach provides more convenient way of dealing with transition between direct gap and indirect gap alloys.
- Change of the dielectric constant of III-N materials due to anisotropy and piezoeffect is included into the model.
- In results, the strain components are outputted in coordinate system related to the crystal lattice, but not to the epilayers.
- PL computations are not supported in the current version. They will be restored in future with account of transport of photoexcited carriers. Also, default value for the absorption coefficient is set to zero (it was used only for PL computations).
- In laser computations, automatic selection of the waveguide mode with highest optical confinement factor is implemented. To use this option, one needs specify 0 for the index of the waveguide mode.
- New solver with improved speed and convergence is implemented. Particularly, it can work with extended precision of the floating point numbers. In case of any problem with convergence, it is recommended to increase the precision up to the maximum value (256 bit).

**NB** Due to the changes listed above, project files generated in version 5.x (and all previous versions) can not be completely supported. An attempt to open the file created in older versions will result in the following automatically implemented procedure:

- Project files of versions 5.14 and 5.15 will be automatically updated as following:
  - Material properties are imported from new default datasets "Wurtzite.matprop" or "Zinc Blende.matprop" supplied with the software. Material properties of the old project will be ignored.
  - Layers defined in previous versions will be recognized, necessary updates in material names and composition will be made (say, alloy names "AlGaX-direct" and "AlGaX-indirect" are both replaced by "AlGaAs") to comply with the new version. However, if the old project includes materials added by the user and the structure includes layers made of those materials, these custom materials will not be recognized. The error message with the list of such materials will appear and update will be cancelled.
  - Global parameters (like temperature, solver settings, and so on) are taken from the project file. New parameters are added with their default values.
  - All simulation results are discarded as they became inconsistent with the new material parameters and physical models.
- Project files of versions released before version 5.14 are not supported now. The user can use the following steps to convert these project files:
  - Open your project file with SiLENSe 5.14 (supplied with the software for this purpose)
  - Update your project to version 5.14 (recognized by the version 6.3) by just saving it with a new name. Now you can open it with version 6.3.
- Project of versions 6.0, 6.1, and 6.2 are converted is a regular way, keeping old material properties and simulation results. One can use "Material Properties -> Import" menu item to import default material properties to use parametric dependence of recombination constants B and  $C_n$  in cubic materials (it is the only new option appeared in version 6.3 compared to versions 6.0 - 6.2).

## 4. Release Notes 5.15

This section describes new options in version 5.15 compared to version 5.14:

- Additional output for laser simulation is added into text export file with band diagram: refractive index (ordinary and extraordinary), field intensity (squared field) of the

waveguide mode selected in "Laser Results" tab, distribution of the free carrier absorption, and product of the free carrier absorption and field intensity of the mode.

This output is added both to laser results and LED results (if the old simplified laser model was used to estimate the threshold based on this LED result).

For LED results, the peak wavelength and FWHM parameters are stored in the project file (there is no need to recalculate them after re-opening of the project file with results).

## 5. Release Notes 5.14

This section describes new options in version 5.14 compared to version 5.13:

- FWHM of the emission spectrum is added into LED Results table.
- An error in position of hole subbands has been fixed in computation of the emission spectrum. The error reveals itself only for spectrum computation and only for AlGaIn QWs of high Al composition, where heavy holes are not the top subband. Results for InGaIn QWs are not effected by the error.
- Additional convergence control has been introduced. In some very rare cases, computations are considered as successfully finished, but results are not converged. Now users can specify an additional check - maximum variation of the Fermi levels between iterations (last string in main solver parameters table). This option allows sort out wrong solutions.
- License end and start dates are shown in About window.

## 6. Release Notes 5.13

This section describes new options in version 5.13 compared to version 5.12:

- Import of custom tabulated radiative lifetimes with dependence on carrier 2D concentration in a QW and temperature is supported. To activate the option, one needs set global parameter "Use imported spontaneous recombination lifetime = Yes" and import tables with lifetime as a function of the carrier 2D concentration for a set of temperatures by using "Material Properties -> Import Radiative Lifetime" menu item.

## 7. Release Notes 5.12

This section describes new options in version 5.12 compared to version 5.11:

- For calculation mode "Series Calculation for SpeCLED" (automatic variation of both p-n junction bias and temperature) the output data for SpeCLED are organized as a



single (\*.txt) file (filename is similar to the project file) for all temperatures (instead of several (\*.sct) files, one per temperature). This way allows running SpeCLED computations with account of lateral carrier diffusion in the active region and surface recombination. Results to be loaded into SpeCLED by using "Table Input" in "Active Region" tab of SpeCLED.

- Default grid is more fine ("mesh refinement factor" of 1.1 is used compared old variant of 2).
- Some minor improvements are done in material properties editor.
- We have fixed several errors related to semipolar orientations:
  - For orientations [10-1-1] and [10-1-3] wrong inclination angles of 61.96 and 32.04 degree were used instead of correct ones of 118.04 and 147.96. Correct angles are used since version 5.12. Older project files with such orientations are converted as the custom inclination angles of 61.96 and 32.04 degree.
  - In version 5.11 and below, results calculated with custom inclination angle , after saving results and opening project file again, spontaneous polarization shown in results was not multiplied by the cosine of the inclination angle (and the same wrong contribution was included into total polarization). The error effected only appearance of the results, but actual electric polarization used in computations was correct.
  - The above error effected spectrum computations: for spectrum computations, effective masses along [0001] direction were used for any custom inclination angle.

## 8. Release Notes 5.11

This section describes new options in version 5.11 compared to version 5.10:

- Calculation of the integral characteristics (like leakage current density and so on) has been slightly changed. After opening of an old file with results, one can see slightly different leakage current density, IQE, etc. The discrepancy is within the accuracy of computations.
- Former IQE parameter (ratio of the current density converted into radiative recombination to the total one,  $j_{rad}/j_{tot}$ ) has been eliminated and replaced by former IQE\_QW (ratio of the current density converted into radiative recombination inside QWs,  $j_{radQW}/j_{tot}$ ).

- Sheet concentrations of electrons and holes,  $n_{2D}$  and  $p_{2D}$ , are shown in the table of results. They are obtained by integration of the 3D carrier concentrations over the QW layers (i.e. layers marked as active region).
- "Export to SpeCLED" window has been simplified. Radio group regarding IQE treatment has been eliminated because we decided always calculate IQE by using QW layers only (see above). The radio-group related to the file format has been eliminated, too. Instead, one can choose the file format in the save dialog. Choosing \*.sct output will provide a file of old format, while choosing \*.txt output enables saving section which can be imported into SpeCLED by using "Table Input" option for the active region. The latter option can be used to prepare export data allowing to study lateral carrier diffusion in the active region by **SpeCLED** (a new option in **SpeCLED** which will be released soon in version 4.15).
- Density of states,  $N_C$  and  $N_V$ , are shown in "Results->Conc" plot along with concentrations of carriers and ionized impurities.
- A small misprint in spectrum computations has been fixed. The only effect is that CH hole band is shifted down by ~4 meV.

## 9. Release Notes 5.10

This section describes new options in version 5.10 compared to version 5.9:

- In laser computations, users can specify their own function for dependence of the gain (and respective wavelength) on the current density (three new parameters in "Laser Parameters" tab: "Use Imported Gain Data", "Peak Gain vs Current Density Function", "Peak Gain Wavelength vs Current Density Function"). In laser calculations without self-consistent treatment of the stimulated recombination ("old style"), these data are used instead of calculation of the material gain in the active region. One can import material gain of the active region and modal gain. If user imports material gain, it is assumed that all QWs have the same contribution to the total gain. Then modal gain is calculated as usual, according to Eq. (10.1) of Physics Summary.
- In laser computations, one can make the laser solver to calculate the absorption in the layers which are not QWs by using the material properties data ("Use Absorption From Material Data" parameter in "Laser Parameters" tab). In this case, the absorption coefficient taken from the material properties dataset will be used instead of the absorption coefficient predicted by Eq. (10.4). This option effects both laser computations with and without self-consistent treatment of the stimulated recombination. Please note this option does not effect the QW layers, as their optical properties and their dependence on the carrier concentration are included into the QW material gain.
- Convergence of PL computations has been improved.
- In module for user-defined functions the following error is fixed: sometimes global user-defined constants appeared to be zero no matter what value has been specified. This error might provide wrong simulation results only in case when user-defined script functions has been used, and this functions use global user-defined constants.
- Some minor improvements has been made, and some minor errors has been. None of these errors lead to wrong simulation results.

## 10. Release Notes 5.9

This section describes new options in version 5.9 compared to version 5.8:

- Laser computations has been improved considerably by adding the stimulated recombination rate into the drift-diffusion model. It allows prediction of the laser operation above the threshold, while previous versions only extrapolated the output power from the differential efficiency calculated at threshold conditions.

## 11. Release Notes 5.8

This section describes new options in version 5.8 compared to version 5.4:

- Variation of the layer composition can now be specified by a script function of the position, or by a tabulated function of the position. The function module is similar to that used for specification of the material properties. One can view and edit functions for composition variation by using "Heterostructure->Functions" menu item. To make the layer composition to be a function, one can pick up the respective function name in the drop-down list for the composition.
- New option for specification of the lattice relaxation is supported now for structures grown in [0001] direction. One can directly specify the relaxed lattice constant  $a$  of the layer (instead of specification of the degree of relaxation). Then this value is used in computation of the strain components in the layer and respective piezoelectric polarization. The relaxed lattice constant  $a$  may be a constant or a function of the position (similarly to the layer composition - see previous paragraph). Old variant of specification of relaxation by degree of relaxation is supported, too.
- **SiLENSe** now can import the simulation results for the layer composition and relaxation obtained by STR **STREEM InGaN** software by using "Heterostructure->Load Layers From STREEM file" menu item.
- Generation of the computational grid is considerably changed. More options for control of the grid is available for users. Details are given in the User Manual, while default grid options resemble old variant and they are well enough for most cases.
- Pause/continue button is added to the solver control window.
- A number of minor errors has been fixed, while non of them is related to a wrong simulation results.

## 12. Release Notes 5.4

This section describes new options in version 5.4 compared to version 5.2:

- Simulation of steady-state resonance photoluminescence (PL) experiment is available. PL simulation is done for zero bias. User can specify the excitation wavelength and power density. The excitation is assumed to be resonance, and carriers are assumed to recombine in the same quantum well (QW) where they were generated. PL computations are done as following. First, simulation of the band diagram at zero bias as done. Next, for each QW the software computes the additional non-equilibrium 2D concentration of electrons and holes (they are the same because of above assumption) from the condition that the recombination rate integrated across the QW is equal to the integrated generation rate. Finally, the PL emission spectrum is calculated in the manner similar to that for EL simulations.

PL simulation can be started by using "Run-> Run PL" and "Run-> Run PL Series" menu items similarly to electroluminescence (LED) computations. PL results are visualized similarly to electroluminescence results and can be seen by using "Window->PL results" menu item.

**NB:** Absorption coefficient is critical for correct description of the generation rate in PL computations. The default database now contains some basic approximation for the absorption coefficient, while users are welcome to correct it according their own data (see below note on material properties).

**NB:** When old project files are updated up to version 5.4, default value of the absorption coefficient is zero. To enable old projects for running PL computations one needs manually import new database of material properties (default is "wurtzite.matprop") into the project by using "Material Properties -> Import" menu item.

- Now all material properties can be specified with user-defined functions depending on the composition (in case of alloys), temperature, and wavelength (for optical properties). Functions can be Pascal-like script or tabulated dependence which can be inputted directly or imported form a text file. The functions module is similar to that used in **SpeCLED** and **SimuLAMP** STR products. The respective changes are made in the properties editor (ProEdit.exe).

**NB:** In version 5.4 material properties are stored in a single file with \*.matprop extension (in older versions, there were two files, for materials and for alloys, with the same filename and extensions \*.mat and \*.mats, respectively). Properties editor can open old files.

**NB:** For the refractive index, users can continue using old-style parameterization for its spectral dependence or specify their own function.

**NB:** User can edit the material properties from **SiLENSe** by using *Material Properties->Edit* menu item . Then the **Properties Editor** window will be opened with the current dataset already loaded. By closing properties editor, one applies save changes into the (\*.sls) project. Technically this option is done by import of the current dataset into a temporary (\*.matprop) file, starting properties editor with this file as a command-line argument, and then importing dataset after closing properties editor. So, it is necessary to save changes in the properties editor in order to get it applied.

- Some errors are fixed in computation of the gain spectrum. Now the resulting gain spectrum will be lower than that in the older versions.
- Results of laser simulation can be saved in the project file.

### 13. 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 band 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 .

### 14. 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.

## 15. 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.



## 16. 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  $\tau_{n,p}^{tot} = \left[ (\tau_{n,p}^{dis})^{-1} + (\tau_{n,p}^{def})^{-1} \right]^{-1}$  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.

## 17. 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 \*.dvs 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).

## 18. 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.

## 19. 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).

## 20. 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 by 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<sup>1</sup>. 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'.

## 21. 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<sup>2</sup>. 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<sup>2</sup>.
- 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.

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<sup>1</sup> 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.

<sup>2</sup> It means that re-running simulations with new version will give the same results.

## 22. 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.

## 23. 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.
- 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 / 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.

## 24. 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.

## 25. 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.

## 26. 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.

## 27. More info

More detailed information about the **SiLENSe** package is available at the site of STR IP Holding: <http://www.str-soft.com/products/SiLENSe>. Evaluation package can be requested by the e-mail address [simuled-support@str-soft.com](mailto:simuled-support@str-soft.com) .