

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

Graphical User Interface Manual

Version 4.12

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1 Introduction

SpeCLED and **RATRO** are 3D modules of **SimuLED** software package designed for modeling of LED operation. **SpeCLED 2008** and **RATRO 2008** share a common graphical user interface (GUI) allowing the user to specify the 3D geometry and physical parameters of the LED die and run the computations.

The heat transfer and current spreading computational domain in **SpeCLED 2008** includes the following chip elements:

- \triangleright n- and p-semiconductor layers
- \triangleright n- and p-electrodes
- \triangleright n- and p-pads
- \triangleright substrate (optionally)
- \triangleright p-spreading layer (optionally)
- \triangleright n- and p-blocking layers (optionally)

Active region is considered as internal zero-thickness surface where non-linear resistance is specified. The boundary conditions on both the current spreading and heat transfer are set on wire plates where the voltage is applied. The potential drop inside the electrodes and pads is calculated. In case of thin pads with considerable potential drop the contact area is smaller than the overall pad and the current spreading inside the pad is accounted for. Boundary conditions for the heat transfer problem assume heat sinks on the pad surfaces or bottom substrate surface.

The ray tracing computational domain in **RATRO 2008** includes the following chip elements:

- > n-semiconductor layer
- \triangleright p-semiconductor layer
- \triangleright substrate

Electrodes, pads, spreading and blocking layers are not considered as bulk objects of the computational domain. However, the light extraction from the contact layers into immersion medium is governed by the characteristics of the immersion medium and by the local surface material, which can represent free semiconductor surface, electrode, spreading layer or pad.

SpeCLED + RATRO 2008 graphical user interface can be supplied in 3 configurations:

- **SpeCLED + RATRO** GUI. The program includes specification of both **SpeCLED** and **RATRO** modules.
- **SpeCLED** GUI. The program includes specification of the die geometry and parameters of the current spreading problem.
- **RATRO** GUI. The program includes specification of the die geometry and parameters of the light extraction problem.

The present document describes all options of the **SpeCLED + RATRO** GUI.

Starting **SpeCLED+RATRO** graphical user interface requires registration of the program. **SpeCLED+RATRO** is supplied on terms of single-node or network license using dongle key protection. The program is delivered with a HASP HL dongle key that should be plugged in a USB port on the PC where **SpeCLED+RATRO** will be used. Registration procedure is described in **SpeCLED+RATRO** Release Notes.

At running the **SpeCLED™** Graphical User Interface after the registration procedure, **Start Program** dialog window is opened (see Fig. 1). The user is asked to start a new project or to open an existing project. At starting a new project the user should select one of the predefined chip configurations and assign its parameters in **Chip Configuration** dialog window (see Fig. 2). When an existing project is opened or the new project configuration is specified, the main window becomes available.

! Note that chip configuration type can only be specified at starting of a new project and can not be modified afterwards.

Fig. 1

Projects of **SpeCLED 2008** are stored in files with extension *.dvx. Note that **SpeCLED 2008** file format is not compatible with file format used in **SpeCLED 3.0** and earlier (*.dvc). To import old projects into **SpeCLED 2008** the user should use a special tool **DVC2DVX_Convertor** that is supplied along with **SpeCLED 2008**.

The main window of the **SpeCLED** shell contains the following tab windows:

- **► Geom** drawing of the LED contours
- **► Grid** generation of the computational mesh
- **Layers** assignment of the drawn contours to LED layers
- **Functions** scripts describing complex temperature and coordinate dependencies that can be used in materials properties and boundary conditions used by **SpeCLED** module. This tab is not included in **RATRO** GUI
- **Materials** manual specification or import of the materials properties used by **SpeCLED** module. This tab is not included in **RATRO** GUI

- **Active Region** import or parametric specification of Active Region properties used by **SpeCLED** module. This tab is not included in **RATRO** GUI
- **Run** assigning materials to the die layers, setting boundary conditions and running the current spreading and thermal computation. This tab is not included in **RATRO** GUI
- **RATRO** assigning bulk and surface optical properties of the LED chip and running the light extraction computation. This tab is not included in **SpeCLED** GUI

2 Chip Configuration Dialog Window

Fig. 2

The **Chip Configuration** dialog window allows the user to select the chip configuration and assign chip vertical dimensions. It contains two frames, **Configuration** and **Dimensions**.

When the **Chip Configuration** dialog is opened at the start of a new project, **Configuration** frame contains 4 predefined die schemes (see Fig. 2), namely:

- \triangleright Planar die without substrate
- \triangleright Planar die on an insulating substrate
- \triangleright Vertical die without substrate
- \triangleright Vertical die on a conducting substrate

The user should select the desired scheme by clicking on the respective image with the mouse left button.

The **Chip Configuration** dialog can also be opened later during the work with the project using **Configuration** menu item. In this case, the user can only change the parameters in the Dimensions frame. On the **Configuration** frame the active chip configuration is only shown, so that it can not be changed. So if the user has to specify a chip with a new scheme, one should start a new project.

Fig. 3

The **Vertical Dimensions** frame (see Fig. 3) allows the user to assign vertical die dimensions, **Additional Layers** frame allows to add optional layers, and **Vertical Mesh** frame is for specification of the vertical mesh. The data specified in the **Project Configuration** window can be edited at any stage of working with the project. The number of parameters depends on the active configuration.

The following parameters characterize the dice without a substrate:

- \triangleright A, μ m height of the p-semiconductor layer
- \triangleright a, μ m height of the n- semiconductor layer
- \triangleright D, μ m thickness of p-electrode
- \triangleright d, μ m thickness of n-electrode

- \triangleright NA vertical meshing of the p-semiconductor layer (number of cells in vertical direction)
- \triangleright Na vertical meshing of the n-semiconductor layer
- \triangleright M, μ m etching depth of the mesa in n-semiconductor layer assigned for a planar die only. M should lie within the following range: $A < M < (a + A)$.

The other parameters specify the shape of the substrate. **SpeCLED™** supports specification of flat (rectangular parallelepiped, see Fig. 4a) and shaped (with flat and sloped zones, see Fig. 4b and Fig. 4c) substrates.

Substrate geometry is defined by the following parameters:

- \triangleright E, μ m height of the sloped part of the wafer
- \triangleright F, μ m height of the vertical part of the wafer
- \triangleright DX and DY degrees of wafer narrowing/enlargement in X and Y directions, defined as the ratios of sizes of the back wafer surface to the heterostructure (nsemiconductor) surface, , see Fig. 5. *x* $DX = \frac{x_s}{x}$ and *y* $DY = \frac{y_s}{x}$ are dimensionless parameters, dice with $DX = 1$ correspond to Fig. 4a, $DX < 1 - Fig. 4b$, $DX > 1 - Fig. 4c$ 4c.
- \triangleright NE vertical meshing of the sloped part of the wafer
- \triangleright NF vertical meshing of the vertical part of the wafer

Fig. 5

Note that while the horizontal dimensions of the heterostructure (semiconductor layers, electrodes, etc.) are defined by the user in **Geom** tab window, the horizontal dimensions of shaped wafers are calculated using the n-semiconductor size and the DX and DY ratios defined along with the vertical dimensions.

The following additional layers can be specified in the die configuration:

- \triangleright N-blocking layer insulating layer under the n-electrode
- \triangleright P-blocking layer insulating layer under the p-electrode
- \triangleright P-Spreading layer ITO layer under the p-electrode
- \triangleright Modified active region this option allows specify lateral variation of the active region properties

Switching between **Configuration** and **Dimensions** frames is made using **Back** and **Next** buttons.

3 Menu Bar

Menu bar in **SpeCLED™** contains the submenus File, Options, Configuration, Picture and Help.

3.1 Menu File

The options available within the **File** menu (see Fig. 6) allow the user to open an existing project file, to save the current project to a file, and to add text notes to the project file.

Fig. 6

- **The menu item New** closes the previously opened project allowing to start specification of a new project.
- ▶ The menu item **Open...** allows the user to open an existing project. This item is designed to load the files in the format *.dvx, which contain all necessary information including the system geometry, materials, mesh, etc.
- **The menu item Save allows the user to store the current project into a project file** (*.dvx) using the current project name. If no project name has been set previously (i.e. the project was built using the shell and was not saved earlier), the **Save** option will work as the **Save As** option.
- The menu item **Save As…** allows the user to store the current project into a project file (*.dvx) with a manual specification of the file name and working directory.
- The menu item **Notes…** opens the window Notes where the user can view, add or edit some text information that is stored in the project file.
- The menu item **Exit** allows the user to close the shell with a confirmation dialog window.

The **File** menu also provides the user with a list of the most recently opened projects.

3.2 Menu Options

The **Options** menu contains the only item **Preferences…,** which opens the **Preferences** dialog window.

3.2.1 Preferences Dialog Window

Fig. 7

The **Preferences** dialog window (see Fig. 7) that includes the following items:

- \triangleright Section *Page Size.* This section governs the size and position of the page where the whole drawing is placed. The page perimeter is shown with dashed white lines. The user can specify the minimum and maximum values of both X and Y coordinates. By default, the page is 1000×1000 microns.
- \triangleright Section Grid. This section contains parameter Grid Step that governs the distance between consecutive nodes of reference grid to which the points can be aligned. By default, it is equal to 10 microns.
- Section X, Y to Display. This section contains parameter Digits After Point that governs the accuracy of specification of point coordinates and other values. It corresponds to the number of digits after decimal point.

- Section Points. This section governs representation of the points. It contains the following parameters:
	- \checkmark Shape. The shape of the symbol used to mark a point. By default, it is circle. Rectangular points are also available.
	- \checkmark Size. The point size (circle diameter or rectangle side) in pixels.
	- \checkmark Width. The width of black contour surrounding the point. Thin (1 pixel) and thick (3 pixels) contours are available.
- \triangleright Section *Marking Points.* This section governs representation of the points used as markers in Point-To-Point mode of line creation. The size of the point itself is the same as the size of the other points and is assigned by the Size parameter in Point section. The Marking Points section contains parameter Size that govern the length of white lines of the cross-hairs.
- Section Lines. This section allows the user to specify the width of the lines. Thin (1) pixel) and thick (3 pixels) lines are available.
- Section *Zoom Scale By Mouse*. This section allows the user to change degree of image scaling by moving the mouse with middle button pressed. A higher scale value requires a smaller mouse displacement for a given zooming.
- \triangleright Section Autosave. This section allows the user to specify the time interval at which the current changes of the project should be saved in a temporary file. If zero interval is specified, no temporary files are created. Note that each saving operation takes some time, so too frequent saving can be annoying for the user. Temporary file is saved in the working directory with extension ".~dvs".

3.3 Menu Configuration

The **Configuration** menu opens the **Chip Configuration** dialog (see Fig. 2 and Fig. 3), described above.

3.4 Menu Picture

The **Picture** menu allows the user to save the current image to a .bmp file or to copy it to the clipboard. It contains the following items:

- **Save To .bmp File**
- **Copy to Clipboard**

3.5 Menu Help

The **Help->About SpeCLED** menu item provides information about the current **SpeCLED™** version and registration of **SpeCLED™**.

4 Geom Tab Window

In **SpeCLED™**, all three-dimensional die elements are represented by a set of prisms which are determined by the structure of their planar base and height value. The **Geom** tab window is designed to provide an easy-to-use specification of the die contours.

- \triangleright For a planar chip configuration, it shows the top view of the die.
- \triangleright For a vertical chip configuration, it shows top and bottom views.

So in this window the user should draw all lines of the die heterostructure in horizontal planes. The die dimensions in vertical plane and shape of the substrate are defined in the **Chip Configuration** dialog window.

If a vertical chip configuration is selected, **Active Side** section above the Graphics Window governs which side if the die is drawn.

- $\frac{1}{\sqrt{2}}$ Top View. The drawing corresponds to a p-side layer.
- Bottom View. The drawing corresponds to an n-side layer.
- Checkbox **Opposite Side Visible** governs whether the lines from the other side are visible. If it is checked, they are shown as grey lines.

Note that for a vertical die the external die contour should be assigned twice, both in Top View and Bottom View drawings. To avoid double specification of the same contour, the user can draw it in Top View, select the whole contour (by clicking on any of its boundaries with Shift key pressed) and copy it into the clipboard using the **Copy Selected** item of the context menu available on pressing the right mouse button. Then one should switch to the Bottom View and paste the contour using the **Paste Selected** item of the context menu.

Along with lines bounding the constructive elements of the die, the contours defined in the **Geom** window may include internal lines used for domain decomposition in the grid generation.

The **Geom** tab window contains Drawing toolbar on the left-hand side, Viewing toolbar at the bottom, Parameters panel on the right-hand side, Object Editor on top of the window, and the Graphics Window.

Fig. 9

4.1 Drawing Toolbar

The Drawing toolbar is located at the left hand side of the **Geom** tab window contains a set of items allowing user to specify and modify the die geometry.

4.1.1 Select object

 The **Select Object** tool allows the user to select points, lines, and arcs with the left mouse button.

A Point is selected when the mouse cursor is positioned in the vicinity of the point. In this case, the point starts flickering in white to identify that this specific point will be selected on clicking the mouse button. A selected point is marked in white.

A Line or Arc is selected when the cursor is positioned on the boundary at a distance from any point (otherwise, the point will be selected instead of the boundary). The selected boundary is marked in white.

Repeated clicking on a selected object deselects it. Consecutive selection a series of objects provides their multiple selections. Clicking on a line that is a fragment of a closed contour with Shift key pressed selects the whole contour.

4.1.2 Select Object in the Rectangle

The **Select Object in the Rectangle** tool allows the user to select a group of points, lines, and arcs by Lasso, providing selection of all objects placed in a rectangular area. Moving the mouse with left button pressed assigns the rectangle dimensions specifying the bottom right corner keeping the top left corner. On the other hand, moving the mouse without pressing the button displaces the rectangle keeping its size, specifying the top left corner.

Note that in the lasso selection the boundaries are identified by the segment end points. So if no end point of a boundary lie within the area (i.e. if a single boundary segment crosses the lasso rectangle), the boundary is not selected.

The last specified position and size of the selection rectangle is saved.

4.1.3 Clear Selection

 The **Clear Selection** tool clears the selection of all objects. This button is duplicated by the "Spacebar" key.

4.1.4 Add Point

 The **Add Point** tool allows the user to add a new individual point. The point is created when the left mouse button is pressed. If the mouse cursor is positioned in the vicinity of an existing point or existing line, the new point is aligned to the existing object.

4.1.5 Align Point to Grid

The Align Point to Grid tool allows the user to align an existing point to reference grid. Note that this tool does not assume prior selection of the points. The user should first press the **Align Point to Grid** button and then click consecutively on the points to be aligned.

4.1.6 Explicit Coordinate Specification

留 The **Explicit Coordinate Specification** tool allows the user to assign coordinates of a point, line or an arc explicitly in a table. This option is an alternative to drawing the lines by clicking the mouse on the Graphics Window. When The **Explicit Coordinate Specification** button is pressed, **Points List** window is shown. The user should select the object to draw (Point, Line or Polyline), assign the coordinates in the table and press **Apply** button.

Fig. 10

4.1.7 Add Line

 The **Add Line** tool allows the user to draw a line. To draw a line the user should consecutively click with the left mouse button on the first and last ending points.

There are two modes of line drawing.

 \triangleright Elastic Lines mode (set by default). While the mouse cursor is moved after the first point is specified, the current line position is previewed for each cursor position. In this mode drawing can not be interrupted by displacement of the view area by the right mouse button, so locations of both points of the line should be visible on the screen at the start of drawing. Thus, this mode is optimal for drawing short lines.

Point-To-Point Line mode. The line is not shown until it is created, while the ending points are marked with crosshairs $\frac{1}{\sqrt{2}}$ symbol. The line is drawn when both points are prescribed. In this mode the user can shift the view area by the right mouse button, so this mode can be preferable in drawing long lines where zoom/move operations are needed to specify the exact point positions.

Switching between the drawing modes is made using the **Mode** section on the Viewing toolbar below the Graphics Window.

4.1.8 Add Vertical or Horizontal Line

 The **Add Vertical or Horizontal Line** tool allows the user to draw a line (see the above section **Add Line** for details) aligning it in vertical or horizontal direction.

When the line is created using this tool, the position of the second ending point is displaced from the exact point under the cursor so that the line is oriented in the strictly vertical or horizontal direction.

4.1.9 Add Rectangle

 The **Add Rectangle** tool allows the user to draw a closed rectangular contour. The rectangle is specified by its diagonal line. So to create a rectangle the user should specify two points: its top left corner and the bottom right corner (or the other pair of opposite corners).

4.1.10 Add Arc By 3 Points

 The **Add Arc by 3 Points** tool allows the user to specify an arc assigning three points lying on it. First the user should specify two arc ending points by clicking the left mouse

button. They are shown as marking points with crosshairs **.** Then the middle point should be assigned. In *Elastic Line* mode the user can move the middle point keeping the left button pressed, the current arc position is previewed. When the left button is released, the arc is created. In *Point-To-Point* mode the arc is shown after all three points are specified.

4.1.11 Add Arc by Center and 2 Points

 The **Add Arc by Center and 2 Points** tool allows the user to specify an arc assigning its center position, radius and angles of the ending points. First the user should specify the arc center (the center of the circle comprising the arc) and first arc ending point by clicking and releasing the left button. These points are shown as marking points with crosshairs

. Then the second ending point should be assigned. When the user releases the left button after assigning the first ending point and moves the mouse, the arc is previewed for each cursor position. Clicking the left button the user specifies the final position of the second ending point.

4.1.12 Add Circle

 The **Add Circle** tool allows the user to draw a closed circle. First the user should specify circle center by clicking the left mouse button. The center is shown as marking point

with crosshairs \bullet . Then the circle radius should be assigned by specifying a point that lies on the circle. The user should click the left button and can move the point keeping the left button pressed, the current arc position is previewed. When the left button is released, the circle is created.

4.1.13 Make Two Arcs Concentric

 The **Make Two Arcs Concentric** tool allows the user to adjust an arc center to center of another arc. The user should first select the arc (circle) to be moved, and then the reference arc (circle).

4.1.14 Move Arc Point

The Move Arc Point tool allows the user to change arc length by moving an arc ending point along the arc. To move an arc point the user should select the point, then press the left button and keeping the button move the mouse towards the new point position. Then the point is displaced strictly along the arc.

4.1.15 Change Arc Radius

 The **Change Arc Radius** tool allows the user to increase or reduce the radius of an existing arc or circle. To change circle radius the user should select the circle (arc), then press the left button and keeping the button move the mouse toward or outward the circle center to increase or decrease the radius, respectively.

4.1.16 Split Line or Arc at a Point

The Split Line or Arc by Point tool allows the user to split a line at a given point. To split the line the user should just specify the splitting point position by clicking the left mouse button. Prior selection of the line (arc) to be split is not required. The point under cursor is automatically aligned to the nearest object which is split. If the splitting point is an intersection point of two or more lines, all of them are split.

4.1.17 Add Normal Splitting An Existing Line, Arc…

 The **Add Normal Splitting an Existing Line, Arc…** tool allows the user to create line normal to an existing line or arc which is split at the intersection point. The user should select the line (or arc) to be split and then to specify the reference point, i.e. a point from

which perpendicular is dropped on the selected line. The reference point can either be an existing point (an ending point of some other lines) or a new point.

Note that creation of a normal to a line is successful if only the reference point is positioned so that its projection is within the selected line, which is actually a finite-length line segment with two ending points. Otherwise, if this segment and the normal line do not intersect (i.e. the intersection point of the normal and the infinite line that comprises the segment lies beyond the segment itself), the intersection point is shifted to the nearest ending point, so that the created line is not normal to the selected line.

A normal to an arc (circle) is a line connecting the reference point and the arc (circle) center.

4.1.18 Split Line, Arc… By Normal Projection

The **Split Line, Arc... By Normal Projection** tool allows the user to split a line at a point created as a normal projection of some reference point. The user should select the line (or arc) to be split and then to specify the reference point, i.e. a point from which perpendicular is dropped on the selected line to find the projection position. The reference point can either be an existing point (an ending point of some other lines) or a new point. Unlike the **Add Normal Splitting an Existing Line or Arc** tool, this tool does not add the line connecting the reference point and the splitting point.

Note that splitting by normal projection is only available when the reference point is positioned so that its projection is within the selected line, which is actually a finite-length line segment with two ending points.

A normal to an arc (circle) is a line connecting the reference point and the arc (circle) center. So the arc is split at the point of intersection of the arc with circle radius oriented toward the reference point.

4.1.19 Add Text

 The **Add Text** tool allows the user to add a text to the drawing. The user should specify the text position with the left mouse button and enter the text in a Text dialog window.

4.1.20 Add Callout

 \mathbf{a} The **Callout** tool allows the user to add a callout to some element of the drawing. The user should specify the text position with the left mouse button and enter the text in a Text dialog window.

4.1.21 Edit Text

 The **Edit Text** tool allows the user to edit an existing text. To edit a text, the user should first press the Edit text button and then click on the text to be edited. Then a Text dialog window will appear.

4.1.22 Increase Font Size

AA The Increase Font Size tool allows the user to increase size of the font used in text and callouts added to the drawing. To enlarge a text, the user should first select the text and then to press the **Increase Font Size** button. A single click application of this tool increases the font size by 10 per cent of its current value.

4.1.23 Decrease Font Size

 The **Decrease Font Size** tool allows the user to decrease size of the font used in text and callouts added to the drawing. To reduce a text, the user should first select the text and then to press the **Decrease Font Size** button. A single click application of this tool decreases the font size by 10 per cent of its current value.

4.1.24 Move Selected Objects by Mouse

 The **Move Selected Objects by Mouse** tool allows the user to move objects (lines, arcs, or points) in an arbitrary direction using the mouse. The user should first select the objects to be moved, then to press the left mouse button, move the mouse cursor in the desired direction, and then to release the mouse button specifying the new object position. If new positions of some points of the moved object are located in the vicinity of the existing objects, the cursor position specifies the intermediate positions only. To finalize the object

displacement the user should clear the object selection (by pressing the spacebar key). Then such points are aligned to the existing points.

Note that releasing the mouse button does not finalize the moving operation (it does not clear the object selection) so that the object can be consecutively moved several times without distortion at the intermediate positions.

4.1.25 Move Horizontally by Mouse

 The **Move Horizontally by Mouse** tool allows the user to move objects in horizontal direction using the mouse. Compared to the **Move Selected Objects by Mouse** tool, the vertical coordinate is fixed during cursor displacement.

4.1.26 Move Vertically by Mouse

 The **Move Vertically by Mouse** tool allows the user to move objects in vertical direction using the mouse. Compared to the **Move Selected Objects by Mouse** tool, the horizontal coordinate is fixed during cursor displacement.

4.1.27 Move Selected Objects by Explicit Shift

 The **Move Selected Objects by Explicit Shift** tool allows the user to move selected objects by explicit specification of the displacement value. First, the user should select the objects to shift, then to press the **Move Selected Objects by Explicit Shift** tool button. It opens the Translation dialog window that has two text fields **Translation along X** and **Translation along Y**, respectively. The shift values should be specified in microns.

Fig. 11

4.1.28 Put Flag

The **Put Flag** tool allows the user to add a mark to some drawing position.

4.1.29 Merge Selected Points

昬 The **Merge Selected Points** tool allows the user to merge some separated close points. To merge some close points the user should first select the points to be merged and then press the **Merge Selected Points** tool button. Then the points will be merged into a single point whose position is determined by the order of the point selection, so that the coordinates of the first selected points are assigned to the new common point.

4.1.30 Merge All Points in the Rectangle

鸥 The **Merge All Points in the Rectangle** tool allows the user to merge all points in the selected window. To merge a group of points the user should first press the **Merge Selected Points** tool button. Then the cursor shape changes to a small rectangle. The user should position this rectangle so that it would comprise the points to be merged. The rectangle has a fixed size in pixels so that if it is too small to surround all needed points the user can change the relative size of the rectangle by zooming out the drawing. Clicking with the left mouse button will merge the points into a single point whose position is determined by one of the merged points that is closest to the rectangle center. This point starts flickering in white to identify this before the points are merged.

4.1.31 Unlink Lines with a Common Point

 The **Unlink Lines with a Common Point** tool allows the user to unlink lines that have a common point. To apply this tool the user should first select the lines (see Fig. 12 **a**) and then press the **Unlink Lines with a Common Point** tool button. Then the lines are separated (see Fig. 12 **b**) and can be edited (moved, etc.) independently.

Fig. 12

4.1.32 Align Selected Points Horizontally

 The **Align Selected Points Horizontally** tool allows the user to align X coordinates of a group of points. The user should first select two or more points and then press the **Align Selected Points Horizontally** tool button. The X-coordinates of all selected points will be changed to the X-coordinate of the first selected point.

4.1.33 Align Selected Points Vertically

圩 The **Align Selected Points Vertically** tool allows the user to align Y coordinates of a group of points. The user should first select two or more points and then press the **Align Selected Points Vertically** tool button. The Y-coordinates of all selected points will be changed to the Y-coordinate of the first selected point.

4.1.34 Multiply Selected Objects

e, The **Multiply Selected Objects** tool allows the user to multiply several objects with moving them in some direction, rotating with reference to a selected point, or flipping vertically or horizontally. This tool was designed to provide an easy specification of repeated contour fragments in some complex, for example, periodical or symmetrical, die geometries.

Pressing **Multiply Selected Objects** tool button opens the **Copy Objects** dialog window that includes three tabs corresponding to different types of the tool operation and a set of buttons governing the following stages of the user actions:

- **►** Select Objects. The initial stage at which the user should select the original objects by the mouse.
- **►** Select Center. For Rotate type the user should specify a point that will be used as the rotation center. For Flip type, the user should specify a point that determines a horizontal or vertical line that will be used as the reference axis.
- **Enter Param**. At this stage the user should specify the parameters described below.
- **Copy Objects**. A button applying the operation.

The following types of the operation are available:

- **EXECOPY** CODY. This operation represents translation of the selected objects in a vertical or horizontal direction. Simultaneous copying in several directions is available. The **Copy** tab includes the following elements (see Fig. 13):
	- Section **Direction** contains checkboxes –X, +X, -Y and +Y providing translation to the left, to the right, downward and upward, respectively.

- **Step**. The distance of the translation.

- **Repeat**. The number of objects to be created in each specified direction. Multiple translation (**Repeat** is above 1) creates equidistant objects

consecutively, so that *i*-s new object is translated by Step value with reference to the $(i-1)$ -s object, i.e. by Step^{*}i with reference to the original one.

Rotate. This operation creates new object by rotation of the selected objects. Simultaneous creation of objects by rotating at consecutively increasing angles is available. The **Rotate** tab includes the following elements (see Fig. 14):

- **Angle**. The rotation angle of the translation (in degrees).

- **Repeat**. The number of objects to be created. Multiple rotation (**Repeat** is above 1) consecutively creates objects so that \dot{r} s new object is rotated by Angle value with reference to the $(i-1)$ -s object, i.e. by Step^{*}i with reference to the original one.

Fig. 14

Flip. This operation represents flip of the selected object with reference to some vertical or horizontal axis. The **Flip** tab includes the following elements (see Fig. 15):

- **Flip Vertical/Flip Horizontal** element allows the user to specify the flip direction.

Fig. 15

4.1.35 Duplicate Selected Objects at a Specified Shift

 $\mathbb{F}^{\mathbb{Z}}$ The **Duplicate Selected Objects at a Specified Shift** tool allows the user to duplicate an object creating the copy at a specified position. The user should first select an object, then specify the starting point of the translation vector (as a rule, a point on the original object), and then specify the ending point of the translation vector (at the new position of this point).

4.1.36 Duplicate Selected Objects at a Preset Shift

 The **Duplicate Selected Objects at a Preset Shift** tool provides a fast way to duplicate an object creating the copy at some predefined position shifted both to the right and upwards with respect to the original object. The user should only select an object and press the **Duplicate Selected Objects at a Preset Shift** tool button.

4.1.37 Duplicate at Preset Shift Horizontally

DHD The **Duplicate at Preset Shift Horizontally** tool provides a fast way to duplicate an object creating the copy at some predefined position shifted to the right with respect to the original object. The user should only select an object and press the **Duplicate at Preset Shift Horizontally** tool button.

4.1.38 Duplicate at Preset Shift Vertically

舌 The **Duplicate at Preset Shift Vertically** tool provides a fast way to duplicate an object creating the copy at some predefined position shifted upwards with respect to the original object. The user should only select an object and press the **Duplicate at Preset Shift Vertically** tool button.

4.1.39 Analyze for Dangling Lines

 The **Analyze for Dangling Lines** tool performs analysis of self-consistency of geometry specification, providing the user information on the presence of dangling lines (in other terms, points with only one contacting line or arc) and partially coincident lines.

4.1.40 Measure Distances and Orientation

耑 The **Measure Distances and Orientation** tool allows the user to measure distances and orientation of lines in the drawing. The user should consecutively specify the first and the last ending points of a vector. A resulting message window contains the following parameters:

- \triangleright Coordinates of each points
- \triangleright Length of the X and Y projections of the vector
- \triangleright Vector length
- \triangleright Angle of the vector orientation in the counter-clockwise direction.

Fig. 16

4.1.41 Delete Selected Objects

 \times The **Delete Selected Objects** tool allows the user to remove any objects from the current layer of the drawing.

4.1.42 Undo

The **Undo** tool allows the user to undo the last action.

4.1.43 Redo

The **Redo** tool allows the user to redo the last action.

4.2 Object Editor

The Object Editor located on top of the **Geom** tab provides an explicit modification of the coordinates of boundary end points (see Fig. 17). It includes two tabs **Selected Object** and **New Object** allowing the user to edit coordinates of a selected existing object or to create a new object by specifying its coordinates. Each tab contains the following items:

- **Civilible Type** combo box specifying the type of the edited object, which can be Point, Line, Arc or Circle. For a selected object, this parameter can not be changed. For a new object, it should be assigned by the user prior to specification of the object coordinates.
- \triangleright The list of the parameters to be specified:
	- \checkmark For a *Point*: X, Y point coordinates.
	- \checkmark For a Line: X1, Y1, X2, Y2 coordinates of first and last ending points.
	- \checkmark For an Arc: Xc, Yc, R, A1, A2 center coordinates, radius, and angles of the arc ending points.
	- \checkmark For a Circle: Xc, Yc, R circle center and radius.
- \triangleright A text field with the parameters. Text field contains both name of the parameters, which are added automatically, and their values, which are entered by the user. Switching the cursor position between values of different parameters can be made by pressing <Tab> (go to the next parameter) and <Shift-Tab> (go to the previous parameter).
- A button **A** Apply.

Fig. 17

4.3 Viewing Toolbar

The Viewing toolbar is located at the bottom of the **Geometry** tab window and contains a set of buttons governing the options of geometry specification and visualization.

4.3.1 Zoom

The **Zoom** section allows the user to refresh and zoom the image. It contains the following buttons:

- **E**
Zoom In button allows the user to enlarge the image.
- **Zoom Out** button allows the user to reduce the image.
- **Show All** button automatically calculates the drawing scale to fit all objects in the drawing.
- **Show Page** button assigns the drawing scale to fit the page. The page is visualized by white dashed lines, its dimensions and position can be specified in the Options dialog window available via Options -> Preferences menu item.
- **Refresh** button forces image refreshing.

4.3.2 Draw Color

The **Draw Color** section allows the user to specify the color of the lines to be drawn. Note that changing the color does not have an effect on the earlier drawn contours.

4.3.3 Pen Width

The **Pen Width** section allows the user to specify the thickness of the drawn lines. Changing the line thickness affects all contours on the drawing.

4.3.4 Drawing Mode

The **Mode** section contains **Elastic Lines** and **Point-to-Point Lines** buttons that allow the user to switch between two modes of line drawing, which are described above in Add Line section.

4.3.5 Grid

The **Grid** section allows the user to specify visualization of reference coordinate grid and alignment of the entered coordinates to the grid nodes.

The **Grid** section contains the following buttons:

- **Show Grid** governs visualization of the reference grid.
- **Draw Aligning To Grid** governs the creation of new objects. If this button is pressed, the ending points of new objects are aligned to the nodes of the reference grid closest to the cursor position.
	- **益** Decrease Step button decreases the Grid Step in two times.
	- **Increase Step** button increases the Grid Step in two times.

The **Grid Step** can also be assigned by the user explicitly using Options->Preferences menu item.

4.3.6 Points

The **Points** section allows the user to specify the modes of point visualization. It contains the following buttons:

Show Points governs visualization of ending points.

 Show Frame Around Close Points enables identification of close points which might correspond to a single physical point but were separated unintentionally during geometry specification.

4.3.7 Select

The **Select** section allows the user to specify the modes of point and line selection. It contains the following buttons:

- **S** Select Lines Only. If this button is pressed, points cannot be selected, which makes easier to pick a line in a complex geometry with close points lines.
- **Select Points Only**. If this button is pressed, lines and arcs cannot be selected, which makes easier to pick a point in a complex geometry with short lines.

5 Layers Tab Window

5.1 Assigning the Layers

When the contours are drawn, the user has to assign them to layers of the chip.

5.1.1 Layers in Planar Chip Configuration

Specification of a planar chip (see Fig. 18) includes assigning the following layers:

p-semiconductor. Surface of the p-semiconductor layer (see Fig. 19). The whole die contour area lying beyond the p-semiconductor is assumed to represent the mesa etched in the die. The area of the n-semiconductor layer is assumed to match the external contour drawn by the user. So it is assigned automatically and should not be explicitly specified.

Fig. 19

p-spreading. Area of the current spreading layer (highly conductive semiconductor like ITO) under p-electrode (see Fig. 20), if it is included into **Chip Configuration**. This layer should lie inside the p-semiconductor.

Fig. 20

p-blocking. Area of the current blocking layer (insulating material) under p-electrode, if it is included into **Chip Configuration**. This layer should lie inside the p-semiconductor.

p-electrode. Area of the metal p-electrode (see Fig. 21). This layer should lie inside the p-semiconductor.

Fig. 21

p-pad. Area of the pad on p-electrode (see Fig. 22). This layer should lie inside the pelectrode.

Fig. 22

p-wire. Area of the electric contact of the pad on p-electrode where the electric potential equals to the applied voltage. This layer should lie inside the p-pad.

Fig. 23

n-electrode. Area of the metal n-electrode (see Fig. 24). This layer should lie inside etched mesa, i.e. outside of the p-semiconductor layer.

Fig. 24

n-blocking. Area of the current blocking layer (insulating material) under p-electrode (see Fig. 25), if it is included into **Chip Configuration**. This layer should lie inside etched mesa, i.e. outside of the p-semiconductor layer.

Fig. 25

n-pad. Area of the pad on n-electrode (see Fig. 26). This layer should lie inside the nelectrode.

Fig. 26

n-wire. Area of the electric contact of the pad on n-electrode where potential equal to zero. This layer should lie inside the n-pad.

5.1.2 Layers in Vertical Chip Configuration

Fig. 27

The areas of the both p- and n-semiconductor layers are assumed to match the external contour drawn by the user. So they are assigned automatically and should not be explicitly specified. Specification of a vertical chip (see Fig. 27) includes assigning the following layers:

p-blocking. Area of the current blocking (insulating material) under p-electrode, if it is included into **Chip Configuration**.

p-spreading. Area of the current spreading layer (highly conductive semiconductor like ITO) under p-electrode, if it is included into **Chip Configuration**.

p-electrode. Area of the metal p-electrode (see Fig. 28).

Fig. 28

p-pad. Area of the pad on p-electrode (see Fig. 29). This layer should lie inside the pelectrode.

Fig. 29

p-wire. Area of the electric contact of the pad on p-electrode (see Fig. 30) where electric potential equals to the applied voltage. This layer should lie inside the p-pad.

n-blocking. Area of the current blocking (insulating material) under n-electrode (see Fig. 31), if it is included into **Chip Configuration**.

Fig. 31

n-electrode. Area of the metal n-electrode (see Fig. 32).

Fig. 32

n Pad. Area of the pad on n-electrode (see Fig. 33). This layer should lie inside the nelectrode.

Fig. 33

n-wire. Area of the electric contact of the pad on n-electrode. This layer should lie inside the n-pad.

5.1.3 Assigning the Layers

To assign a layer, the user should do the following:

- \triangleright Select the layer to be specified in the list of layers. By default, all layers are empty, so no contour in the Graphics Window will be colored.
- \triangleright Select the block(s) which to be added to the selected layer. The selected blocks are colored with the color corresponding to the selected layer. Each layer can consist of an arbitrary number of contours, which can be either adjacent to each other or separated. There are two selection modes which can be chosen by the two buttons in the Select Mode rectangle below the list of the layers (see Fig. 33):
	- \checkmark Selecting one block by one click with the left mouse button
	- \checkmark Selecting all blocks inside the rectangle
- **Press Apply** button to confirm addition of the selected blocks to the selected layer.

For a vertical chip configuration either n- or p-side elements are shown at one time. The user should select the edited side of the die using the **Active Side** buttons above the Graphics Window.

In addition to the layers to be assigned, the list of shown layers includes an item Mosaic. If it is selected, all contours are checked with colors corresponding to all layers in which the given domain is included. So, for example, the p-pad contour is colored with colors of p-pad, p-electrode and p-contour.

Button **Draw 3D** activates the 3D visualization of the die geometry.

5.2 3D View Mode

The **3D View Mode** (see Fig. 34) provides intuitive visualization of the specified die geometry, including the substrate. It contains the following elements:

Fig. 34

- \triangleright List of the die layers at the left hand side of the window. The user can check the layers to be shown.
- \triangleright Graphics window presents the 3D die geometry. The image is controlled by the following mouse operations:
	- \checkmark Image translation (displacement) right button.
	- \checkmark Image rotation left button.
	- \checkmark Zooming in wheel (rolling downwards)
	- \checkmark Zooming out wheel (rolling upwards)
- **Color** button, allowing the user to assign the colors to each die element.
- **Move** section contains arrow buttons allowing the user to move the image. It provides another possibility of the image displacement in addition to shift by mouse.
- **Zoom** section contains two buttons allowing the user to zoom in and zoom out the image. It provides another possibility of the image scaling in addition to zoom by mouse.

- **Z-Scale** section allows the user to scale the image by assigning the multiplication factor used to draw the layer height. The factor can be increased or decreased using the arrow buttons at the right hand side of the text field either by 1 (slow z-scale variation) or by 10 (fast z-scale variation).
- **Default View** button restores the initial scale and position of the image.
- **Copy To Clipboard** button copies the image to the clipboard.
- **Save To File** button stores the image to a .bmp file.
- **Elose** button closes the 3D view and switches back to main mode of the Layers tab window.

6 Grid Tab Window

Fig. 35

The **Grid** tab window (see Fig. 35) is designed to specify and visualize the computational grid.

Mesh is generated in all closed contours for which fragmentation is assigned for all boundaries.

Boundaries at which the fragmentation is not assigned are marked by large yellow circles.

The control panel at the left hand side of the Graphics Window includes the following elements governing the grid generation:

Section Mode. The following modes of grid generation are available:

- **Selected Edge**. This mode provides specification of the grid fragmentation independently for each individual boundary. The user should first select the boundary and assign its fragmentation. Multiple selections are also available. If several boundaries are selected, the fragmentation is assigned to all selected boundaries.

- **All Edges**. This mode provides automatic fragmentation of the whole geometry using a single user defined parameter. Note that since the user defined parameter represents a number of intervals (see description of Interval parameter below) rather than the interval length, in this mode the user should first select a reference boundary.

Section **Interval**. This section provides specification of the number of intervals and interval length to be assigned. It contain the following elements:

 \checkmark Interval text field contains the number of intervals to be assigned to the selected boundary. If fragmentation is assigned to a group of boundaries (in the automatic mode or in case of multiple boundary selections in the manual mode) which can have different length, this parameter is first converted to the grid density (length of an interval) using the length of the selected boundary (in case of multiple boundary selections in the manual mode the first selected boundary is used). Then the found grid density is assigned to all (in automatic mode) or all selected (in manual mode) boundaries.

A group of buttons **2 3 10 13 20 23 30** provides a fast assignment of some predefined Interval values.

Fig. 36

- Section **Refinement** allows the user to specify a continuous increase of the internodal distance (i.e. distance between consecutive grid nodes) towards some of the edges of the selected boundary or to the center from both edges (see Fig. 36). It is only available in the Selected Edge mode. It contains the following elements:

- Text field **Power** specifying the exponent of the power function used to define the internodal distance variation. Power $= 1$ corresponds to a uniform point distribution. The higher is power, the more considerable internodal distance increase is applied. Fig. 36 presents an example of grid refinement for a Power of 1.7.

- Up and Down Arrows providing an easy way to increase or decrease the digits of the Power decimal representation. The left arrows govern the digit before the point, while left arrows govern the digit after the point.

 \checkmark Direction of increase of the internodal distance. The following variants are available: **Forward** (the internodal distance increases from the first ending point towards the second ending point), **Backward** (the internodal distance increases from the second ending point towards the first ending point), and **Symmetrical** (grid refinement towards the ending points).

 Section **T-Grid Options** provides specification of triangular grid generation. The following options are available:

Fig. 37 Fig. 38

- **Adv.Front**. The advancing front method builds internal cells close to equilateral triangles whose side size is equal to the boundary edge size, using no additional parameters (see Fig. 37).

- **Delauney**. The Delauney method builds cells by scattering the internal points in the domain (see Fig. 38) using the parameter Cell Size Ratio that is specified in the text field located at the right hand side of the of the T -Grid Options section. Fig. 38 presents an example of Delauney grid generation for a cell size ratio of 1.30.

► Section Auto Grid Type allows the user to specify the desired mesh type. The following options are available:

- **Try To Create Q-Grid** (default). In this case the automatic generator tries to generate quadrangular grid in all domains. If the domain can not be represented as a quadrangle, triangular grid is generated. The user can also manually specify the blocks where triangular grid should be generated using the *Blocks* section described below.

- **All Grids Should Be T-Grids**. In this case the automatic generator generates triangular grid for all domains regardless to their shape.

- **►** Button Apply applies the specified parameters keeping selection of the boundaries.
- **►** Button **Store** applies the specified parameters clearing selection of the boundaries.
- Section **Grid Contrast** allows the user to vary the brightness of the mesh lines with respect to the main geometry lines.

Below the Graphics Window the status bar provides information of the number of cells in grid.

In a vertical die n- and p-sides of the chip are meshed independently. So for a vertical chip configuration the user should assign both n- and p- grids.

7 Functions Tab Window

The **Functions** tab window allows the user to specify a set of functional and piecewise linear dependencies to be used in specification of the materials properties. **Functions** window contains two tab windows, namely, **Functions** and **Piecewise-Linear Approximation**.

The tab **Functions** contains the following elements (see Fig. 39):

Fig. 39

- Section **Global User-Defined Constants** on top of the window allows the user to define a set of global parameters that can be used in different functions.
- Section **Functions** containing the list of defined functions and the following buttons:

- **✓** Button **New** adds a new function.
- Button **Delete** removes the selected function.
- Button **Rename** allows the user to rename the selected function.
- **►** Tab **Editor** provides specification of the function. It contains the following items:

- Section **Arguments of the Function** contains list of variables to be used as arguments of the function. The available variables include X , Y (planar coordinates), Z (vertical coordinate counted starting from the active layer), and T (temperature).

- Section **Code** contains the text definition of the function. The function returns the value assigned to the variable Result.

- Button **Compile** provides compilation of the function text and checks for the errors.

- Button **Built-In Functions** opens a dialog window providing a list of built-in functions (see Fig. 40). The user can either type the function name in the code or just select the needed function in the list and press button **Copy to Code**.

Fig. 40

- Button **Import** allows the user to load functions defined in another project.

- Button **Code Example** provides a set of code fragments to be used as examples of function programming.

 Tab **Graph** provides graphical visualization of the specified function. It contains the following items (see Fig. 41):

- Button **Create Graph** opens a dialog window allowing the user to select the X-variable, Y-variable (this can be Result variable or some other variables defined in the function code), and ranges of X-variable variation.

- Button **Edit Ranges** allowing the user to change ranges of the X-variable variation for an existing plot.

 \checkmark The graph plotting Y-variable vs. X-variable.

Fig. 41

 Tab **Debugger** allows the user to trace the code execution and check the intermediate results. It contains the following items (see Fig. 42):

 \checkmark Section containing the lines of the function code, which are executed consecutively.

- Button **Execute Line** providing execution of the code of the current line.
- Button **From Beginning** providing restart of the code debugging.

- Section **Variables** at the right hand side visualizing the current values of all variables defined within the function.

- Button **Edit Value** allowing the user to assign manually the value of a selected variable during the code execution.

Fig. 42

7.1.1 Functions Dialog Window: Piecewise-Linear Approximations Tab

The tab **Piecewise-Linear Approximations** contains the following elements (see Fig. 43):

- Section **Approximations** containing the list of defined approximations and the following buttons:
	- Button **New** adds a new piecewise-linear approximation.
	- Button **Rename** allows the user to rename the selected approximation.

- Button **Import** allows the user to load points of an approximation defined in an ASCII text file as two columns of numbers. File with extension .txt or .dat can be loaded. Note that the points defined in the file are assigned to the selected approximation. So to read an approximation from the file the user should first create a new (empty) approximation and then import the data into it.

- Button **Delete** removes the selected approximation.
- Section **Argument** contains list of variables to be used as argument of the approximation. The following arguments are available: X , Y (planar coordinates), Z (vertical coordinate counted starting from the active layer), and T (temperature).

- Section **Points** containing the list of points (table with two columns corresponding to the argument and value of each point) in the current approximation and the following buttons:
	- Button **Add** adds a new point to the approximation.
	- Button **Delete** removes the selected point from the approximation.

- Button **Change** opens a dialog window where the user can enter the argument (X-axis) and value (Y-axis) of the approximation. The values should be separated by a white space, comma or semicolon.

Section **Plot** visualizing the specified approximation.

Fig. 43

8 Materials Tab Window

The **Materials** tab window allows the user to specify the physical properties of the semiconductor and metal materials to be assigned to the die elements. It contains the following sections (see Fig. 44):

Fig. 44

8.1 Specification of Materials Properties

Section **Materials** containing the list of materials defined in the current project and the following buttons:

- ▶ Button **New** adds a new material. Pressing this button opens a New Material dialog window specifying the type of the material. Generally, the following types are supported: Semiconductor (can be used for semiconductor layers and for the substrate), Conductor (can be used for substrate and for semiconductor layers), Insulator (can be used for insulating substrate only), and transparent conductive oxide (ITO). ITO material can be added only to a project with p-spreading layer activated in the **Project Configuration** window.
- **►** Button Copy duplicates an existing material, creating another material with the same characteristics. This provides an easy specification of a group of materials with

similar properties, allowing the user to avoid second definition of common characteristics and to assign the changed parameters only.

- Button **Delete** removes the selected material.
- **▶ Button Rename** renames the selected material.
- **Button Import** provides importing materials from other project files. After the user selects the file with materials, Import dialog window is opened (see Fig. 45). It contains the list of materials in the selected file at the left hand side and the list of materials in the current project at the right hand side. The user should check the materials to be imported and press the **Import** button.

Import from D:\SpeCLED2\Tests\testP0_05c.dvx ⊻ SP	
testP0_05c.dvx	Current project
$\sqrt{}$ n-Ga $\overline{\text{N}}$ Au ⊽ Ψ _{p-GaN}	
g Select all 極 Import	X Close

Fig. 45

8.2 List of Properties

Section **Properties** contains the list of characteristics of the given material and section **Property Description** with specification of each material parameter.

8.2.1 Conductor and Insulator Materials

Conductor materials provides the user direct control of the electrical and thermal conductivity:

- **COND** Thermal conductivity $[W/(mK)]$
- **ECOND** Electric conductivity $[(\Omega \, m)^{-1}]$ (not required for insulators)

8.2.2 Semiconductor Material

Semiconductor material allows the user to specify the electrical conductivity in terms of the material parameters. For a semiconductor material the user should specify the following parameters (their meaning depends on the semiconductor type, n- or p-)

- **COND** Thermal conductivity $[W/(mK)]$
- **MOB_XY** and **pMOB_Z** Carrier mobility in lateral and normal direction, respectively.
- **▶ DOPING** –Concentration of dopant atoms (donors or acceptors) [cm⁻³]
- \triangleright **Ei** Activation energy of the dopant $[eV]$
- **▶ DOS** Conduction band or valence band density of states [cm⁻³]
- **g-factor** Degeneracy factor for electrons or holes

8.2.3 ITO Material

ITO material is treated in a special way because of its complex properties. For a Spreading Layer material the user should specify the following obligatory parameters:

- \triangleright Thickness of the spreading layer [nm]
- Electric conductivity of the spreading layer $[1/(\Omega \cdot cm)]$. Sheet resistance is calculated automatically to help the user.
- \triangleright Thermal conductivity of the spreading layer [W/(m·K)] The electron heat conductivity may be considerable in ITO material, so the user can add this contribution.
- \triangleright Specific contact resistance to the underlying p-semiconductor

Also, one can estimate the optical properties of the ITO which are closely related to its electrical properties. To do it, one need specify some additional parameters: electron concentration, electron effective mass, and lattice dielectric constant. Then resulting optical properties are calculated automatically and their wavelength dependence is shown (see Fig. 46).

! Note that optical properties are calculated just for user convenience. They are NOT automatically transferred into the RATRO input data.

Fig. 46

8.3 Specification of Materials Properties

Each parameter can be specified by a constant value, predefined temperature dependence, or a used-defined function of temperature or coordinates. So the following options are available:

Constant (see Fig. 47). For a constant specification of the selected material characteristic, the Property Description section contains a text field **Value** and button **Edit** allowing the user to change the value.

Fig. 47

Polynomial (see Fig. 48). For a polynomial specification of the selected material characteristic, the Property Description section contains the following items:

Property description COND - Heat Conductivity, VW(m*K) Parametric Dependence constant C A+B/T C polynomial C expression C function C piecewise linear Polynomial P(T)=15+6.3e-3*T+1.23e-7*T^3 Polynomial coefficients 15 TAD TChart 150 6.3e-3 T^{A1} $\begin{array}{|c|c|c|}\n\hline\n0 & T^2 \\
1.23e-7 & T^3\n\end{array}$ 140 130 120 110 100 90 $\overline{80}$ 70 60 50 40 30 20° 350 420 490 560 630 700 770 840 910 980 1050 280 Ranges from 300 to 1000 **Later Edit ranges** Add Coefficient $\begin{tabular}{|c|c|} \hline Scale X & Scale Y \\ \hline @ linear & @ linear \\ \hline C & log & C & log \\ \hline \end{tabular}$ Xaxis Line Width Y axis # Default # # Default 滑Edit **X** Delete $\sqrt{2}$

Fig. 48

 \checkmark A text string presenting the polynomial expression corresponding to the current values of coefficients.

- Section **Polynomial Coefficients** presenting the list of assigned coefficients

 \checkmark Button **Add Coefficient** allowing the user to add the coefficient at the next degree of temperature with respect to the highest degree already assigned. So the coefficients should be introduced consecutively, starting from T^0 (the free term). If some coefficient is missed in the polynomial approximation, zero value should be explicitly assigned.

- Button **Edit** allowing the user to change the value of the selected coefficient

 \checkmark Button **Delete** allowing the user to remove the last term in the polynomial approximation.

- Plot visualizing the property variation with temperature. Button **Edit Ranges** allows the user to change the range of the argument variation in the plot.

Piecewise Linear (see Fig. 49). For a piecewise linear specification of the selected material characteristic, the Property Description section contains the following items:

- Section **Points** containing the list of points (table with two columns corresponding to the argument and value of each point) in the current approximation

✓ Button New adds a new point to the approximation.

- Button **Delete** removes the selected point from the approximation.

✓ Button Edit opens a dialog window where the user can enter the argument (X-axis) and value (Y-axis) of the approximation. The values should be separated by a white space, comma or semicolon.

- Button **Import** allows the user to load points of an approximation defined in an ASCII text file as two columns of variables. File with extension .txt or .dat can be loaded.

 \checkmark Plot visualizing the property variation with temperature.

A + B/T (see Fig. 50). For a temperature dependence of the selected material characteristic defined as $f(T) = A + B/T$, the *Property Description* section contains a text field **Values** and button **Edit** allowing the user to change **A** and **B** parameters. The values should be separated by a white space, comma or semicolon.

Expression (see Fig. 51) allows the user to specify a simple (expressed by a single formula) temperature dependence of the selected material characteristic. In this mode the Property Description section contains the following items:

Property description nMOB - Lateral Electron Mobility, cm^2/(V*s) Parametric Dependence C A+B/T constant polynomial c expression C piecewise linear C function Expression | Expression 250*(300/T)^1.5 **SEdit** 260 nMOB - Lateral Electron Mobility, cm⁺2/(... 240 Expression 250*(300/T)^1.5 220 200 \vee Ok <Enter> X Cancel <Esc> 180 160 140 120 100 80 60 40 350 420 490 560 630 700 770 840 910 1050 280 980 Scale X Scale Y Line Width Y axis Xaxis Clinear Clinear # | Default | | | | Default | $\sqrt{2}$ Ranges from 300 to 1000 H Edit ranges

Fig. 51

 \checkmark A text string presenting the polynomial expression corresponding to the current values of coefficients.

- Button **Edit** allowing the user to enter the formula. The expression syntax can be seen using the Code Example window available from the Functions dialog window.

 \checkmark Plot visualizing the property variation with temperature.

- Button **Edit Ranges** allows the user to change the range of the argument variation in the plot.

Function (see Fig. 52) allows the user to specify a complex temperature dependence of the selected material characteristic. In this mode the Property Description section contains the following items:

- Combo box **Function** where the user can select an existing function. The functions should be specified earlier using the Functions dialog window. The functions are identified by the user-defined names preceded by "#" symbol.

- Button **Edit Functions** allows the user to create a new function without leaving the Materials dialog providing an access to the Functions dialog window.

Fig. 52

9 Active Region Tab Window

The **Active Region** tab window allows the user to specify the I-V characteristics of the active region for a set of temperature values. The user can either import them from files generated by **SiLENSe™** code in the mode Computed by SiLENSe, to prescribe them using an approximation in the mode *Parametric Approximation* or assign them manually in Table Input mode. The approximations are described in details in the Physics Summary documentation.

Mode of the active region I-V characteristics is selected using radio buttons at the bottom of the window. This selection activates the respective tab window.

9.1 Use of I-V Characteristics Computed by SiLENSe

In the Computed by SiLENSe mode, control panel at the left hand side of the **I-V Characteristics** window contains the following elements (see Fig. 53):

- **EXECUTE:** List of files with active region I-V characteristics at different temperatures.
- **Button Load** allows the user to import active region I-V characteristics from other projects or from one or several files (*.sct) generated by **SiLENSe™** software for the given structure of the chip active region for a given temperature.

Button **Delete** removes the selected characteristic.

Button Delete All removes all imported characteristics.

Fig. 53

9.2 Parametric Specification of I-V Characteristics

In the Parametric Approximation mode, control panel at the left hand side of the **Active Region** window contains the following elements (see Fig. 54):

Fig. 54

- Section I-V Characteristics contains the following parameters of the I-V characteristics approximation:
	- Saturation current density j_0 , A/cm²
	- \checkmark Specific band gap E_G , eV
	- \checkmark Active layer resistance ρ_A , Ω cm²
	- \checkmark Non-ideality factor m
- Section Internal Quantum Efficiency (IQE) contains the following parameters of the IQE approximation:
	- \checkmark Active Region Thickness d, nm
	- \checkmark Radiative Recombination Constant B, cm³s⁻¹
	- Auger Recombination Coefficient C, cm^6s^{-1} .
	- \checkmark Non-radiative lifetime τ , ns
	- \checkmark Power Factor γ
- \triangleright Section *Wavelength* allows the user to assign the emission wavelength.
- \triangleright Button Restore Defaults assigns the default predefined values to all parameters.

- \triangleright Button Store as Defaults allows the user to set the specified values as default parameters.
- \triangleright Button Apply allows activates the entered values and refreshes the plots at the righthand side.
- Eist of temperatures for which the I-V characteristics and IQE has been calculated and plotted.

9.3 Manual Specification of I-V Characteristics

In the Manual mode the user can assign the current-voltage characteristics, IQE and emission spectrum in a table form. The control panel at the left hand side of the **Active Region** window contains the following elements (see Fig. 55):

Fig. 55

- \triangleright Table containing several sections corresponding to different temperatures. It has the following columns:
	- \checkmark U, V forward bias

- \checkmark j, A/cm^2 current density
- \checkmark IQE internal quantum efficiency
- \checkmark Wavelength, nm emission wavelength

To remove a table row corresponding to a given bias the user should select any cell in this row with a single click and press **Delete** key on the keyboard. Note that button **Delete** located below the table removes the whole temperature section as described below.

► Section **Temperature Block** allows the user to add sections of the table for a given temperature. It contains the following buttons:

 \checkmark New – create a new section. After pressing this button, a dialog window appears where the user has to assign the temperature value

- \checkmark Edit modify the temperature value
- \checkmark Delete removes the temperature section
- **Button Sort Table** sorts the table rows in each temperature section according to voltage values.
- Button Import allow import of the active region characteristics specified by the table from another (*.dvx) project file or from a text file (*.txt) of the following format: data for each temperature start from a line containing the temperature, following by the table of 4 columns (p-n junction bias, current density, IQE, and emission wavelength) separated by space or tab symbols. Double slash and all next symbols in the string are ignored. A sample short file is shown below:

300 // fist block for T=300K

9.4 Visualization of Active Region I-V Characteristics

At the right hand side of the **I-V Characteristics** tab window the loaded or assigned by the user active region parameters are plotted as follows.

- Section **Current Density** (available in Computed by SiLENSe and Parametric Approximation modes) contains plot presenting the current (mA) as a function of voltage (V). The selected characteristics (characteristics corresponding to the selected temperature) are drawn in yellow line while all other characteristics drawn as blue lines. Both current and voltage can be plotted in linear or logarithmic scale.
- Section **IQE** (available in Computed by SiLENSe and Parametric Approximation modes) contains plot and datasheet presenting the internal quantum efficiency as a function of current (mA).

Fig. 56

- Tab **Spectra** is available in Computed by SiLENSe mode and provides visualization of the spectra corresponding to the selected I-V characteristics for each voltage value. It contains the of voltage values (in V) and a chart plotting the spectra for the selected voltage.

- Tabs **j**, **IQE** and **Wavelength** is available in Table Input mode and provides visualization of the I-V characteristics, IQE and emission wavelength.

10 Run Tab Window

The **Run** tab provides assigning materials to the die layers, setting boundary conditions and running the computation (see Fig. 57).

Fig. 57

10.1 Heat Transfer

Section **Heat Transfer** specifies the problems to solve. The following options are available:

- **Isothermal Current Spreading**. The current spreading is modeled in an isothermal die at a given temperature assigned in section **Device Temperature**.
- **Coupled Current Spreading and Heat Transfer**. The current spreading and heat transfer are modeled in self-consistent approach, accounting both for the effect of the current spreading on heat transfer and the effect of the temperature non-

uniformity on current spreading. In this mode, temperature assigned by the user is considered as the die temperature used at the initial iteration.

10.2 Light Extraction Efficiency

A user-defined parameter used in the heat transfer simulation to find the heat sources due to light absorption in the crystal. Besides, this parameter is used in the calculation of the total output power of the LED shown in Report section of **SimuLEDView**.

Accurate computation of this parameter is made by **RATRO**. If the user has both **SpeCLED** and **RATRO**, the computations can be made in two iterations as follows:

- An initial **SpeCLED** computation of the emission distribution with some estimation of the light extraction efficiency.
- A **RATRO** computation of the extraction efficiency using the obtained emission distribution.
- **EXECUTED** computation with the calculated light extraction efficiency.

10.3 Volume Conditions

Section **Materials** provides selection of the materials or die element, including the n- and psemiconductor layers, n- and p-electrodes and pads, p-spreading layers, and the substrate. In **Run** tab window, materials are referenced by their names. Characteristics of the materials are specified in the **Materials** tab window.

10.4 Boundary Conditions

Section **Boundary Conditions** provides specification of the following parameters:

- \triangleright Heat Transfer boundary conditions, which are specified by the heat transfer coefficient and ambient temperature on the surfaces that can be used as the heat sinks, namely the n- and p-pads and the substrate back side. One can specify either a value or a name of a script-function defined in the **Functions** tab window.
- Current Spreading boundary conditions include specification of the contact resistances on n-electrode and p-electrode in Ohm \cdot cm².

10.5 Run

The **Run** section allows the user to specify the direct current and start the computations. Also, one can tune solver options here. There are three computation modes listed in the *Current* tab: *Single Calculation*, *Series Calculation*, and *Series Calculation for SimuLAMP*.

Single Calculation tab allows the user to run the computation of the current spreading for a given value of the total current in the die. This value should be assigned by the user in **Total Current** text field. The computation involves fitting of the total current in the die starting from a given voltage. The fitting process is governed by the following parameters:

- **Initial Voltage, V.** Initial value of the forward voltage for which the first iteration on the current spreading at the initial temperature is solved.
- **Voltage Fitting Step, V**. The value of voltage increase (decrease) at the first iterations of the current spreading. The initial iteration results in some current distribution with a certain value of the total current. If this value is less (higher) than the specified current, the initial voltage is increased (decreased) by the Voltage Increment for the second iteration. The next values of the voltage are determined automatically in order to find the voltage providing the specified current.

Series Calculation allows the user to run the computations of the die operation in a wide range value of the current values. This mode allows the user to find the die I-V characteristics. In this mode the user should assign the lower and the upper values of the total current. First, a single calculation is done for the lower current limit. Then the found voltage is increased by the **Voltage Variation Step** and the current spreading is solved at this voltage. The voltage is increased consecutively until the found value of the total current becomes greater than the upper limit of the range of the total current assigned by the user. Thus, in the series computation is made for the range of I-V characteristics specified by the ending values of the current. But the intermediate points of this I-V characteristics are distributed for equidistant values of the voltage. This is made for saving the computation time, provided by avoiding the voltage fitting for each intermediate value of the total current.

Series Calculation for SimuLAMP is designed in order to make an input file for the **SimuLAMP** software containing main LED characteristics for a certain range of temperature and current. The difference with the series computations is that there is also another loop over the list of temperatures specified by the user. The first kind boundary conditions are used at the heat sink surfaces, because the results will be used in SimuLAMP, where the heat resistance between the chip and external LED surface is simulated directly (contrary to

the third kind boundary conditions in usual SpeCLED run, where the heat resistance outside the die is simulated with the heat transfer coefficients). As a result, a text file with ***.tivc** extension is generated for import into **SimuLAMP** software. Output *.cgs files are not generated.

10.5.1 Solver Parameters

Solver Parameters tab contains a set of the computational parameters affecting the convergence of the iterative process. Usually, most of these parameters should not be modified by the user. Below, we will describe them in details and indicate what parameters to be likely changed to resolve convergence problems.

 Current Spreading. Parameters of the solver applied to solution of the electric current spreading problem at given forward voltage at given temperature. It contains the following parameters:

- ∆**J**. The limit variation of the current density. The problem is assumed to be converged if the variation of the current becomes lower than this value.

- **U-Residual Preliminary** and **U-Residual Final**. The limit variation of the electric potential. The problem is assumed to be converged if the variation of the potential becomes lower than this value. Preliminary value is used at the intermediate steps of fitting the current, while final value is used to obtain the final solution.

- **U-Residual Limit** and **U-Number of Iterations**. The limit residual and the maximum number of iterations of the solution of the linear set of equation which is solved by a cycle of local iterations at each iteration of the non-linear problem. Normally, these parameters should not be modified by the user.

- **U-Inertion** and **U-Relaxation** – inertial factor and linear relaxation factor applied to the solution of the non-linear problem. These parameters considerably affect the convergence of the current spreading problem and can be modified by the user in case of divergence or too slow computation. **Automatic** mode enables automatic update of these parameters by the solver according to the solution history, which usually provides satisfactory results. For manual setting, the *Inertial Factor* should be a small value above than zero (for Velocity, Inertial Factor should always exceed zero). As a rule, a lower Inertial Factor value provides faster convergence rate, while a higher value provides more stable convergence by improving ill-conditioned linear set of equations. In

case of solution divergence at the default value, this parameter should be increased. Reasonable values of the inertial factor are in the range 10^{-5} (fast convergence) – 10^{-3} (slow convergence) Linear Relaxation can lay within the interval $0 <$ Relaxation \le 1. Higher Relaxation value provides the fastest convergence rate, while the lower values provide more stable convergence. In case of solution divergence at the default relaxation value, this parameter should be lowered. Reasonable values of the relaxation are in the range 0.2 (slow convergence) – 0.9 (fast convergence).

- **Active Region Parameters (I-V Linearization Method** and **Relaxation)**. It is important what method is used for linearization of the non-linear conductivity of the active region, and what is the relaxation. Usually, tanget method is better and faster for planar structures, while secant method is recommended for vertical ones. But it is recommended to try another method in case of too slow or unstable convergence. The **Relaxation** parameter is a value between 0 and 1, and lower values provide more slow and stable iteration process.

 Heat Solver. Parameters of the solver applied to solution of the heat transfer problem at given current density distribution. It contains the following parameters:

- ∆**T.** The limit variation of the temperature. The problem is assumed to be converged if the variation of the temperature becomes lower than this value.

- **T-Residual Limit** and **T-Number of Iterations.** The limit residual and themaximum number of iterations of the solution of the linear set of equation which is solved by a cycle of local iterations at each iteration of the non-linear problem.

- **T-Inertion** and **T-Relaxation.** The inertial factor and linear relaxation factor applied to the solution of the non-linear problem.

Usually, convergence of the heat transfer problem is quite fast and stable, so that the default parameters should not be modified by the user.

Coupling. These parameters determines the global convergence limit and significantly influence the computation time.

- ∆**J.** In Single Calculation mode, the program iterates the voltage until the difference between the obtained current and the prescribed current becomes lower than that parameter. Increase of this parameter allows to get results

faster. For instance, if one prescribed the current of 350 mA, it may be OK to get results for 245 mA. Note that this parameter does not change the accuracy of results (like parameters in the current spreading section), it just indicates how close we wil approach to the prescribed current.

- ∆**T.** The limit variation of the maximum temperature. The global iterations, i.e. consecutive solution of the current spreading and the heat transfer problems, is stopped as the variation of the maximum temperature becomes lower than this value.

All the solver parameters set in the **SpeCLED** graphical user interface before starting the solver can later be changed run-time in the solution monitor window. The changes are applied only after the "Update" button is pressed!

Fig. 58

10.5.2 Output

Output tab contains a set of zones which are stored in the output files. The following options are available:

- Active Region. 1 zone representing the active region.
- \triangleright Metal Contacts. 4 zones representing the p- and n- electrodes and pads.
- \triangleright Spreading Layers. 1 zone representing the p-spreading layer.
- \triangleright Z-Planes. A set of zones representing horizontal die sections at the center of each cell of the computational grid. The number of zones depends on the number of cells in p- and n-semiconductor layers and substrate in vertical dimension.
- \triangleright 3D. A 3D structure of the die allowing visualization of the die geometry in the visualization tool.
- **Cross Section.** A vertical cross-section of the conducting substrate allowing visualization of the current spreading in the substrate in vertical dies.
- **!** In case of series computations the above settings affect the output file corresponding to the lowest current only. All other files contain the active region only to save the hard disk space.

11 RATRO Tab Window

The **RATRO** tab provides specification of the optical parameters of the chip bulk materials and surfaces and running the ray tracing computation (see Fig. 59).

11.1 Global Parameters

Section **Global Parameters** is used for specification of the global parameters of the light extraction problem. It includes the following sections:

 Emission Parameters. **Emission Wavelength** is the user-defined wavelength of the emission that affects all wavelength-dependent parameters. The corresponding

photon energy $\hbar\omega = \frac{2\kappa\hbar}{\lambda}$ $\hbar\omega\!=\!\frac{2\pi\hbar\,c}{2}$ is shown in **Photon Energy** text field.

Polarization Effect. A flag governing the account of the light polarization in the computations. If it is checked, TE and TM rays are traced. For polarized light, section **Initial Emission Polarization** specifies the polarization of the emission from the active region, i.e. the probability of emission of TE or TM ray. If this flag is not checked, the reflection and transmission coefficients of each ray are calculated as

an average value of the TE and TM polarizations. For instance, the average reflection coefficient 2 $R = \frac{R_{TE} + R_{TM}}{2}$.

Intensity Distribution section governs the distribution of the emission intensity over the active region. Two options are available:

√ **Distribution from SpeCLED.** Distribution of the intensity of emission from the active region is imported from a file generated by **SpeCLED** as a result of solving the current spreading problem. In this case the file name is shown at the text field below the Global Parameters section. The button on the right of the text field opens the File Open dialog allowing the user to select the file in *.cgs format with results of **SpeCLED** computations. Note that this file should be obtained for the same die geometry that is specified in the opened project.

- **Uniform Intensity Distribution.** Uniform distribution of the intensity of emission from the active region is assigned.

Computational Parameters sections contains the following parameters:

- **Far-Field Radius**. Radius of the top and bottom hemispheres used for visualization of the far-field light distribution and the radiation patterns.

- **Number of Rays**. The number of rays (in millions) simulated in the ray tracing procedure. Increasing Rays will increase the accuracy of the obtained results but require greater computation time. A typical Number of Rays value may lie in the range of $10 - 100$ millions.

√ Far-Field Mesh. The number of cells along the diameter of the far-field sphere. Increasing of the mesh accuracy increases the radiation pattern resolution. However, use of the high mesh accuracy requires also an increase of the number of rays traced.

Threshold Ray Intensity (%). The value of ray intensity below which it is considered absorbed by the medium and its tracing stops. It is measured as a fraction of the initial intensity at which it is emitted from the active region.

- **Detector Angle (degree).** The software allows simulation of the image of the chip taken by an optical system collecting the rays emitted at the angle to the normal below the specified value. The result is shown in the Detector Image section of the output *.cgs file. For the detector angle value of 90 and higher the result is the same as the top (bottom) chip face in the Near-Field section. For a

lens of diameter D at the distance H from the chip, the angle can be calculated

$$
\text{as } \theta = \arctan\biggl(\frac{D}{2H}\biggr).
$$

11.2 Bulk Properties

The **Bulk Properties** tab (see Fig. 59) allows the user to specify the optical properties of the bulk materials of the die. It includes the following sections: **p-Semiconductor**, **n-Semiconductor**, **Substrate**, and **Immersion Medium**. For each of them, the user needs specify the refractive index and absorption coefficient. It can be done by selecting one of the pre-defined materials or by selecting "Other" item and manual specification of the optical properties. Note that "Other" is not a name of an additional material whose parameters are assigned to all domains to which it is applied, but a way of specification of the parameters explicitly for the domain selected.

Refraction Index section. It includes the following sections:

 \checkmark Type of the dependence of the refraction index on the wavelength. Two options are supported:

Constant. A text field with the refraction index value is shown. This value can be modified only if "Other" is selected. Otherwise, the value specified for the material is used.

Parametric Approximation. A first-order Sellmeier approximation 2 1 2 2 1 $2^2(\lambda) = 1 + A_1 \frac{\lambda}{\lambda^2 - \lambda^2}$ λ) = 1 + A₁ λ^2 − $n^2(\lambda) = 1 + A_1 \frac{\lambda^2}{\lambda^2}$ is used. Text fields show the approximation

parameters. Note that this approximation can only be applied if λ_1 is smaller than the emission wavelength. The coefficients can be modified only if "Other" is selected. Otherwise, the values specified for the material are used. Special text field shows the refraction index value at the operating wavelength.

 \checkmark Plot illustrating the refraction index variation with the wavelength.

Absorption Index section. It includes the following sections:

 \checkmark Type of the absorption index dependence on the wavelength. Two options are supported:

Constant. A text field with the absoprtion index value is shown. This value can be modified only if "Other" is selected. Otherwise, the value specified for the material is used.

Parametric Approximation. Background absorption and free-carrier absorption are assumed to contribute to the absorption index for the quant energies below the energy gap: $\alpha(\lambda) = a_0 + a\lambda^2 n$. Here a_0 is the background absorption, *n* is the carrier concentration, and a is a fitting parameter depending

on the carrier mobility μ and effective mass m_{eff} as $\alpha_n = \frac{q}{4\pi^2 M m^2 m^2}$ ref ϵ_0 2 1 2 3 $n = 4\pi^2 \mu m_{\rm eff}^2 n_{\rm ref} \varepsilon_0 c$ *q* π ⁻ μ m_{eff} n_{ref} \mathcal{E}_{e} $\alpha_{\rm n} = \frac{q}{\sqrt{q_0 q_0^2 + \frac{q_0^2}{q_0^2 + \cdots + q_n^2}}}$,

where n_{ref} is the refractive index. The coefficients can be modified only if "Other" is selected. Otherwise, the values specified for the material are used. Special text field shows the absorption index value at the operating wavelength.

 \checkmark Plot illustrating the value of the absorption index.

Materials Editor button (see Fig. 60) opens the material editor where the user can edit the parameter of the pre-defined materials. It includes the following sections:

Fig. 60

- **Materials**. List of pre-defined materials.

- **Chip Layers**. List of chip domains to which the selected material can be applied.

- **Refraction Index** section.

- ❖ Constant value.
- Coefficients of the parametric approximation.

- **Absorption Index** section.

- ❖ Constant value.
- Coefficients of the parametric approximation.

∕ Restore Defaults button allows the user to restore the default parameters assigned to the materials.

The **Active Region** parameters includes the angular distribution of the emitted light, as well as parameters describing re-absorption of the light by the active region.

> - **Thickness** and **Absorption Index** are used to calculate re-absorption of the emitted light in the active region. Each time a ray crosses the active region its magnitude is multiplied by the factor of $exp(-d\alpha / cos(\theta))$, where θ is the angle between the ray direction and normal to the active region, d is the total thickness of the narrow-gap layers which can re-absorb emitted light, and α is the power absorption index of these layers.

> - **Emission Distribution**. Specification of the angular distribution of the emission from the active region. Three options are supported and the resulting distribution is shown in the plot:

> **Isotropic**. The active region is assumed to emit isotropic light, i.e. power emitted into a unit space angle does not depend on the ray direction (recommended choice).

> **Lambert's Law**. The active region is assumed to emit as a lambertian surface. The power emitted into a unit space angle depends on the polar angle θ as $I(\theta) \sim I_0 \cos \theta$.

> **Table**. This option allows input of custom angular distribution. The distribution can be loaded from a text file using the **Load** button. The file should contain two columns of values separated by tab. First column is for the angle in degrees, second is for the probability. Zero angle refers to the normal direction in top direction (from n-side to p-side).

11.3 Surface Properties

Fig. 61

11.3.1 Surface Properties Tab window

The **Surface Properties** tab (see Fig. 61) allows the user to specify the optical properties of all interfaces of the chip. Note that since the surface reflection, absorption and transmission coefficients depend on the refraction indices of the adjacent materials, the bulk properties should be assigned prior to the surface properties. For each surface, the user needs specify the optical model and, optionally, its parameters. The meaning of the selected surface is indicated by the hint right to the list of surfaces. Also, the selected surface is highlighted in the schematic drawing below the list of surfaces. The reflection, absorption and transmission coefficients obtained for the selected model and parameters are visualized in the plot as a function of the incident angle. Note that change in the parameters to be confirmed by the **Apply** button.

11.3.2 Surface models

The following models are supported:

 Smooth Surface. This type can be assigned to all metal-free surfaces, i.e. the nand p-semiconductor layer free surfaces, substrate or n-semiconductor layer bottom surfaces and heterostructure/substrate interface. Besides, this type is automatically assigned to all lateral chip surfaces. For a smooth surface, the reflection and transmission coefficients are calculated for TE and TM polarized waves according to the Fresnel's relationships:

Reflection and transmission coefficients for wave amplitudes:

$$
r_{TE} = \frac{n_1 \cos \varphi_1 - n_2 \cos \varphi_2}{n_1 \cos \varphi_1 + n_2 \cos \varphi_2}, \quad t_{TE} = \frac{2n_1 \cos \varphi_1}{n_1 \cos \varphi_1 + n_2 \cos \varphi_2}
$$

$$
r_{TM} = \frac{n_2 \cos \varphi_1 - n_1 \cos \varphi_2}{n_2 \cos \varphi_1 + n_1 \cos \varphi_2}, \quad t_{TM} = \frac{2n_1 \cos \varphi_1}{n_2 \cos \varphi_1 + n_1 \cos \varphi_2}
$$

Reflection and transmission coefficients for light intensity:

$$
R_{TE} = r_{TE}^2, \quad T_{TE} = \frac{n_2 \cos \varphi_2}{n_1 \cos \varphi_1} \cdot t_{TE}^2, \quad R_{TM} = r_{TM}^2, \quad T_{TM} = \frac{n_2 \cos \varphi_2}{n_1 \cos \varphi_1} \cdot t_{TM}^2
$$

The incidence and reflection angles obey the relationship

 $\varphi_1 = \varphi_2$.

The incidence and refraction angles obey the relationship

$$
\frac{\sin \varphi_1}{\sin \varphi_2} = \frac{n_2}{n_1}.
$$

- **Mirror**. This type can be assigned for any surface. For a **Mirror** surface, the reflection and refraction angles correspond to the case of a smooth surface, but the reflection (R) and transmission (T) coefficients are assigned by the user, while the absorption coefficient (A) is found as $A = 1 - R - T$. The assigned values are used unless the incidence angle exceeds the total internal reflection angle. In case of total internal reflection $T = 0$, $R = 1 - A$, while A is assumed to be constant in the whole angle range.
- **► Full Absorption.** A type that can be assigned to n- and p-pads. It corresponds to the **Mirror** surface with $A = 1$.
- **Multiple Layer**. This type can be assigned to the n- and p- electrodes, pads and to p-spreading layer. A multiple layer can consist of one or several layers of different

materials and thickness. The effective reflection, absorption and transmission coefficients of such surface are calculated by the program accounting for the interference in the multilayer contact. The user should specify the number of layers, material and thickness of each layer. Material should be selected from the predefined list. For all pre-defined materials the wavelength-dependence of the refraction and extinction coefficients are taken from a database stored in **Material** folder. The user can edit database or even add new materials. To specify arbitrary user-defined optical properties (n,k) one need choose 'other' item in the drop-down list. Table with the layer parameters also includes the parameters of the media above (first row) and below (last row) the multiple layer itself.

 Hexagonal Facets, **Rectangular Facets**, and **Hemisphere Facets** (see Fig. 62). These types can be assigned to all metal-free surfaces, i.e. the n- and psemiconductor layer free surfaces, substrate or n-semiconductor layer bottom surfaces and heterostructure/substrate interface. They represent regularly patterned surfaces with hexagonal and rectangular facets, respectively. The user should assign the geometric parameters of each facet.

Fig. 62

Patterned surface is considered as a set of local surfaces with different orientation. For instance, surface patterned with hexagonal pyramids has 7 different types of local surfaces: surface parallel to the boundary and six different facets of the pyramid. Probability of light interaction with i-th local surface is calculated as *j j* $f_i = A_i \cos \theta_i / \sum A_j \cos \theta_j$, where A_i is the area of the i-th local surface and θ_i is the

angle between the ray direction and normal to the local surface. Summation is done only for the surfaces "visible" for the particular direction of the incident ray, i.e. shaded surfaces are excluded. Probabilities f_i are used to determine with which local surface interacts the ray. Then transmission and reflection probabilities are calculated using "smooth surface" model for the particular ray direction and the local surface.

 Multiple Layer on Facets. This type is combination of 'Multiple Layer' and 'Facets' options to described a patterned surfaces covered with some layer refractive layer (say, metal electrode on top of the facetted semiconductor or ITO layer). The ray tracing is done in a way described for the facets of the same geometry, while probabilities of the ray refraction, transmission, and absorption are computed from the multiple layer model.

12 Graphics Window

All tab windows contain the Graphics Window that is designed to specify and visualize the layout of all die layers, providing mouse specification of the objects to be created or modified. Multiple boundary selection is also available. The cursor view depends on the type of the active operation.

The following basic operations are available within the Graphics Window:

 \triangleright Image translation (displacement of the whole image including the origin of coordinate system, i.e. the coordinates of all objects are unchanged).

 \checkmark Right mouse button is pressed and the mouse is moved along the translation direction.

- \triangleright Zoom In (enlarging the image).
	- \checkmark The mouse wheel is rolled towards the user.
- \triangleright Zoom Out (reducing the image).
	- \checkmark The mouse wheel is rolled away from the user.

 \triangleright Selecting a point.

 \checkmark In the selection mode, the left mouse button is pressed on the point. When the mouse cursor is positioned in the vicinity of a point so that clicking the mouse button will lead to its selection, this point starts flickering in white. A selected point is marked in white.

 \triangleright Selecting a boundary.

 \checkmark In the selection mode, the left mouse button is pressed on the boundary at a distance from any point (otherwise, the point will be selected instead of the boundary). The selected boundary is marked in white.

- \triangleright Deselecting an object (point or a boundary).
	- Second selection of a selected object clears its selection.
- \triangleright Selecting a group of objects (points or boundaries).

- Consecutive selection a series of objects provides their multiple selections. To suppress multiple selection (i.e. to select a different object only when some other objects are already selected) the user should manually deselect them in advance.

- \triangleright Filling a contour (assigning a closed contour to the current die layer).
	- \checkmark In the Fill mode, the left mouse button is pressed inside of the contour.
- \triangleright Specifying an ending point of a new boundary.

 \checkmark New point: The left mouse button is pressed at a distance from any existing point. If a new point should be added near an existing point, the user should zoom in the image so that the point positions on the screen become far enough from each other.

 \checkmark Selecting an existing point: The left mouse button is pressed in the vicinity of an existing point which starts flickering to identify this.

The color of an unselected point in the *Graphics Window* depends on the number of boundaries adjacent to it.

- If it is equal to 0 (an individual point) or 1 (an ending point of a dangling boundary), it is filled in red.
- \triangleright Otherwise, it is filled in green.

The color of unselected boundaries (lines or arcs) forming a closed contour is brown. Individual unselected boundaries that do not form closed contour are marked in yellow.