SimuLase Designer

Quick-Start Guide, Version 3.0

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Contents

Preface

The following is a brief description of the main functionality of **SimuLase™** 's main features. For more details please see the corresponding Sections in the full manual of **SimuLase™** that can be found under the Help-menu of the program or downloaded at '**www.nlcstr.com\ SimuLaseDemo.htm**'.

SimuLase^{TM} comes with an example for a more complex structure than the basic default structure. To load this structure go to '**File | Open Structure**' and load the structure-file 'C:\Program Files\NLCSTR\SimuLaseX64\SampleLayeredStructure.sls'.

All entries that are typed into any of the fields of **SimuLase^{TM}** have to be confirmed by hitting the enter key.
Numerical entries have to be in the format $ABCDEF.GHI$, using a decimal point if necessary.
Large numbers can be entered using the format $A.BeN$ for $A.B \times 10^{N}$.

1 Design Structure

Figure 1: Design Structure panel

The 'Design Structure' tool is the default page that appears when SimuLase^TM is started. Initially the chart displays a basic 3-layer structure. A pre-existing structure layout may be loaded by selecting **File | Open Structure...**.

The main chart window displays the currently loaded device as a series of colored layers stacked horizontally. Superimposed on top of this device representation are plotted one or more graphs showing either the band edges (confinement potential, optionally computed using a classical Poisson-**drift-diffusion** model and/or a microscopic Schrödinger-Poisson model), wavefunctions and associated energy levels or the refractive index profile and the lowest confined mode across the device.

The controls above the main chart enable the user to construct a layered device and dynamically view various aspects of the resulting device. The controls are arranged into three functional groups:

**Group 1** allow viewing and editing of the material properties of a single layer;

Group 2 controls the algorithms used to simulate the device and the resulting data view;

Group 3 enables the addition of new layers or the removal of existing layers.

The individual controls in each of these functional groups are detailed in the following sections.

Group 1: Layer Properties

The various controls in Control **Group 1** detail the physical properties of the current layer. Changing any of the displayed values for the current layer will automatically cause the corresponding plots in the chart to be updated.
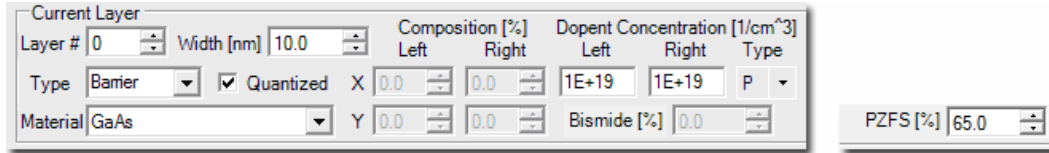
Layer # A single layer is selected by changing the number field in this control (or using the mouse wheel or scroll arrows to cycle through layer numbers). Layers are numbered sequentially starting with layer 0. The currently selected layer is highlighted in green

Width [nm] The width the current layer in nanometers.

Type The function of the layer in the device. A layer can be one of three types, '**Barrier**', '**Well**' or '**Cladding**'. The program uses these to determine the number of relevant subbands. It searches the number of bands that are confined in any of the wells, i.e., connected sequence of layers marked 'Well' within the quantized region. Also, if a GainDatabase is loaded for well or barrier material in the calculation of reflection and transmission spectra, the absorption/gain and carrier induced refractive index changes are added to the background refractive index in all layers marked 'Well' or 'Barrier', correspondingly. No GainDatabase data is associated with layers of the type 'Cladding'.

Quantized Only layers marked as quantized are included in the microscopic calculations of wavefunctions, bandstructures, for solving the Poisson-Schrödinger problem of potential modifications due to local charge inhomogenities and for calculating optical properties like gain/absorption. Creating a quantized region begins with a single layer of type 'Well' which may then be surrounded by layers of type 'Barrier'. Currently any structure may contain only a single continuous quantized region. Every quantized region has to include at least one layer of type 'Well'. The actual quantum well can be made of several layers of type 'Well' and there can be several separate ells in the quantized region.

Material Layer material which may be a binary, ternary or quaternary material.

Composition[%] This set of four numeric values sets the concentrations X and Y of the material compound at the Left and Right hand edges of the current layer. A linear gradient in concentration is assumed across the layer.

Dopant Concentration This set of two numeric values and a N-type or P-type selector set the dopant type and concentrations at the Left and Right hand edges of the current layer.

Z/Nitrogen/PZFS [%] In quinternary materials, this field allows to set the additional composition 'z'. For dilute Nitrogen (GaInNAs) it allows to set the Nitrogen content. In AlInGaN it allows to set the strength of the internal piezoelectric and spontaneous polarization fields. Here, all strain-related internal fields throughout the structure are scaled according to this ratio from the nominal literature value. We found for this parameter a value of 65% to be appropriate in most cases. For quinternary materials and dilute Nitrides the program currently allows only layers with constant 'z' composition across the layer.

Group 2: Algorithm and Data View Selection

The various controls in Group 2 specify the computational algorithm used to compute properties of the quantized region and dictate which aspects of the computed data should be plotted.
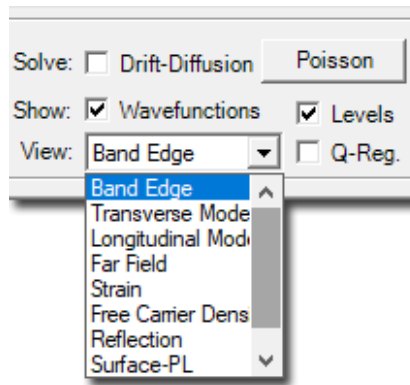
Drift-Diffusion If this box is checked the Poisson drift diffusion problem describing possible band edge modifications due to local charges from ionized dopants and free carriers are solved.

Poisson Click this button to solve the microscopic Poisson-Schrödinger model for the quantized region. A fully coupled 8x8 kp-model is used in this calculation. The number of subband states that are used in this calculation is set on the 'Advanced'-panel.
Note: It is assumed that the potential modifications due to charges that are quantized in the wells are small as compared to the global potentials due to ionized dopants and/or externally applied Voltages. Thus, we do not use a self consistency loop that couples the classical Poisson drift diffusion problem to the quantized Poisson-Schrödinger problem.

Wavefunctions If checked, in addition to the confinement potentials the wavefunctions are shown. The number of wavefunctions to be shown is set on the 'Advanced'-panel.

Levels Show energy levels associated with the wavefunctions in addition to band edges.

View This field allows to switch from displaying the confinement potential and wavefunctions ('Band Edge' view) to displaying the transverse or longitudinal optical mode together with the corresponding optical confinement factor and refractive index profile, the far field for transverse modes, the strain or the free carrier density due to ionized dopants. In the 'Surface Emitter Mode' (select by clicking the icon: ⬇ in the top menu) it also allows to show the reflection/transmission spectrum, the surface-PL spectrum and the LI-characteristic.

Q-Reg Provides a "zoomed-in" view of the 'Quantized Region', i.e., the region of the device containing layers marked as quantized that are used in the microscopic calculations.

Group 3: Add/Remove Layers

The various controls in Control Group 3 enable the addition or removal of one or more layers to or form the layered structure. The 'Add/Remove button performs an operation on the
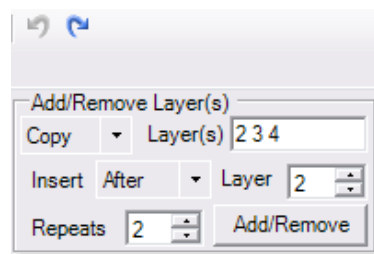
structure according to the values of all active controls contained in the group. For example with

the setting shown in the figure above, clicking **Add/Remove** will *"***Copy** *layers* **2, 3, 4** *and* **insert** *them* **After** *layer* **2**, **Repeat***ing this operation* **2** *times"*. Using the drop-down arrows the user can select either a **Copy, Clone** or **Delete** operation and similarly may select **After** or **Before** to specify the insertion location.

The **Repeats** numeric value may be used to construct periodic arrangements of layers. For example a Bragg mirror can be created by first defining two layers that define the unit cell for the mirror and then cloning those two layers N times by setting the **Repeats** numeric value to N. The designer first creates a substructure composed of the cloned layers and then inserts that substructure at the appropriate location specified in the Insert **(After | Before)** numeric box. While the attributes 'well/barrier' will be transferred to the clones or copies, the new layers will not be part of the 'quantized region' unless they are manually marked to be part of it.

The **Clone** operation differs from the **Copy** operation in that cloned layers share the same material properties. Changing any property of a cloned layer like width, dopant concentration etc., will cause the same change in all clones of that layer. The **Clone** operation is most commonly used (with Repeats set to a value greater that 1) to construct periodic arrangements, such as Bragg mirrors, where layers shares common properties.

The **Delete** operation permanently removes all layers listed in the Layer(s) numeric box. If a layer is part of a series of clones, all corresponding layers in the clones will also be deleted.

The **undo** and **redo** buttons, ↶ ↷, allow to undo or redo changes made with the controls of this group.

2 Advanced Tab

The various controls contained under the Advanced tab are use to specify parameters related to the whole structure such as Lattice Temperature operating wavelength etc.
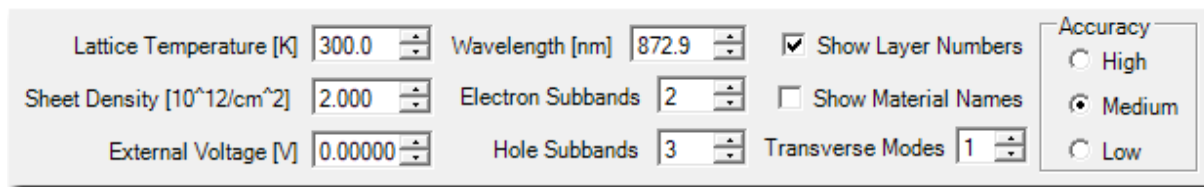
Lattice Temperature The temperature of the device. This temperature is assumed to be also the carrier temperature.

Sheet Density The sheet carrier density in the quantized region as used for the quantized Poisson-Schrödinger problem. Equal electron and hole densities are assumed. This is the density related to external optical or electrical pumping. Intrinsic, dopant related carrier densities are assumed to be negligible in the Poisson-Schrödinger calculation. This density is also used if absorption/gain is included in the calculation of the longitudinal mode and reflection and transmission spectra.

External Voltage A possible external voltage applied across the device.

Wavelength The wavelength at which the device is assumed to operate. This is used in the calculation of the mode profiles and optical confinement factors as well as the calculation of reflection and transmission spectra. See Sec. 7.1 of the full manual for a discussion of the confinement factor calculation.

Electron/Hole Subbands Specifies the number of confinement wavefunctions and subband levels which are displayed in the chart. Also specifies the number of subbands that are used to solve the Poisson-Schrödinger problem for the structure display. The numbers are not used for the GainDatabase calculation and have to be reset there.

Accuracy Allows changing the number of grid-points used for the calculation of the wavefunctions and levels. The calculation-time increases with the accuracy level which can become noticeable especially if the Poisson-Schrödinger problem shall be calculated.

Show Layer Numbers Labels each layer on the chart with its associated layer number.

Show Material Names Labels each layer on the chart with the type of material used in the layer.

Transverse Modes Specifies the number of transverse modes and corresponding far fields that shall be displayed.

3 Main GUI Components
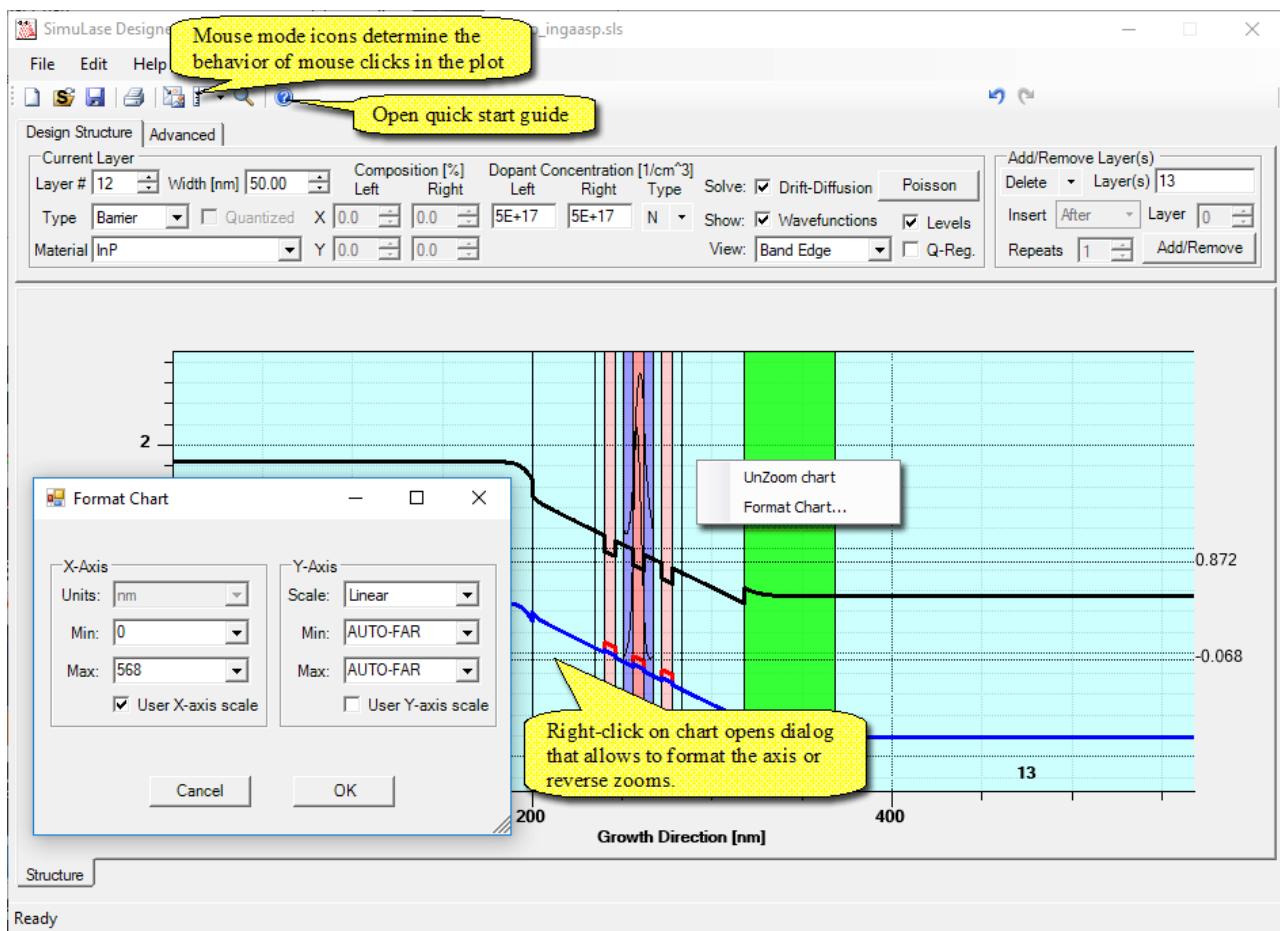
Figure 2: Overview of the main GUI panel.

The main GUI components are shown below. Information about a structure is saved in files with the extension ".sls". To load a structure select '**File | Open Structure**' or click the icon. To save a structure go to '**File | Save Structure**' or click the icon. To create a new

structure starting from the default structure go to 'File | New Structure' or click on the icon
.

3.1 Formatting the Axes

The layout of the chart may be formatted by 'right-clicking' the mouse to display a pop-up menu.
Selecting the 'Format Chart' option displays the dialog box shown as an insert in Fig.2. Use
this dialog to format the X-axis units (electron Volts or nanometers), the Y-axis scale (Linear or
Logarithmic) and the physical extents of each axis. When changing numeral entries these
have to be confirmed by hitting the 'enter' key.
By default a chart will auto-scale the X and Y-axes so as to include all data points within the
chart area and also present well-rounded major and minor tick mark spacing of the chart axes.
Three auto-scale modes are provided:
'AUTO-EXACT' sets the Max and Min value of the axis to the exact Max and Min values
in the displayed data sets.
'AUTO-NEAR' sets the Max and Min value of the axis to the next minor tick mark that
encompassed displayed data sets.
'AUTO-FAR' sets the Max and Min value of the axis to the next major tick mark that
encompassed displayed data sets.
The user may override the default auto-scale settings (AUTO-EXACT for the X-axis and AUTO-
FAR for the Y-axis) by clicking the User (X or Y)-axis scale check box. A user defined
numeric value for either Max or Min (or both) may be entered.
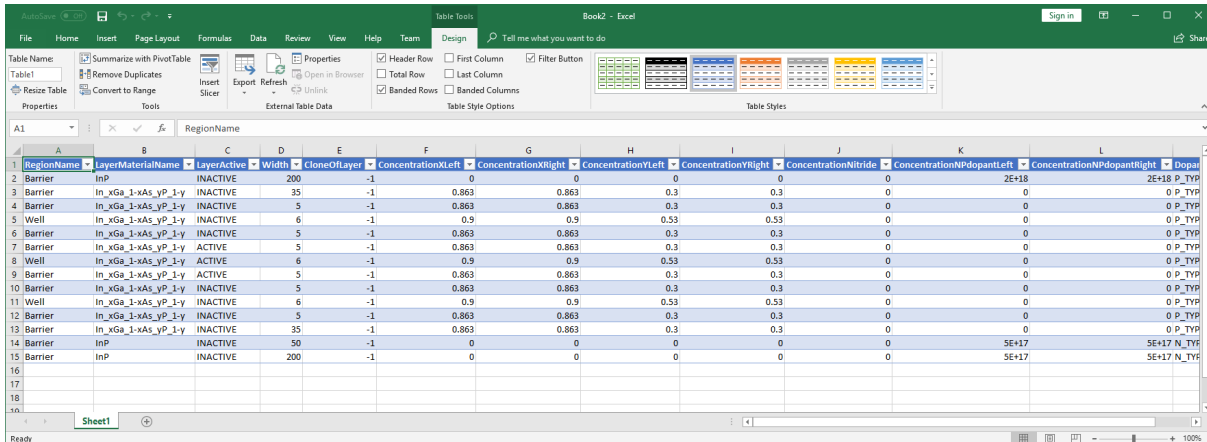
Chart legends may be repositioned by clicking the icon on the main toolbar and using the
left button mouse to select and move the legend to a new location.

3.2 Save/Reload/Export a Structural Layout

The structural layout can be saved and reloaded using 'File | Save Structure' and 'Open
Structure' from the main menu or the icons and , respectively. The structural information
is saved in xlm-format in an *.sls file which can be read externally using, e.g., Microsoft Excel.

Figure 3: Structure file, *.sls, in Windows Excel.

3.3   Exporting a GainDatabase for other Software

GainDatabases can be exported into a format that allows to import the data contained in them into other software products for further evaluation using 'File | Export Database as' from the main menu. Currently, this option allows to export a database in a format that can be imported into Crosslight Inc.'s Lastip software. It also allows to produce reduced GainDatabases containing just subsets of the original database. For more info on this feature see the full manual.

3.4   Saving or Printing Chart Images

An image of the current chart (in *.BMP, *.JPG, *.GIF, *.TIFF or *.PNG format) may be stored in a file by selecting 'File | Save as Image' from the main menu.
High resolution printouts are available by selecting 'File | Print' from the main menu.

3.5   Exporting Displayed Data

The currently displayed data can be exported into ASCII-format data files by selecting 'File | Export Data' from the main menu.