



SpeCLED

Spreading of Current in Light Emitting Diodes

RATRO

Ray-Tracing Simulator of Light Propagation

Software for 3D Modeling of
Current Spreading, Temperature Distribution and
Light Extraction in LED Chips

Release Notes

Version 5



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1 SpeCLED & RATRO v 5.0 (June 2020)

This update of SpeCLED & RATRO is focused on micro-LEDs and includes all-new RATRO solver. Please find below list of improvements:

- All-new **RATRO** solver with the following new options:
 - ✓ Simulation of complicated sloped mesa shape and/or lens. This option can be used for micro-LEDs or LEDs with complicated profile of the substrate. In **Project Configuration** window, one can specify a user-defined script function which will provide dependence of the vertical position z as a function of lateral position (x,y) . This modified chip shape will be used in RATRO computations. See Sec. 11.4 "Specification of sloped mesa sidewalls in RATRO" of User Manual for more details. The installation package includes an example of micro-LED with sloped sidewalls in a shape of truncated square pyramid.
 - ✓ New solver does not support parameters "substrate x-extension" and "substrate y-extension" of "Project Configuration" window (values of 1 are used regardless what specified in the user interface).
 - ✓ New model for patterned surfaces (direct tracing of rays inside the pattern).
 - ✓ Specification of user-defined optical models at sidewalls of n-semiconductor and p-semiconductor.
 - ✓ Automatic correction of integral **SpeCLED** results (LEE , P_{out} , EQE , and WPE) after the end of **RATRO** computations (see Sec. 11.5 "Correction of SpeCLED results after **RATRO** computations" of User Manual for more details).
 - ✓ Parallel computations in **RATRO** solver.
- Output of **SpeCLED** and **RATRO** results into .dcr format. New visualization tool **View 2D** provides a better flexibility in inspecting simulation results.
- More precise control of convergence in lateral carrier diffusion post-processing computation in **SpeCLED**.

2 SpeCLED & RATRO 2008 v 4.15 (December 2016)

Please find below list of improvements of SpeCLED & RATRO:

- Analysis of lateral carrier diffusion in the active region and non-radiative recombination at the mesa side walls is available as a post-processing option after the main **SpeCLED** computations (which remain the same). Set of respective parameters (surface recombination coefficient, diffusion coefficients, and solver parameters) is added in "Run" tab. This option is available only with the active region characteristics specified as a table, where additional data are added. The table can be specified manually or imported from a text file. Please note that **SiLENSe** version 5.11 support export of the heterostructure simulation results in the format supporting this option.
- A number of improvements is done regarding solver settings controlling fitting of the specified current by adjusting the voltage:
 - ✓ New computation mode is added in **SpeCLED** - a set of fixed currents. No one can specify a set of currents and the solver will process them all with fitting the applied voltage to get the specified current with specified accuracy (contrary, in older version of series calculations only minimum current was calculated exactly and then the voltage was increased by a fixed step until the current reach the specified maximum, covering some range of I-V curve). New option is useful when one wants compare results for different input data at exactly the same set of currents.
 - ✓ Smart process of automatic choose of the initial voltage and first step in fitting the specified current is implemented in solver. To use this option, one need use "auto" check box for the initial voltage. Old-style manual specification of the initial voltage is supported, too. It might provide more fast computations if one already know the resulting voltage (because only slight changes are done in the input data) and the initial voltage and first step are chosen appropriately.
 - ✓ The parameters controlling the accuracy of the current fitting are now specified in relative units, i.e. the ratio of the current discrepancy to the total current (while older versions operate with absolute value of the discrepancy). Old projects are converted in such a way to keep the same accuracy.
- Support of additional blocking layer between p-electrode and p-spreading layer.

3 SpeCLED & RATRO 2008 v 4.14 (December 2014)

Please find below list of improvements of SpeCLED & RATRO:

- Export and import of the selected fragment of the geometry to/from a text file is implemented. This option allows copy some geometry objects from one project to another. The option is available in the context (pop-up) menu of the drawing in the "Geom" tab.
- Scaling of the selected fragment of the geometry is implemented. This option is available in the "Multiply Selected Object" tool of the "Geom" tab.
- Batch simulation option is improved in such a way that user can save the batch simulation settings and use them for another project file (no need to specify again the settings).

4 SpeCLED & RATRO 2008 v4.13 (October 2013)

Please find below list of improvements of SpeCLED & RATRO:

- Support of lateral variation of the heterostructure properties is now extended: the user can specify up to 4 different regions with modified active region properties. The number of modified active regions is chosen in the "Project Configuration" modal window.
- Batch simulations with variation of the material properties are supported now. One need choose "Variable" type for material properties which will be varied. See Sec. "Run->Batch variation of material properties" of GUI manual for detailed instruction. The respective example is added into the installation ("Examples/Variation_of_Material_Properties" folder).
- Some minor errors in the user interface were fixed.

5 SpeCLED & RATRO 2008 v4.12 (March 2012)

This update allows simulation of non-rectangular chips in both SpeCLED & RATRO. Please note that 3D view option of the user interface will show a rectangular substrate, while in simulations the actual user-defined shape is used. One can check the geometry in the 3D view of the resulting *.cgs files.

Also, some minor errors in the user interface were fixed.



6 SpeCLED & RATRO 2008 v4.11 (November 2011)

This update includes considerable improvements both in SpeCLED & RATRO. Below, they are listed in brief.

- Lateral variation of the heterostructure properties is now supported in the following way (check box "Modified Active Region" in the "Project Configuration" modal window enables this option). The user can specify two different sets of the active region parameters in the "Active Region" tab, and specify the lateral position of the modified active region in "Layers" tab.
- In the "Active Region" tab, import of users text files is enabled for the table specification of the active region. Now users can easily input their own data for the heterostructure characteristics by making a text file with tables with the p-n junction bias, current density, IQE, and emission wavelength for one or more temperatures.
- In plots appearing in the "Active Region" tab, the values under the cursor are shown in the left top corner of the plot.
- Script function for material properties can now depend on the block identifier shown in the left top part of "Layers" tab next to the cursor coordinates. It enables more convenient specification of the lateral dependence of the material properties.
- Thermal boundary conditions can be specified with user-defined script functions for the heat transfer coefficient and ambient temperature.
- In the "Layers" tab, selection of all blocks within a rectangle is supported.
- License information is shown in the "About" window.

7 SpeCLED & RATRO 2008 v4.10 (June 2010)

This update includes considerable improvements both in SpeCLED & RATRO. Below, they are listed in brief.

- Support of simultaneous specification of p-spreading and p-blocking layers.
- New model for ITO p-spreading layer. Support of vertical mesh in p-spreading layer.
- Redesign of 'Material' tab in order to improve input of material properties and support semiconductor substrates as well as direct input of the electrical conductivity of the semiconductor layers. Also, insulator materials may be used for insulating substrate like sapphire.
- More flexible specification of the solver parameters provides more precise convergence control, as well as allows obtain preliminary results faster.

- Support of custom angular distribution of the heterostructure emission (in addition to existent options of isotropic and Lambertian distributions)
- Support of multiple layers and facets on substrate sidewalls
- Generation of the input data for SimuLAMP software
- Support of Senselock dongle keys

8 SpeCLED & RATRO 2008 v4.09 (February 2010)

This update concerns only RATRO module. The main improvements are listed below in brief.

- Patterning with hemispheres is supported
- Simultaneous use of 'Multiple Layer' and 'Patterning' options for the same surface is supported. It makes surface specification much more flexible, for instance, it will be possible to simulate a patterned surface covered with a metal layer.
- Tool for fast calculation of the scattering properties of a patterned surface is built-in into the interface. In result, the user is able to see probability of light reflection, transmission, and absorption at the patterned surface in a way similar to that used for other surfaces.
- Refractive and absorption indices (n , k) of the materials available for using in 'Multiple Layer' surface are stored in a set of text files now. Now, users can modify optical properties of these materials (which were hardcoded in previous versions), as well as add their own new materials.

9 SpeCLED & RATRO 2008 v4.08 (May 2009)

This update concerns mainly SpeCLED solver. The main improvements are listed below in brief:

SpeCLED solver:

- Automatic choice of solver parameters 'Urelax' and 'UInert' is added. The user can switch on/off auto update of solver parameters by using Automatic check box (see page 'Status' of the solver log). In automatic mode, solver decrease relaxation and increase inertia in case of current oscillations.
- Global current balance is also controlled now. Ideally, the total current through the n-pad, active region, and p-pad to be the same. The discrepancy (in mA) is shown by the blue line in DeltaJ chart. Criterion is that discrepancy to be below 0.1 mA (this level is not shown)



- Names of output variable are changed to improve clearness. The meaning is the same, SimuLEDView documentation is updated.
- Output file names in serial computations include `_ser` suffix to avoid overwriting results of single computations with full info (while series results include active region and integral parameters only, except to the first point). Also, output file names may contain digits after decimal point to avoid overwriting of the results at low currents. For instance, older solver will give the same name to results at 1.8 and 2.2 mA current.
- In report section, averaged IQE is added. The averaging is done with weight of j_z , so averaged IQE describes the overall efficiency of current conversion into the light.
RATRO:
- 'Mirror' and 'Multiple layer' surfaces are available for all surfaces of 'Surface properties' list. - In 'Multiple layer' surface, 'repeat' button is added, which copies two last layers. This option facilitates input of DBR mirrors.

10 SpeCLED & RATRO 2008 v4.07 (March 2009)

This update is focused mainly on improvement of the user interface. Also, new options in RATRO are added. The main improvements are listed below in brief.

10.1 SpeCLED & RATRO GUI

- Import of lateral 2D geometry from DXF file is supported.
- Import of the script functions from other project files is fixed.

10.2 SpeCLED solver and output

- SpeCLED solver now can open log files (*.spl) of completed simulations to show the solution history.
- Some errors caused solver crash are fixed.
- Visualization of the solution process is improved.
- New parameters are added for interactive control of the solution process.
- Report section of output (*.cgs) file is refined, main input parameters are included into report.



10.3 RATRO solver and output

- Multi-layer cover can be specified on the substrate sidewalls.
- User-defined optical properties of blocking layers may be specified.
- Optical losses for all volumes and surfaces are shown in report.
- Report section of output (*.cgs) file is refined, input parameters are included into report.

10.4 Features Added in SpeCLED & RATRO 2008

SpeCLED 2008 and RATRO 2008 have been radically modified compared to SpeCLED 3.0 with RATRO 1.2. Detailed description of the operation with SpeCLED 2008 and RATRO 2008 can be found in the SpeCLED 2008 Getting Started, SpeCLED 2008 Getting Started and SpeCLED - RATRO Graphical User Interface Reference Guide documents. The main new features are listed below in brief.

10.5 Support of New Die Elements in SpeCLED

- A current spreading layer like ITO placed on the p-contact layer is available.
- Substrate was included into the computational domain. Current spreading and heat transfer in conducting substrates and heat transfer in insulating substrates are supported.
- Electrode pads were included into the computational domain. Voltage drop inside the pads is taken into account.

10.6 Modification of the SpeCLED + RATRO Graphical User Interface

- The way of specification of the die design was considerably modified (see *SpeCLED - RATRO Graphical User Interface Reference Guide*, sections *Chip Configuration Dialog Window* and *Layers Tab Window*).
- Manual input of the active region properties was implemented (see *SpeCLED -RATRO Graphical User Interface Reference Guide*, section *Manual Specification of I-V Characteristics*)
- Manual specification of the computational grid in vertical dimension was implemented (see *SpeCLED -RATRO Graphical User Interface Reference Guide*, section *Chip Configuration Dialog Window*).



10.7 Support of New Options in RATRO

- Stand-alone **RATRO** software tool now can be used without **SpeCLED**. Specification of the die geometry is made within **RATRO** graphical user interface. In this case uniform emission distribution from the active region is assumed.
- New model of the die surfaces were implemented (see *SpeCLED - RATRO Graphical User Interface Reference Guide*, section *RATRO Tab Window - Surface Models*):
 - A model of a multiple metal layer contacts to be applied to p- and n-electrodes.
 - A model of regularly patterned surfaces to be applied to free semiconductor or substrate surfaces.
- Specification of wavelength dependence of refraction and absorption indices of the semiconductor, substrate and epoxy materials was implemented (see *SpeCLED - RATRO Graphical User Interface Reference Guide*, section *RATRO Tab Window - Bulk Properties*).
- Light polarization model was implemented.
- Both isotropic and Lambert laws of emission from the active region are supported.

11 Features Added in SpeCLED 3.0

11.1 Support of Current Blocking Layers

SpeCLED can now account for the current blocking by insulating layers made of dielectric materials which are formed between metallic electrodes and contact layers of an LED heterostructure to control the current pattern. Both n-blocking layer and p-blocking layer can be considered.

- Geometry of the blocking layers should be specified using *N-Blocking Layer* and *P-Blocking Layer* tabs of the *Geometry* window, respectively.

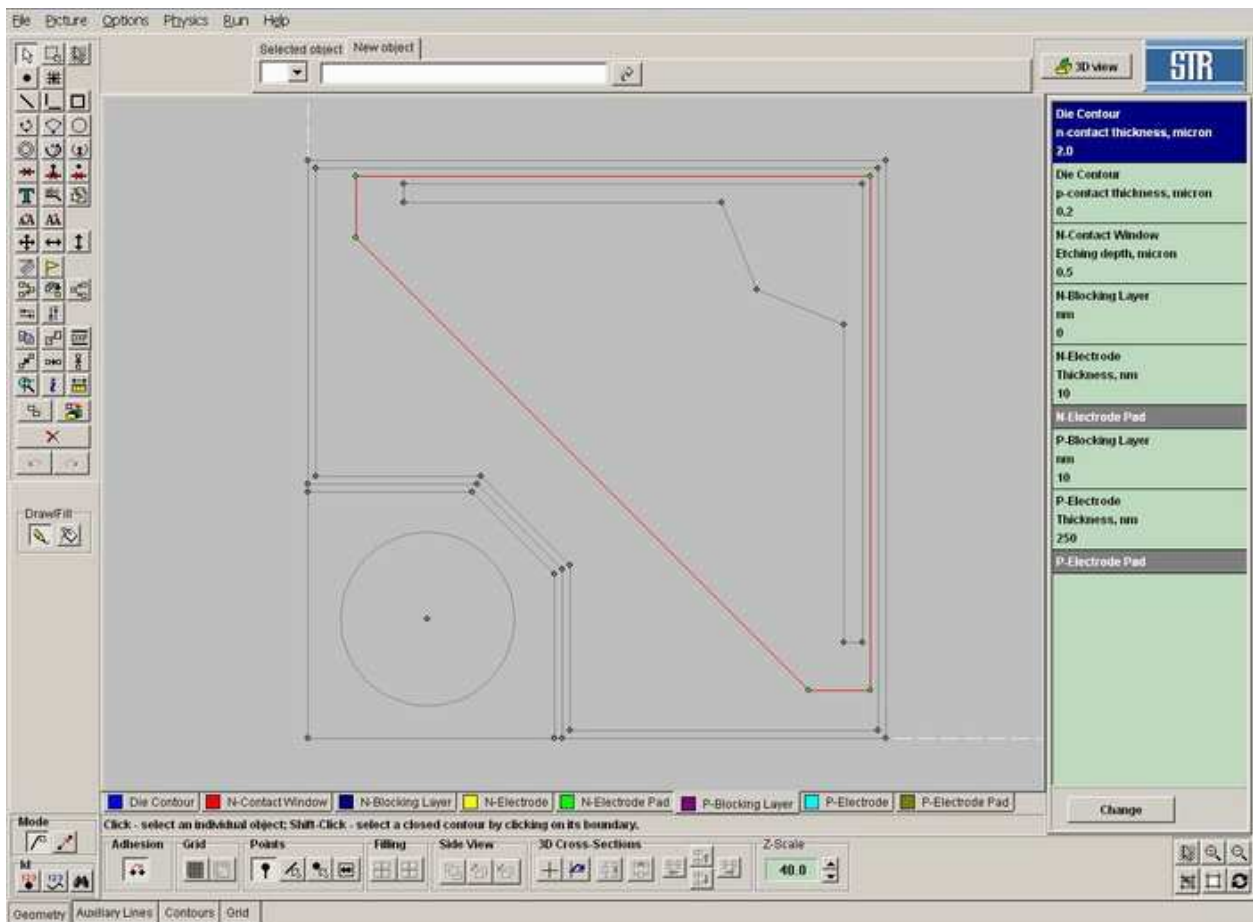


Fig. 1. Specification of p-blocking layer in Geometry window.

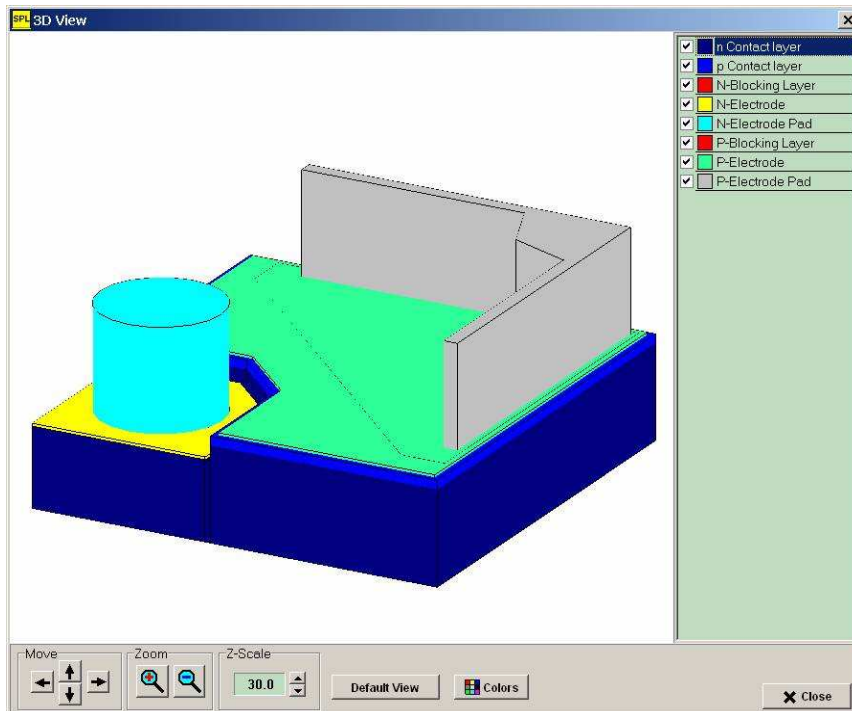


Fig. 2. 3D view of chip with p-blocking layer. All elements are shown

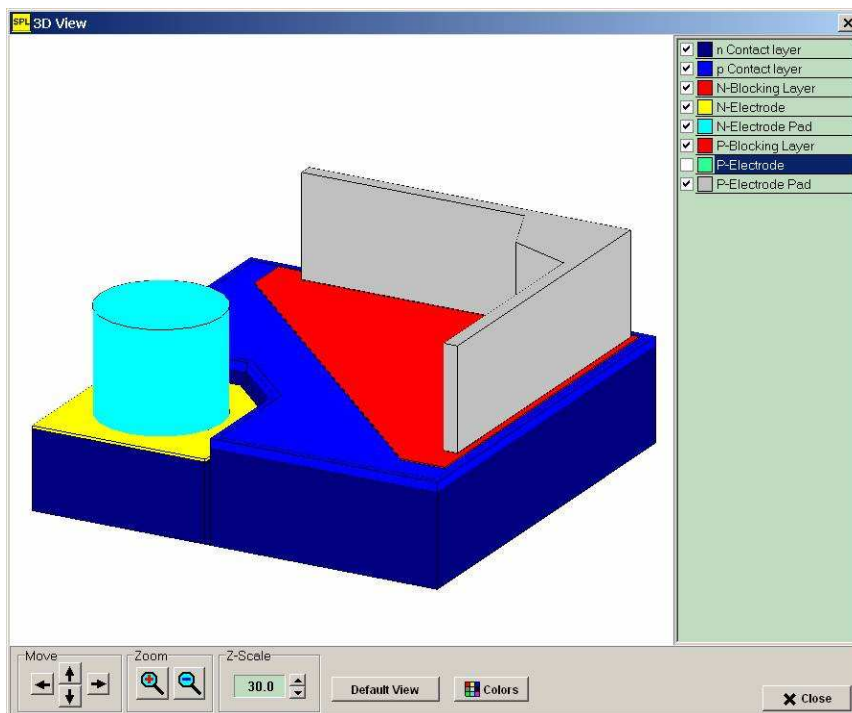


Fig. 3. 3D view of chip with p-blocking layer. P-electrode covering the p-blocking layer is hidden.

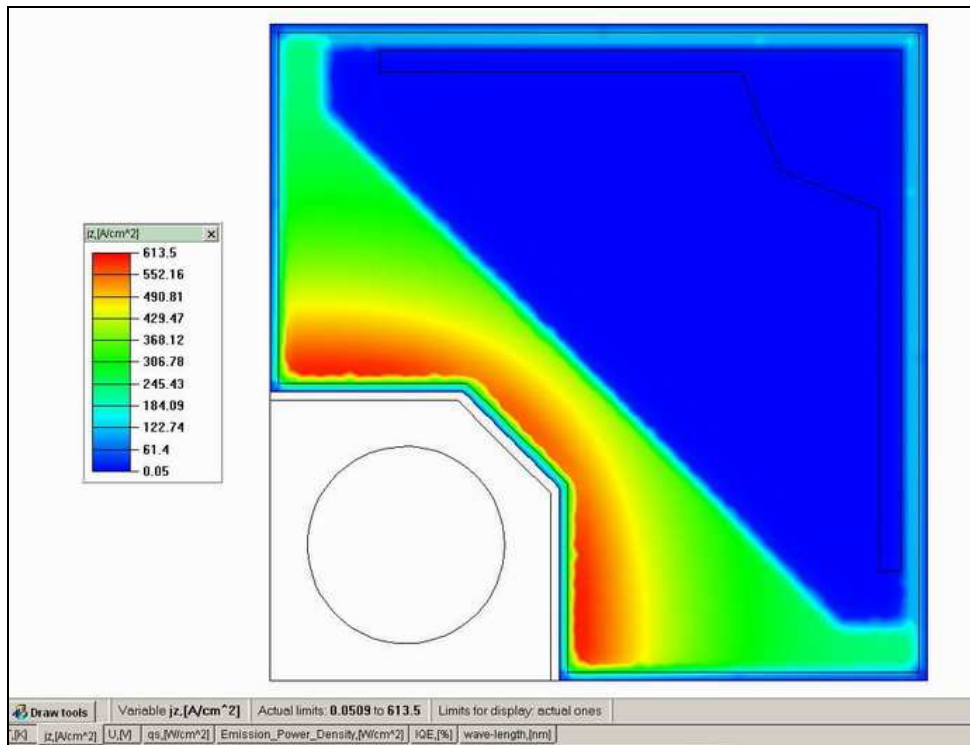


Fig. 4. Current distribution across the active layer. Chip with p-blocking layer.

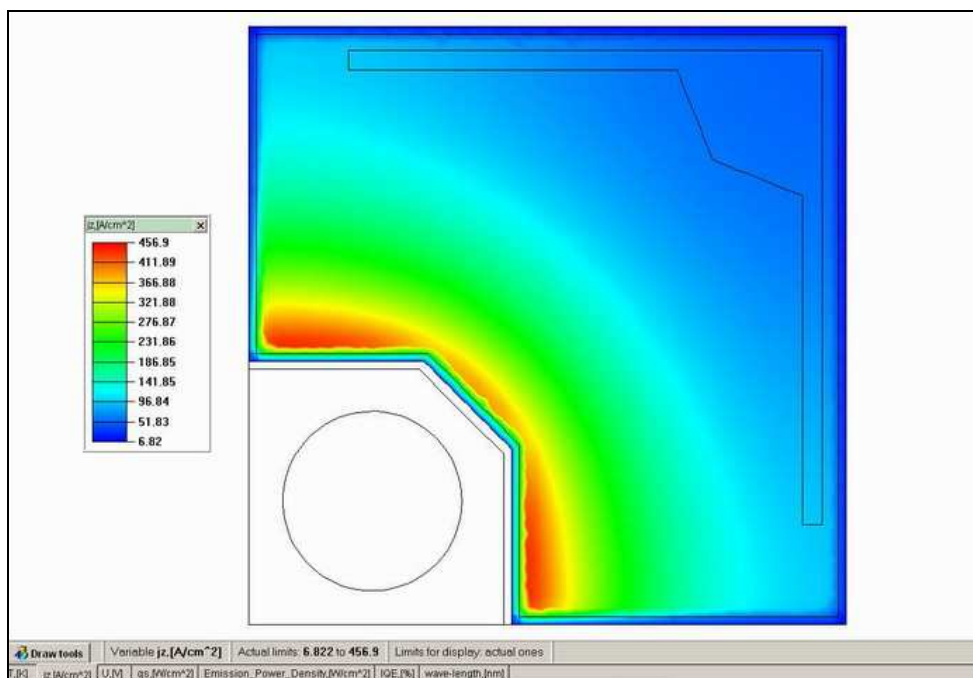


Fig. 5. Current distribution across the active layer. The same chip without p-blocking layer.

- In addition to the current blocking by dielectric films, the implementation of a model of current spreading in the layers made of highly conductive semiconductor materials, like

ITO, is under development. When it is finalized, the user will be able to assign either current blocking layer or current spreading layer under the p-electrode. This should be done using the same GUI element, the tab on the *Geometry* window named *P-Blocking Layer*. Selection of the actual type of this layer (i.e. blocking (dielectric) layer or spreading (highly conductive) layer) should be made in the *P-Blocking/Spreading Layer* tab of the *Physics* dialog window. In **SpeCLED 3.0**, the option *Blocking Layer* is only available in this dialog window.

11.2 Fixing Errors in SpeCLED Graphical User Interface

Several errors in SpeCLED Graphical User Interface have been fixed.

12 Features Added in SpeCLED 2.1

12.1 Import of the Die Geometry from DXF Files

As an alternative to the manual geometry specification, the die contours can be imported from a Drawing Exchange Format (DXF) used by the **AutoCAD** graphic editor and most of other CAD systems.

SpeCLED can recognize the following DXF primitives:

- LINE
- POLYLINE
- CIRCLE
- ARC

If the initial CAD drawing includes some other CAD elements (Reference Blocks, Splines, etc.), it should be converted into the acceptable format prior to saving in a DXF file. In **AutoCAD** the **EXPLODE** command should be used to convert all contours to the primitives listed above. Depending on the initial elements, this command should be applied once or several times consecutively, until all contours are formed by the appropriate elements.

Besides, before exporting a CAD drawing, the user should delete all irrelevant objects, such as fillings, hatchings, dimension lines, etc. It is also recommended to copy all relevant



contours to a new file before saving it in DXF format to eliminate storage of the removed elements in the file.

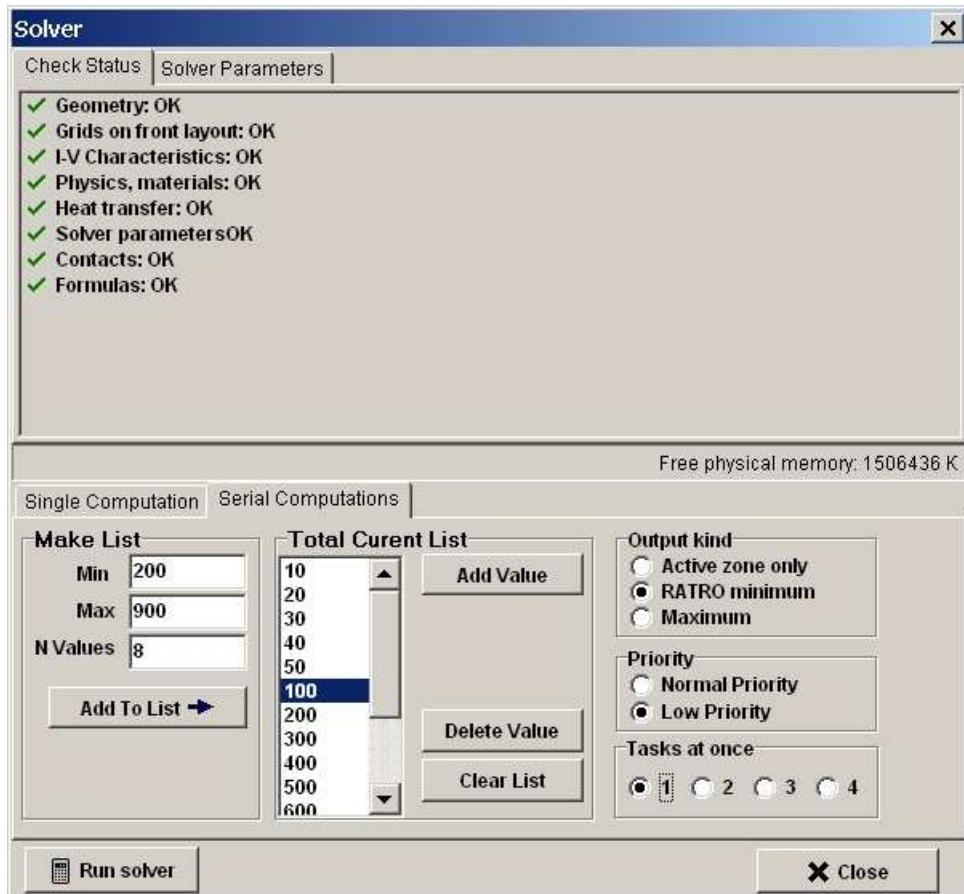
All geometrical elements contained in the imported file are loaded in **SpeCLED** program into one layer. Specification of the correspondence of different contours forming the die with the layers used in **SpeCLED** can be made in two ways:

- The user can split the die geometry in the external tool used to create DXF file (e.g., **AutoCAD**) prior to the exporting procedure. In this case, six individual DXF files should be created, each corresponding to a separate layer. Then the user should consecutively switch between layers in **SpeCLED** and import the respective file to the current layer.
- The user can first import the whole die geometry specified in a single DXF file to one layer, e.g., Die Contour and then to move the contours to the corresponding layers using tools **Move Lines to another Layer** and **Copy Lines from another Layer**.

12.2 Series computations

Series computation for a user-defined sequence of currents was implemented, while in the earlier versions the user was able to start a computation for a single value of current only which required a lot of computations to obtain a voltage-current characteristic.

The **Solver** dialog window allowing the user to start the computations contains the following items:



Single Computation tab allows the user to start a computation of the current spreading at a given total current. It contains the following parameter:

- **Total Current** text field allowing the user to assign the total current through the chip (in mA). The resulting current and temperature distribution corresponds to some calculated value of the total current that differs from the assigned *Total Current* not more than by a *Current Fitting Accuracy* value.

Serial Computations tab allows the user to start a sequence of computations of the current spreading for a wide range of total current, providing prediction of the whole I-V characteristics. It contains the following parameters:

- **Make List** section allows the user to assign an equidistant series of the total current values and add it to the list of currents. It contains the following items:
 - ✓ **Min** – the minimum current value.
 - ✓ **Max** – the maximum current value.

- ✓ **N Values** – the number of values, including the **Min** and **Max**. For example, specification of **Min** = 100, **Max** = 1000 and **N Values** = 10 creates the series 100, 200, 300 ... 900, 1000.
- ✓ **Add To List** button applies addition of the created series to the list of currents.
- **Total Current List** section contains the whole list of current sequence for which the computations should be carried out and the buttons **Add Value**, **Delete Value** and **Clear List**.
- **Tasks At Once** section specifies the number of simultaneously running computational processes. If value = 1 is specified, computation for a single value of current is run at a time. Each new computation is run automatically after the previous one is finished. If value exceeds 1, several computations are run simultaneously, which can be efficiently used on multi-CPU computers.

12.3 New IQE vs. Current Dependence

A new approximation of the dependency of the active region internal quantum efficiency on the total current was implemented. Unlike approximation used in the earlier versions, it involves physical heterostructure characteristics and accounts for the IQE dependence on temperature.

- The relationship between internal quantum efficiency (IQE) η and current density j is approximated using a parametric setting as follows:

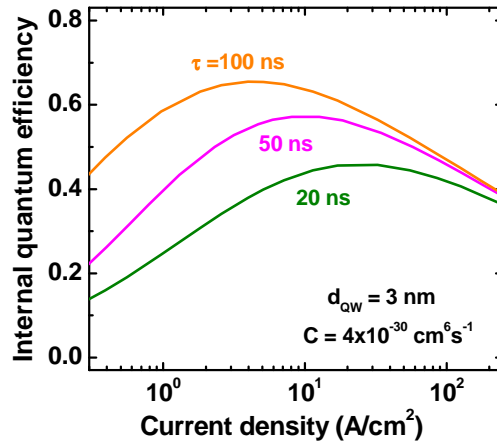
$$j(N) = qd \cdot (N / \tau + BN^2(T/T_0)^{-3/2} + CN^3(T/T_0)^\gamma)$$

$$\eta(N) = (qd / j) \cdot BN^2(T/T_0)^{-3/2}$$

Here:

- N is the non-equilibrium carrier concentration in the active region
- q is the electron charge
- d is the active region thickness (in the case of MQW structure it is the total thickness of all quantum wells)
- τ is the non-radiative lifetime (typically equal to 20-100 ns)
- B is the radiative recombination rate constant at T_0 (typically equal to $2-3 \times 10^{-11} \text{ cm}^3 \text{ s}^{-1}$)
- C is the Auger recombination coefficient at T_0 (typically equal to $1-10 \times 10^{-31} \text{ cm}^6 \text{ s}^{-1}$)
- T_0 is the room temperature

- This parametrization procedure produces the behavior of $\eta(j)$ similar to that observed experimentally and allows much more easier parameter fitting to measured external efficiency versus forward current.



12.4 Fixing Errors in SpeCLED Graphical User Interface

- ✓ An error arising at switching to electrode contour layer after removing of all lines on electrode pad layer
- ✓ An error arising at fast switching between different layers in GUI
- ✓ Several errors in the procedure of drawing of arcs
 - ✓ An error with the range check of the *Mesa Depth* specification
- ✓ An error with displacement of lines occurring at copying contours to a different layer
- ✓ An error with automatic mesh generation in the geometries containing arcs
- ✓ A user-friendly diagnostics of the absence of computational mesh specified for both sides of the vertical structures at the start of the computation
- ✓ Acceleration of the user operation with complex die designs by reducing the number of operations followed by total geometry analysis
- ✓ Specification of individual color to each die layer in 3D View
- Automatic saving of the project file after start of the computation run

12.5 Fixing Errors in SimuLEDView

- ✓ An error arising at loading large number of active region files
- ✓ An error arising at switching between different planes



13 Features Added in SpeCLED 2.0

13.1 Vertical LEDs

In addition to planar LEDs, computation of the current spreading, light emission and heat transfer in multilayer vertical LED dice was implemented.

Before specification of the die geometry, the user should select the basic type of the LED geometry. The current version of **SpeCLED** supports the following die types:

- Planar die (one-side electrode configuration). N-electrode and p-electrode are on the same side of the die, so that n-contact window is etched in the p-contact layer.
- Vertical die (two-side electrode configuration). N-electrode and p-electrode are on the opposite sides of the die.