

# SimuLase



## Quick-Start Guide, Version 3.0

May 8, 2019

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The following is a brief description of the main functionality of **SimuLase<sup>TM</sup>**'s main features. For more details and optimum usage please see the corresponding Sections in the full manual of **SimuLase<sup>TM</sup>** that can be found under the 'Help'-menu of the program or downloaded at '[www.nlcstr.com/SimuLaseDemo.htm](http://www.nlcstr.com/SimuLaseDemo.htm)'.

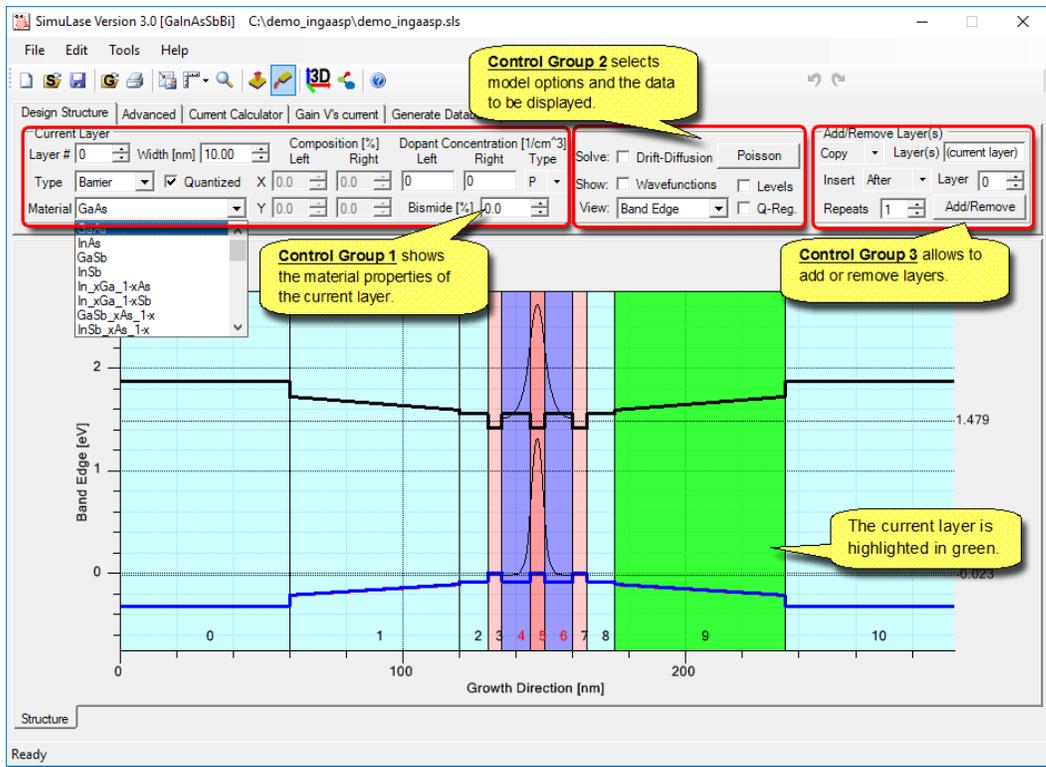
In order to test the various tools **SimuLase<sup>TM</sup>** offers to investigate data you can download a Demo-GainDatabase including various InGaAsP-based wells and radiative and Auger losses from our website at <http://www.nlcstr.com/SimuLaseDemo.htm>. There you can also download some experimental spectra that can be compared to the theoretical data using the **PL-Analyzer** tool.

All data required to reproduce the example of an edge-emitting structure can be downloaded from our website at '[www.nlcstr.com/SimuLaseDemo.htm](http://www.nlcstr.com/SimuLaseDemo.htm)'. This example can be loaded into the free demo-version of **SimuLase<sup>TM</sup>** that can also be downloaded at that link. The example includes the structure file, the theoretical gain databases and the experimental PL-data. This data is also included in the DVD on which the full version of **SimuLase<sup>TM</sup>** is shipped. Here, the folder '**demo\_ingaasp**' contains the full structure. '**unbroadened\_pl**' contains the GainDatabase for the PL-analysis. '**experimental\_pl**' contains the experimentally measured PL spectra and '**broadened\_gdb**' contains the GainDatabase for the current calculation.

**SimuLase<sup>TM</sup>** 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 file 'C:\Program Files\NLCSTR\SimuLase\SampleLayeredStructure.sls'.

All entries that are typed into any of the fields of **SimuLase<sup>TM</sup>** have to be confirmed by hitting the enter-key. Numerical entries have to be in the format  $ABCD.EF$ , 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



The 'Design Structure' tool is the default page that appears when **SimuLase™** 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 structure 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.

The image shows a software control panel for configuring a layer. It includes the following fields and controls:

- Current Layer**: Layer # 0, Width [nm] 10.0
- Composition [%]**: Left 0.0, Right 0.0
- Dopant Concentration [1/cm<sup>3</sup>]**: Left 1E+19, Right 1E+19, Type P
- Type**: Barrier,  Quantized
- Material**: GaAs
- X**: 0.0, **Y**: 0.0
- Bismide [%]**: 0.0
- PZFS [%]**: 65.0

**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 of 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 as '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 inhomogeneities 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'. 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'.

**Material** Layer material which may be a binary, ternary, quaternary or quinary 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/Bismide/PZFS [%]** In quinary materials, this field allows to set the additional composition 'z'. For dilute Nitrogen (GaInNAs) or dilute Bismide (AlInGaAsSbBi) it allows to set the content of the dilute material. In wide bandgap 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 quinary materials and dilute materials the program currently allows only layers with constant 'z' composition across the layer.

## Group 2: Algorithm and Data View Selection

The various controls in Control Group 2 specify the computational algorithm used to compute optical 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 is 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

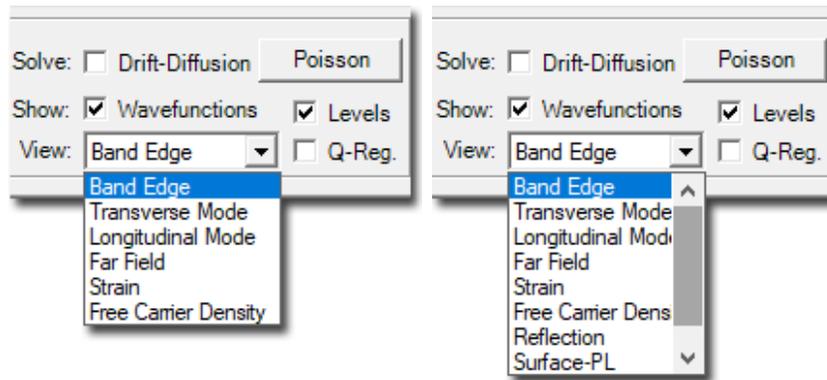


Figure 1: Data view options in edge-emitting mode (left) and surface-emitting mode (right).

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, Repeating 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.

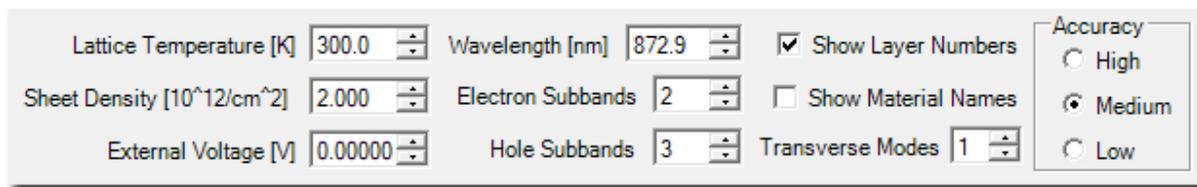
The **Clone** operation differs from the **Copy** operation in that cloned layers share the same material properties. Changing any property of a cloned layer like width, dopant concentration etc., will cause the same change in all clones of that layer. The **Clone** operation is most commonly used (with Repeats set to a value greater than 1) to construct periodic arrangements, such as Bragg mirrors, where layers share 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 used to specify parameters related to the whole structure such as Lattice Temperature operating wavelength etc.. These are used only while setting up the structure. Corresponding parameters - if relevant - have to be set separately for the generation of GainDatabases.



**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.

**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 to change 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 Generate Database

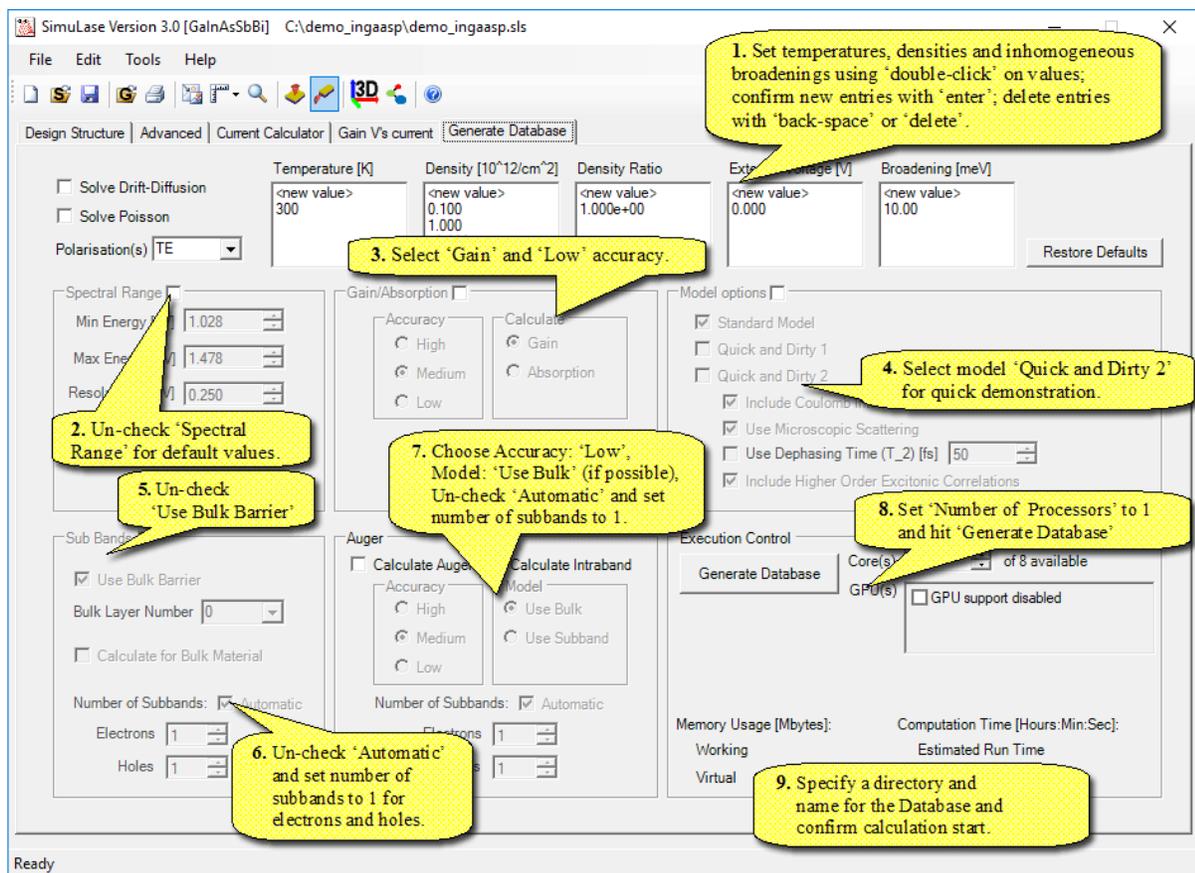


Figure 2: Overview of the 'Generate Database' panel with instructions for a very **quick demonstration run**.

The details of the various selections that can be made on this panel are explained in the main manual.

In order to get a feeling for how **SimuLase**<sup>TM</sup> generates GainDatabases, follow the steps as indicated in Fig.3 and leave all other options in their default setting. With these settings the

model is reduced to a two-band model without any Coulomb effects. The calculations should only take a few tens of seconds for each density/temperature-combination. You can then load the created database into the other tools of **SimuLase™** to view the absorption, PL, etc. by using **'File | Open Gain Database'** and opening the file that starts with the **'Name'** you have chosen for the database followed by the extension **'.gdb'**. For setting up realistic GainDatabases one should always use the **'Standard Model'** which includes Coulomb effects like excitonic resonances, Coulomb enhancement of the absorption or density dependent bandgap renormalization as well as electron-electron and electron-phonon scattering that describe the broadening of the spectra and higher excitonic resonances as source terms for the spontaneous emission. All of these effects are essential to obtain the quantitatively predictive quality for the results that separates **SimuLase™** from any other available software tool.

## 4 Main GUI Components

The main GUI components are shown below. To load a GainDatabase select **'File | Open Gain Database'** or click the **'G' Folder'** symbol, .

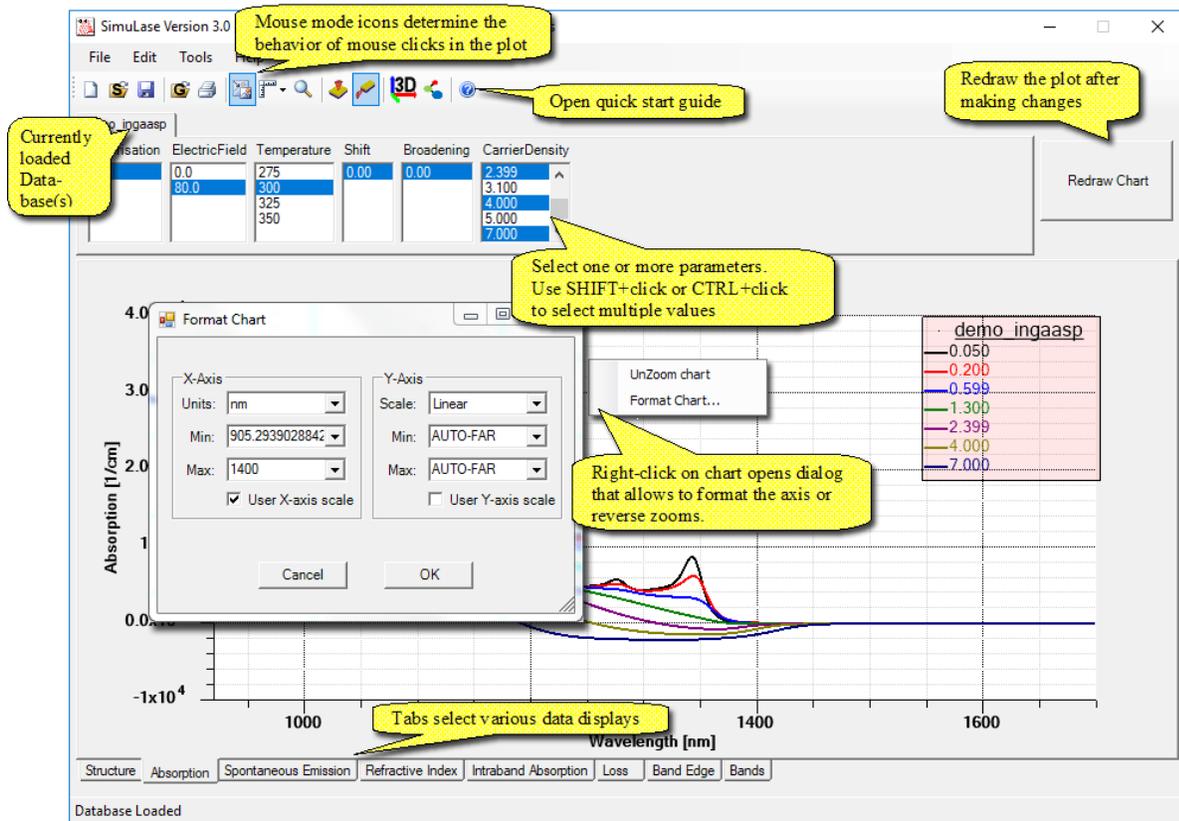


Figure 3: Overview of the main GUI plotting panel.

By clicking on one of the tabs below the plot window, **'Spontaneous Emission'**, **'Refractive Index'**, **'Absorption'**, or **'Losses'**, . . . , the respective data are shown for the selected parameters (Polarization(s), Electric Field(s), Temperature(s), Shift(s), (inhomogeneous) Broadening(s)

and Carrier Densities(s)). At least one entry has to be selected for each of these parameters to display data. To hide all data de-select all entries for at least one of the parameters. To de-select an entry press the 'control' key and click on the entry.

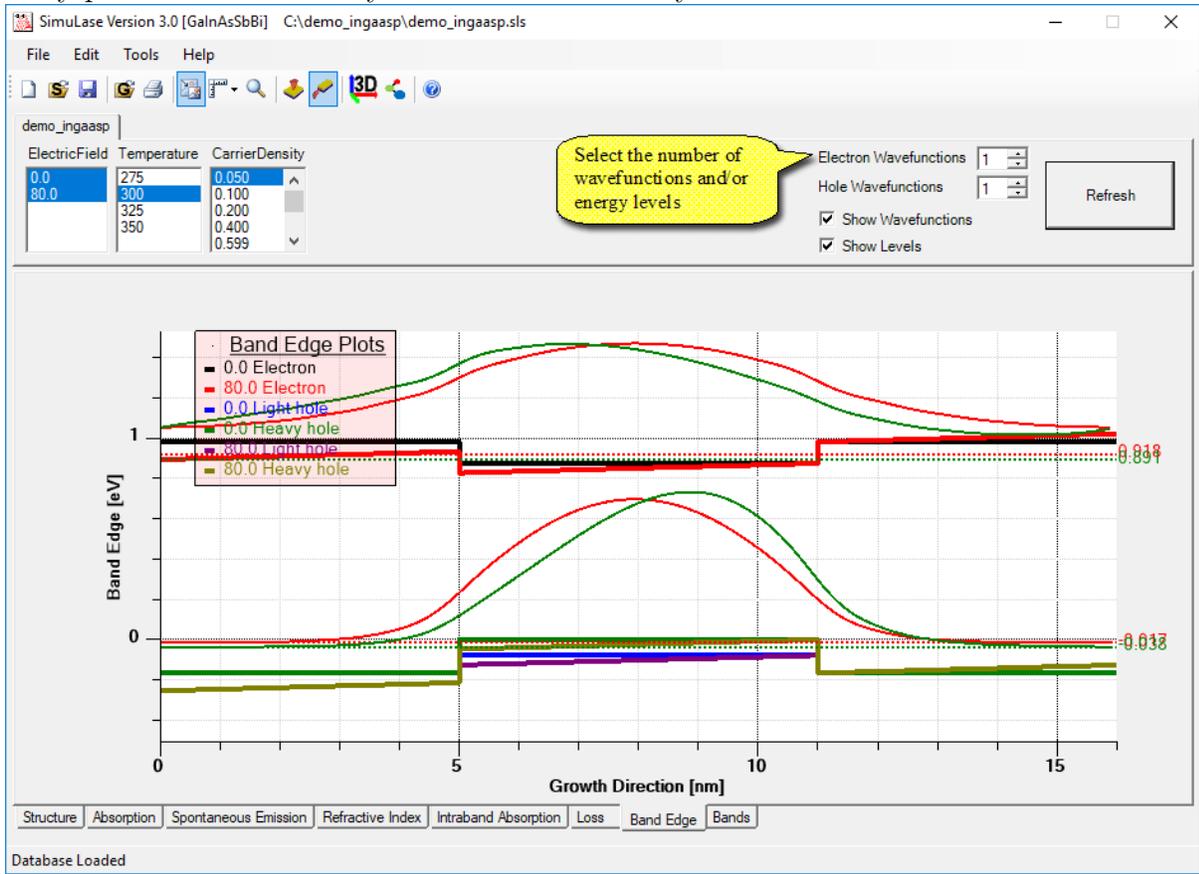


Figure 4: 'Band Edge' plot window.

The tabs 'Band Edge' and 'Subbands' display the confinement potential and subbands for the structure for which the database has been created. One or more energy levels and/or wave functions may be superimposed on the confinement potential by choosing the desired number and activating 'Show Wavefunctions' and/or 'Show Levels'.

### 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.3. 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.

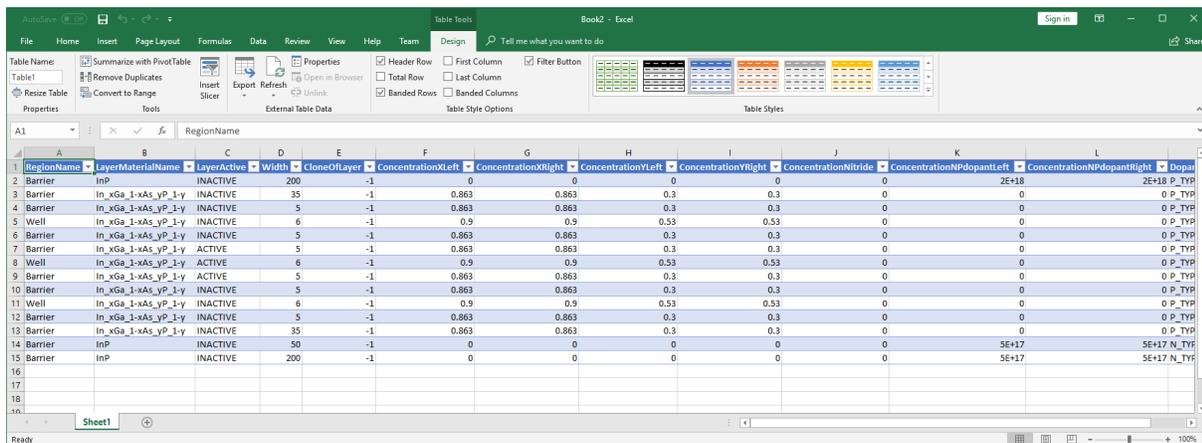
'**AUTO-FAR**' sets the Max and Min value of the axis to the next major tick mark that encompassed displayed data sets.

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.

## 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. The structural information is saved in xlm-format in an \*.sls file which can be read externally using, e.g., Microsoft Excel.



RegionName	LayerMaterialName	LayerActive	Width	CloneOfLayer	ConcentrationXLeft	ConcentrationXRight	ConcentrationYLeft	ConcentrationYRight	ConcentrationNlride	ConcentrationNPdopantLeft	ConcentrationNPdopantRight	Dopant
Barrier	InP	INACTIVE	200	-1	0	0	0	0	0	2E+18	2E+18	P_TYP
Barrier	In_xGa_1-xAs_vp_1-y	INACTIVE	35	-1	0.863	0.863	0.3	0.3	0	0	0	P_TYP
Barrier	In_xGa_1-xAs_vp_1-y	INACTIVE	5	-1	0.863	0.863	0.3	0.3	0	0	0	P_TYP
Well	In_xGa_1-xAs_vp_1-y	INACTIVE	6	-1	0.9	0.9	0.53	0.53	0	0	0	P_TYP
Barrier	In_xGa_1-xAs_vp_1-y	INACTIVE	5	-1	0.863	0.863	0.3	0.3	0	0	0	P_TYP
Barrier	In_xGa_1-xAs_vp_1-y	ACTIVE	5	-1	0.863	0.863	0.3	0.3	0	0	0	P_TYP
Well	In_xGa_1-xAs_vp_1-y	ACTIVE	6	-1	0.9	0.9	0.53	0.53	0	0	0	P_TYP
Barrier	In_xGa_1-xAs_vp_1-y	ACTIVE	5	-1	0.863	0.863	0.3	0.3	0	0	0	P_TYP
Barrier	In_xGa_1-xAs_vp_1-y	INACTIVE	5	-1	0.863	0.863	0.3	0.3	0	0	0	P_TYP
Well	In_xGa_1-xAs_vp_1-y	INACTIVE	6	-1	0.9	0.9	0.53	0.53	0	0	0	P_TYP
Barrier	In_xGa_1-xAs_vp_1-y	INACTIVE	5	-1	0.863	0.863	0.3	0.3	0	0	0	P_TYP
Barrier	In_xGa_1-xAs_vp_1-y	INACTIVE	35	-1	0.863	0.863	0.3	0.3	0	0	0	P_TYP
Barrier	InP	INACTIVE	50	-1	0	0	0	0	0	5E+17	5E+17	N_TYP
Barrier	InP	INACTIVE	200	-1	0	0	0	0	0	5E+17	5E+17	N_TYP

Figure 5: Structure file, \*.sls, in Windows Excel.

## Exporting a GainDatabases

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 Sec. 3.1 of the full manual.

## Saving/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.

## Exporting Displayed Data

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

## 5 General Tools

Some analysis tools that are independent of the device geometry (edge- or surface emitting) can be found under the tab 'Tools' of the main menu.

### 5.1 PL Analysis Tool

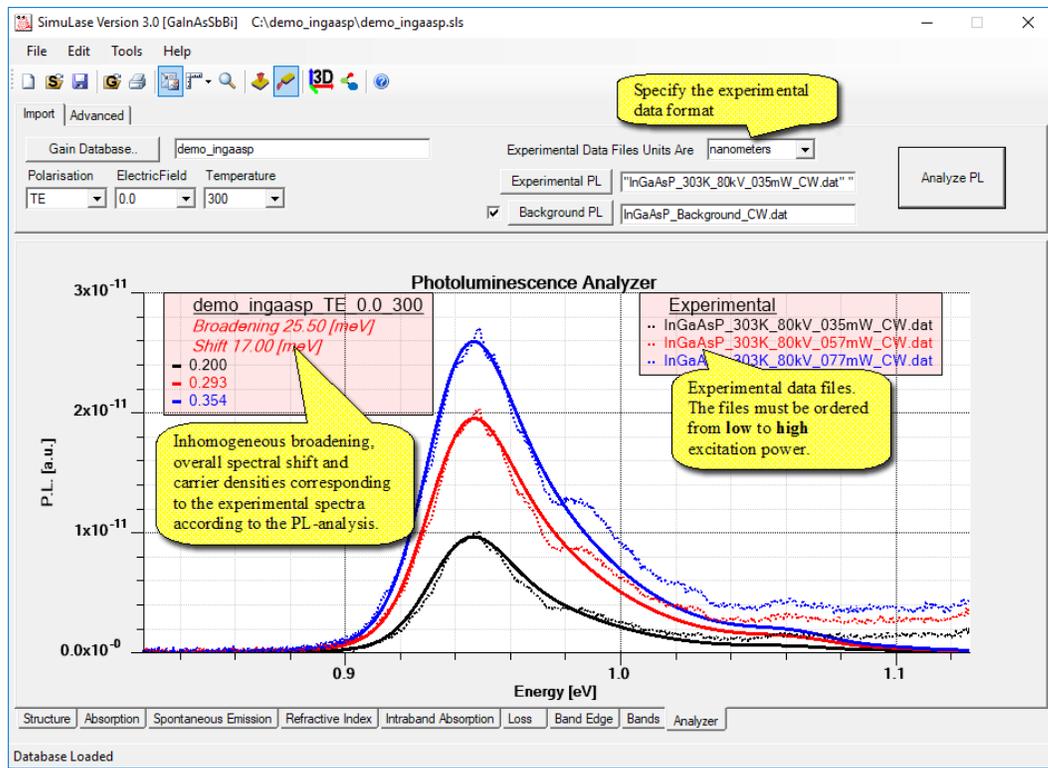


Figure 6: Main PL-Analysis panel.

The PL Analyzer tool allows to compare theoretical material PL-spectra to measured data in order to obtain information about the inhomogeneous broadening and spectral mismatches between nominal and actual structure. The results provide direct insight into device growth quality. In contrast to the 'Surface-PL' panel, here the PL is assumed to be the pure material PL that is not disturbed by cavity effects. This is usually the case in edge-emitting devices or for PL that has been measured from the edge of the device.

The tool may be activated by selecting 'Tools | Analyze Experimental PL' from the menu bar. Performing a PL analysis requires the following steps:

- 1) Select a gain database that matches the material system of the experimental PL spectra to be analyzed. Click on 'Gain Database' and select a pre-computed gain database.

- 2) Select the parameters, like polarization and temperature, that most closely match the experimental conditions. The corresponding theoretical PL spectra from the database are plotted.
- 3) Import the experimental PL data (in order of increasing excitation power) by clicking the '**Experimental PL**' tab and importing the data. In the current version of **SimuLase™** the experimental data has to be in two-column ASCII format. The first column containing the transition energy in [eV] or the wavelength in [nm]. The second column containing the PL data. Specify the data format using the '**Experimental data file units**' selector box.
- 4) If available, load an experimental background noise spectrum data file using the '**background**' tab. This background will be subtracted from all experimental spectra.
- 5) Click the '**Analyze PL**' button to perform an analysis).
- 6) Analysis results may be improved by "clipping" noisy tails from the experimental data and selecting suitable control points on the '**Advanced**' tab.

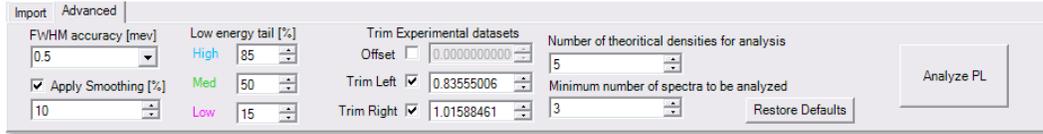


Figure 7: Advanced PL-Analysis panel.

On the '**Advanced**' tab, details of the analysis can be influenced by choosing low-energy matching points, high energy cut-off, the desired accuracy ('**FWHM accuracy**' tab), as well as the number of theoretical spectra used for the analysis.

The '**Offset**' can be used to subtract a constant background value from the experimental spectra - similarly to subtracting a background-noise spectrum.

'**Trim Left**' and '**Trim Right**' allow to exclude low- and high-energy tails in the experimental spectra from the analysis. Low energy tails are often covered by noise where the ideal spectra fall off below the bandgap. On the high energy side experimental spectra often show enhancements of the PL beyond the ideal theoretical PL. This is usually due to non-thermal carriers in the experiment which arise in particular when using CW-excitation. These carriers have not relaxed toward the bottom of the wells - occupying higher subbands - and lead to an enhancement beyond the ideal thermal equilibrium situation assumed in the theory (see e.g. the features at 0.98 eV in Fig.6). These parts should be excluded from the analysis.

The Analysis should focus on the spectral region around the main peak that gives the best information about the inhomogeneous broadening and spectral shifts - starting where the PL reaches about 20% of the maximum to where the PL falls off again to about 50% of the peak value.

The theoretical spectra to the lowest carrier densities are used since experimental data usually is taken under low excitation conditions. The '**Number of theoretical densities for analysis**' should be increased if no good match is found when considering only the lowest densities.

If one has a very large experimental database loaded, one might want to save computation time and/or to focus on the qualitatively best spectra one can choose a subset of spectra to be analyzed by specifying the '**Minimum number of spectra to be analyzed**'. The analysis tool internally selects then a subset of experimental spectra of that size that matches closest average criteria. The final results are displayed only for these spectra.

In case of noisy experimental spectra one can apply a smoothing algorithm by choosing '**Apply Smoothing**' in order to eliminate artificial local peaks in the spectra which might obscure the

true spectral location of the PL maximum. The percentage value chosen for smoothing is given as the percentage of the estimated inhomogeneous broadening present in the experimental data.

After choosing the desired settings, click the '**Analyze PL**' tab. After a short calculation, the best matching theoretical curves appear on the screen superimposed to the experimental data. In order to obtain the agreement, usually

## 6 General Tools

Some analysis tools that are independent of the device geometry (edge- or surface emitting) can be found under the tab '**Tools**' of the main menu.

### 6.1 PL Analysis Tool

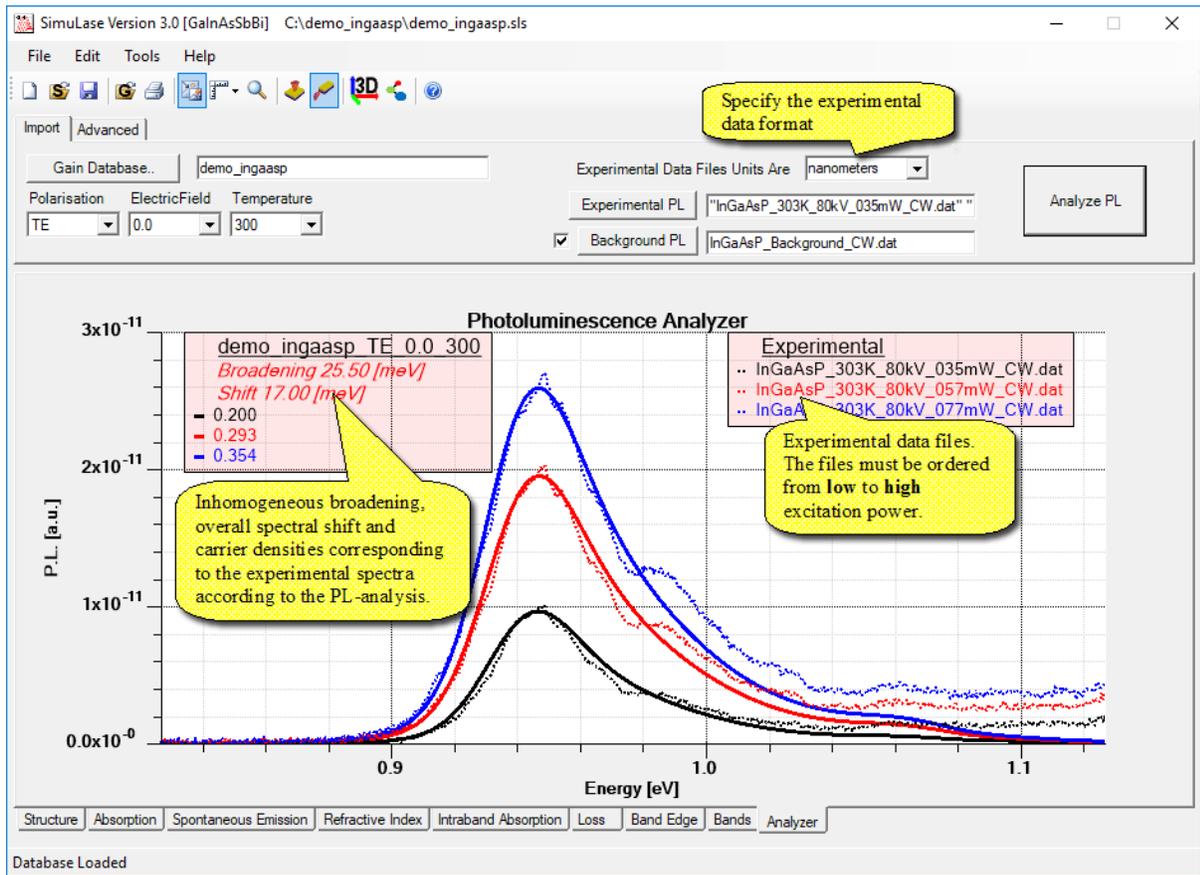


Figure 8: Main PL-Analysis panel.

The PL Analyzer tool allows to compare theoretical material PL-spectra to measured data in order to obtain information about the inhomogeneous broadening and spectral mismatches between nominal and actual structure. The results provide direct insight into device growth quality. In contrast to the 'Surface-PL' panel, here the PL is assumed to be the pure material PL that is not disturbed by cavity effects. This is usually the case in edge-emitting devices or for PL that has been measured from the edge of the device.

The tool may be activated by selecting '**Tools | Analyze Experimental PL**' from the menu bar. Performing a PL analysis requires the following steps:

- 1) Select a gain database that matches the material system of the experimental PL spectra to be analyzed. Click on '**Gain Database**' and select a pre-computed gain database.
- 2) Select the parameters, like polarization and temperature, that most closely match the experimental conditions. The corresponding theoretical PL spectra from the database are plotted.
- 3) Import the experimental PL data (in order of increasing excitation power) by clicking the '**Experimental PL**' tab and importing the data. In the current version of **SimuLase™** the experimental data has to be in two-column ASCII format. The first column containing the transition energy in [eV] or the wavelength in [nm]. The second column containing the PL data. Specify the data format using the '**Experimental data file units**' selector box.
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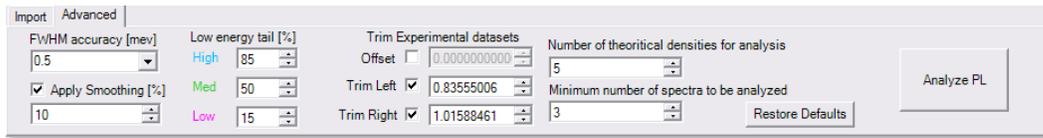


Figure 9: Advanced PL-Analysis panel.

On the '**Advanced**' tab, details of the analysis can be influenced by choosing low-energy matching points, high energy cut-off, the desired accuracy ('**FWHM accuracy**' tab), as well as the number of theoretical spectra used for the analysis.

The '**Offset**' can be used to subtract a constant background value from the experimental spectra - similarly to subtracting a background-noise spectrum.

'**Trim Left**' and '**Trim Right**' allow to exclude low- and high-energy tails in the experimental spectra from the analysis. Low energy tails are often covered by noise where the ideal spectra fall off below the bandgap. On the high energy side experimental spectra often show enhancements of the PL beyond the ideal theoretical PL. This is usually due to non-thermal carriers in the experiment which arise in particular when using CW-excitation. These carriers have not relaxed toward the bottom of the wells - occupying higher subbands - and lead to an enhancement beyond the ideal thermal equilibrium situation assumed in the theory (see e.g. the features at 0.98 eV in Fig.6. These parts should be excluded from the analysis.

The Analysis should focus on the spectral region around the main peak that gives the best information about the inhomogeneous broadening and spectral shifts - starting where the PL reaches about 20% of the maximum to where the PL falls off again to about 50% of the peak value.

The theoretical spectra to the lowest carrier densities are used since experimental data usually is taken under low excitation conditions. The '**Number of theoretical densities for analysis**' should be increased if no good match is found when considering only the lowest densities.

If one has a very large experimental database loaded, one might want to save computation time and/or to focus on the qualitatively best spectra one can choose a subset of spectra to be analyzed by specifying the '**Minimum number of spectra to be analyzed**'. The analysis tool

internally selects then a subset of experimental spectra of that size that matches closest average criteria. The final results are displayed only for these spectra.

In case of noisy experimental spectra one can apply a smoothing algorithm by choosing '**Apply Smoothing**' in order to eliminate artificial local peaks in the spectra which might obscure the true spectral location of the PL maximum. The percentage value chosen for smoothing is given as the percentage of the estimated inhomogeneous broadening present in the experimental data.

After choosing the desired settings, click the '**Analyze PL**' tab. After a short calculation, the best matching theoretical curves appear on the screen superimposed to the experimental data. In order to obtain the agreement, usually it is necessary to inhomogeneously broaden the ideal theoretical spectra (to take into account the experimentally unavoidable local composition and/or well width fluctuations) and to apply a spectral shift. Physically, this shift often appears as a consequence of deviations between nominal and actual composition and/or quantum-well width. The computed broadening and shift can be read from the legend in the display window. This legend also shows the theoretical densities chosen for the best agreement with the experimental data.

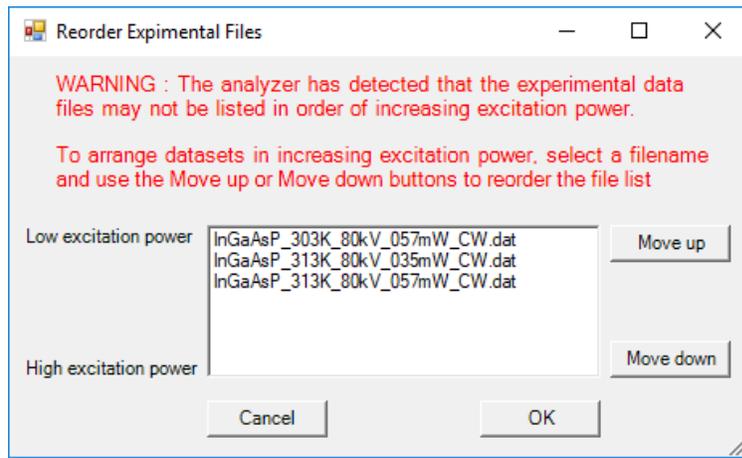


Figure 10: Re-arrange experimental PL panel.

The analyzer requires that the experimental datasets be imported in order of increasing excitation power. Internally, the analyzer arranges the imported data files by sorting the file names in alphabetical order. The resulting ordering of the data files is visible in the '**Experimental**' legend that appears on the plot window next to the experimental data plots. If, after clicking the '**Analyze PL**', button the analyzer determines that the experimental data files are NOT in correct order the following dialog is displayed.

The order of data files may be rearranged by selecting a file name and using the '**Move up**' or '**Move down**' buttons. Once all file have been correctly reordered from low (on top) to high excitation power (at the bottom) click OK, the experimental PL data will be redisplayed in the plot window and the PL analysis may be reapplied by clicking the '**Analyze PL**' button.

## 6.2 Generating Shifted and Broadened Databases

Shifted and inhomogeneously broadened copies of existing GainDatabases may be generated by selecting '**Tools | Shift and Broaden Database**' from the main menu bar. The dialog Fig.11 will be displayed. Select an existing GainDatabase using the '**Gain Database**' button, enter

the desired shift and broadening, select a directory into which the new database shall be stored and click OK. A new database will be generated in the destination directory with all spectra shifted and broadened by the requested amount. All other data unaffected by the shift and broaden operations, like wavefunctions and band structure etc., will be copied to the destination directory. The new database that may be loaded into the viewer, like any other Gain Database, using the '**File | Open Gain Database**' from the main menu bar.

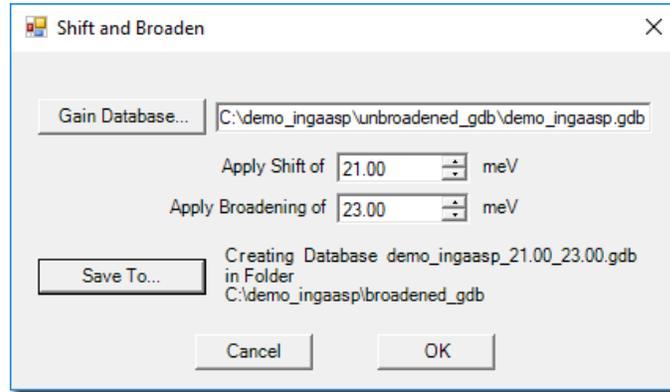


Figure 11: Dialog to create shifted and/or broadened copies of existing GainDatabases.

### 6.3 Linewidth Enhancement Factor Tool

The linewidth enhancement factor tool may be activated by selecting **Tools | Linewidth Enhancement Factor** from the menu bar.

#### Linewidth Enhancement Factor | Carrier Density

This tool calculates the linewidth enhancement factor spectrum ( $\alpha(\omega)$ ) for a specified carrier density ( $N$ ) using:

$$\alpha(\omega, N) = \frac{n(\omega, N + \Delta_N) - n(\omega, N)}{a(\omega, N + \Delta_N) - a(\omega, N)}, \quad (1)$$

where  $n$  is the refractive index in the units as displayed in the '**Refractive Index**'-window,  $a$  is the material absorption and  $\Delta_N$  is an infinitesimal density change.

Since the linewidth enhancement factor is given by the ratio of two differentials, it can vary dramatically when viewed on an extended energy/spectral-range. One usually has to zoom into the relevant region of the spectra.

#### Linewidth Enhancement Factor | Electric Field

This tool calculates the linewidth enhancement factor spectrum ( $\alpha(\omega)$ ) for a change in electric field/applied Voltage ( $F$ ) using:

$$\alpha(\omega, F_0, F_1) = \frac{n(\omega, F_0) - n(\omega, F_1)}{a(\omega, F_0) - a(\omega, F_1)}, \quad (2)$$

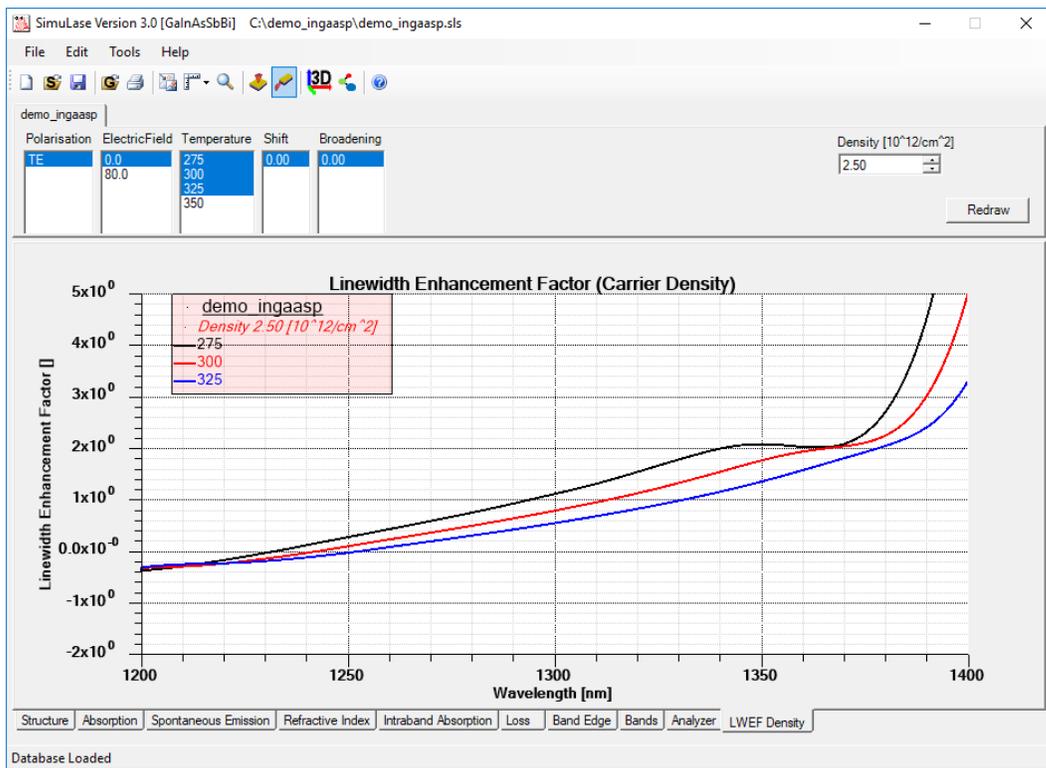


Figure 12: Linewidth Enhancement Factor tool for the calculation of the LWEF for a given carrier density.

where  $n$  is the refractive index in the units as displayed in the 'Refractive Index'-window,  $a$  is the material absorption and  $F_0, F_1$  are two electric field values from the list of fields for which the database has been set up.

## 7 Tools for Edge-Emitters

**SimuLase™** offers some tools that are most useful for analyzing edge emitting structures. They can be accessed by clicking on the icon  in the top panel or by selecting 'Tools | Edge Emitter Mode'.

### 7.1 Current Calculator Tool

Once the edge-emitting mode has been selected, the 'Current Calculator' tool appears as a tab above the plot panel.

While **SimuLase™** does not model the electrical pump injection problem that is crucial for a quantitative analysis of the operating characteristics of electrically pumped devices, this tool allows to determine basic characteristics like the threshold current or internal quantum efficiency for somewhat idealized cases and allows to study their dependence on various parameters like the number of wells or the absorption loss. It also allows to calculate the input-output characteristics

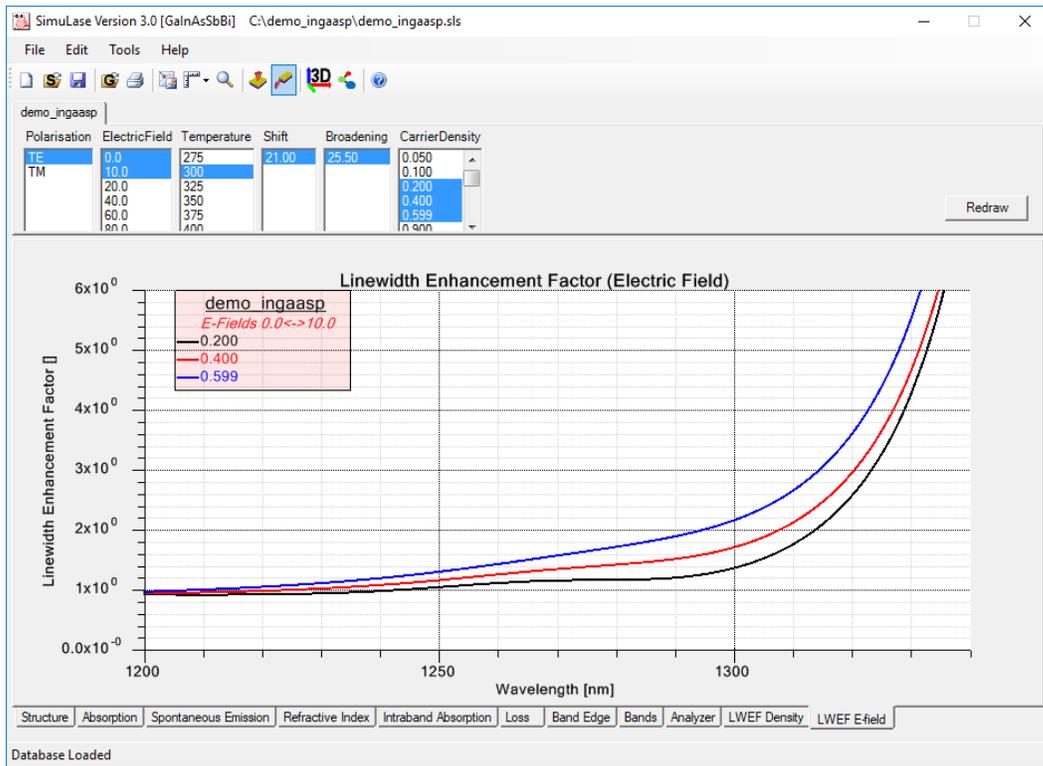


Figure 13: Linewidth Enhancement Factor tool for the calculation of the LWEF for a change in the electric field across the active region.

using a model that is accurate for the case of optical pump injection and can be used to study dependencies in the case of electrical pumping.

The tool requires a gain database and the corresponding structure should be loaded in the 'Design Structure' window. The 'quantized region' for which the database has been set up should be marked correctly in the structure. Then the program automatically determines the number of wells in the structure (identical copies of the quantized region) and scales the data in the database accordingly. This is important for the case where - as typically suggested - the database has been set up for only one well of a multi-well structure.

The tool has two operating modes:

- (1) One determines the threshold characteristics like threshold current, lasing wavelength and IQE, for the fixed temperatures for which the database has been set up. Here, internal heating is neglected.
- (2) One calculates the input-output characteristics taking into account heating due to non-radiative losses.

Mode (1) requires only very limited and usually rather well known input. Assuming that internal heating is not too relevant at threshold, it gives correct results that are independent of the way of pumping.

Mode (2), while more powerful than mode (1), requires to know more input parameters, like the thermal impedance. It is a complete model for the case of optical pumping. However, it does not consider heating mechanisms that occur in electrical pumping like Joule heating and

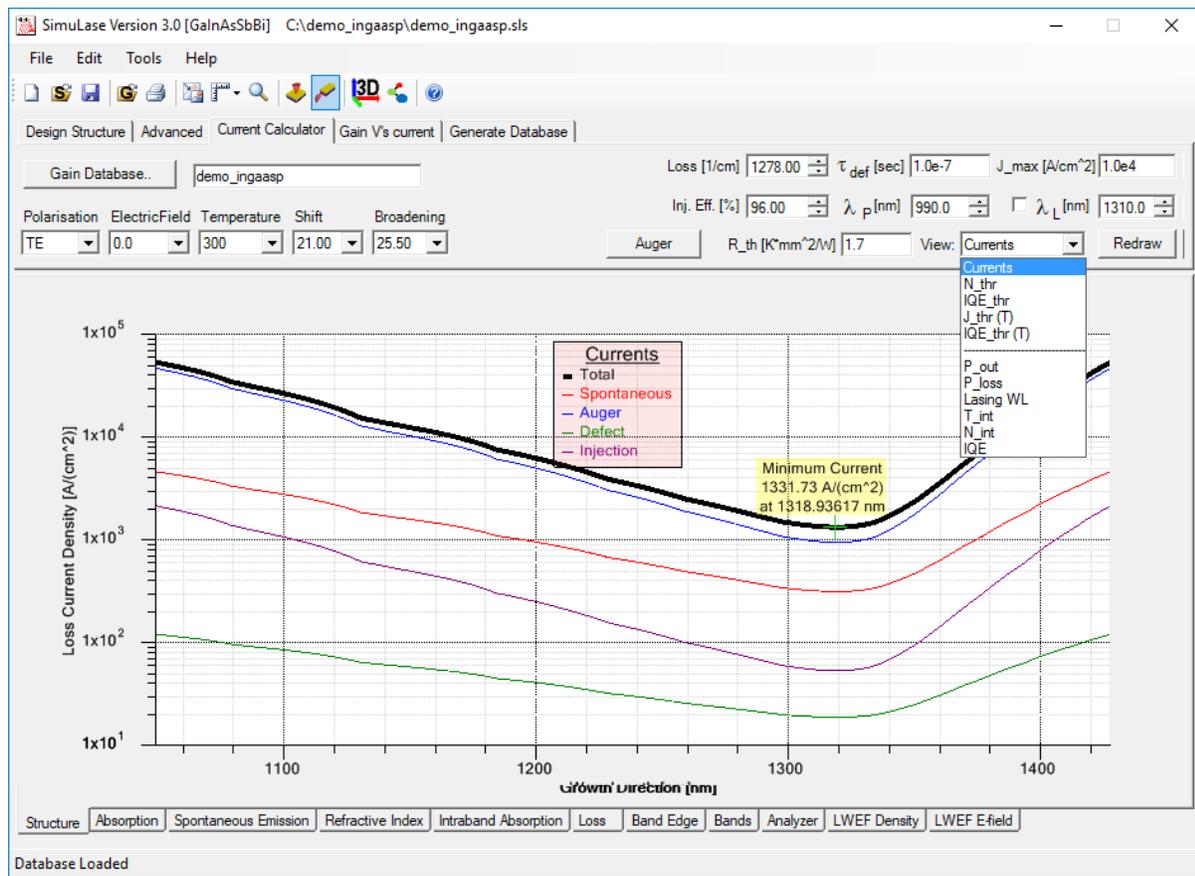


Figure 14: Current Calculator tool displaying threshold characteristics.

Thomson-Peltier heating. The influence of these can only be roughly approximated within this model. Thus, the absolute accuracy is questionable for electrically pumped cases. However, the model should allow to determine general trends of the operating characteristics correctly also for this pump mode.

Three different models for the Auger losses can be chosen. When selecting 'Use Auger Data from Database,' the microscopically calculated Auger losses from the database are used. If the database was not set up including Auger losses, they are assumed to be zero. When selecting the 'CN3' model the classical  $CN^3$  cubical density dependence is assumed. The density-activated defect recombination model, 'DADR', was found to be appropriate for AlInGaN materials. Details of the Auger models can be found in the main manual.

## Threshold Characteristics

As mentioned above, the calculations require a gain database and the corresponding structure has to be loaded in the 'Design Structure' window. The structure is used to determine the number of wells, i.e. the number of repeats of the quantized region for which the gain database has been set up within the full structure. Thus, the number of wells can be varied by adjusting the structure accordingly.

For these calculations internal heating is neglected. The temperature for which the calculations are done is selected from the ones available in the database. The user has to specify the total

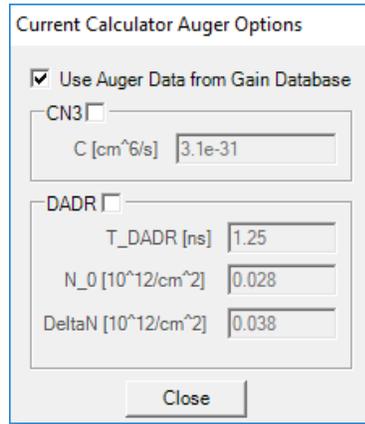


Figure 15: Panel allowing to choose between different Auger models.

material absorption loss in the field '**Loss**'. This is usually given by the sum of the out-coupling loss plus the internal absorption loss. If this is known as a modal loss for the full structure, it has to be divided by the optical confinement factor for the structure. The confinement factor can be calculated using the 'View | Transverse Mode' option from the 'Design Structure' panel. It is calculated for the temperature and wavelength as specified in the 'Advanced' options panel. One also has to specify the defect recombination time in the field ' $\tau_{def}$ ', and the injection efficiency in the field '**Inj. Eff.**'. The latter accounts for pump injected carriers that are not captured into the wells.

The tool looks up from the database what carrier density is required to yield enough gain to overcome the absorption losses. Then the loss currents due spontaneous emission (radiative loss) and Auger losses (according to the selected Auger model) are calculated from the database data for this density. If the database contains data for TE and TM polarization, the corresponding spontaneous emission losses are combined assuming that one third of the spontaneous emission goes into TM-modes and two thirds go into TE-modes. The defect recombination loss is calculated using the specified recombination time.

This evaluation is done for all wavelengths for which optical gain is found in the absorption/gain spectrum that is specified in the database selection fields. The resulting currents are plotted as function of the wavelength.

In a free running device, the threshold lasing wavelength and current is given by the point of minimum total current. For wavelength selective devices, like edge emitters with surface gratings, the fixed lasing wavelength can be set by checking the box next to the field ' $\lambda_L$ ' and specifying the value there. All calculations will then be done for this fixed wavelength.

The tool also allows to display the corresponding intrinsic carrier densities,  $N_{thr}$  and internal quantum efficiencies, ' $\text{IQE}_{thr}$ ' (spontaneous emission loss current divided by total loss current). It also calculates the threshold current and internal quantum efficiency for all temperatures within the database if it contains data for more than one temperature. The data is determined at each temperature from the wavelength of minimum total current or the specified lasing wavelength. The results are displayed by selecting ' $\mathbf{J}_{thr}(\mathbf{T})$ ' and ' $\mathbf{IQE}_{thr}(\mathbf{T})$ '. Exponential fits according to characteristic temperatures ( $T_0$ ) and ( $T_1$ ), respectively, are shown in these plots.

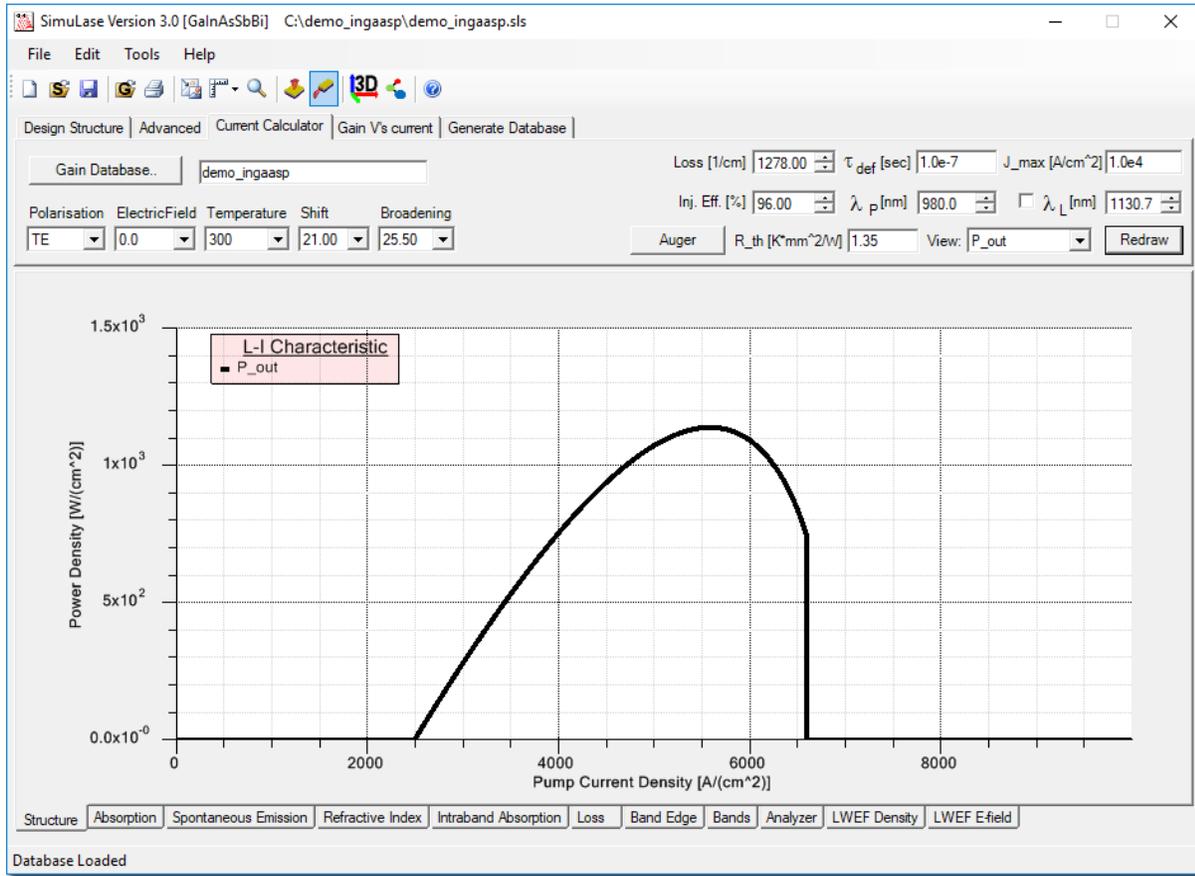


Figure 16: Current Calculator tool displaying input-output characteristics.

## Input-Output Characteristics

Besides the input required also for the threshold calculations described above - database, structure, optical loss, defect recombination time and injection efficiency ( $\eta_{inj}$ ), the calculations of the input-output characteristics require some additional input to model the internal heating.

Here, the heat sink temperature is given by the temperature set on the 'Advanced' panel. A maximum pump current for which the data shall be calculated has to be set in the field ' $J_{max}$ '. The thermal impedance of the device has to be specified in the field ' $R_{th}$ '. A pump wavelength has to be set in the field ' $\lambda_p$ '.

The operating characteristics are determined directly from the balance of powers,  $P_{pump} = P_{out} + P_{heat} + P_{rest}$ , where  $P_{heat}$  is the amount of pump power that is converted to heat and  $P_{rest}$  is power lost to spontaneous emission that leaves the device without contributing to heating. For each temperature in the database the intrinsic carrier density at lasing is determined by looking for the density for which the gain is high enough to lead to enough gain to compensate for the optical losses as specified in 'Loss'. If a fixed lasing wavelength has been specified in the field  $\lambda_L$ , the gain has to be high enough at this wavelength. Otherwise, the gain maximum selects the lasing wavelength.

Then, the spontaneous emission, Auger and defect losses are calculated for this density. It is assumed that all these losses contribute to heating except for a fraction of the spontaneous emission that escapes the device. The results usually do not depend significantly on this fraction.

We currently assume that 50% of the spontaneous emission escapes in all cases.

For each pump power,  $P_{\text{pump}}$ , additional heating losses are given by the amount of carriers that are not captured in the well,  $P_{\text{pump}}(1 - \eta_{\text{inj}})$ , and the quantum defect,  $P_{\text{qd}}$ , i.e. the difference between pump energy and lasing energy.

The intrinsic temperature increase due to this heating power,  $\Delta T_{\text{heat}}$  is calculated using:

$$\Delta T_{\text{heat}} = P_{\text{heat}} R_{\text{th}}. \quad (3)$$

Finally, the operating point is determined by interpolating between the data for the fixed temperatures of the database in order to look up the temperature,  $T$  for which the heating losses lead to a temperature increase satisfying  $T = T_{\text{HS}} + \Delta T_{\text{heat}}$ . Here  $T_{\text{HS}}$  is the heat sink temperature. If such a temperature exists for a given pump power the device will lase with non-zero output power.

This model works for optically pumped devices. In electrically pumped devices there is of course no well defined pump wavelength. Carriers will also lose part of their energy to relaxation from the barrier into the wells, but the total energy loss depends on the positions of the Fermi levels, dopant levels and overall band bending due to space charges and applied Voltages - all of which are pump current dependent. Joule heating and Thomson-Peltier heating are not taken into account. Thus, this model is not an exact tool for this situation. It should merely be seen as a help to estimate overall trends in the performance like their variation with optical losses, number of wells or heating as varied with the parameter  $\lambda_L$ .

The following data can be displayed through the '**View**' pull-down menu:

**P\_out:** Input-output characteristic.

**P\_loss:** Various power losses:

**P\_SE:** Spontaneous emission loss

**P\_aug:** Auger loss

**P\_def:** Defect recombination loss

**P\_qd:** Quantum defect

**P\_inj:** Injection loss

**Lasing WL:** Lasing wavelength

**T\_int:** Internal temperature

**N\_int:** Internal carrier density

**IQE:** Internal quantum efficiency

## 7.2 Gain vs. Current Tool

The '**Gain vs. Current**' tool allows to investigate the absorption/gain for a specific current. This tool helps e.g. to see how the gain for a fixed pump-current changes with temperature.

Databases are loaded using '**Load DB**' the gain vs. current tool may be activated by selecting '**Tools | Gain V's Current**' from the menu bar. After selecting a parameter set the user may view plots of the gain (absorption) as function of the loss current and the number of wells.

The '**Current**' is the assumed intrinsic loss current density solely due to radiative and Auger losses as included in the Gain Database and the 'Auger' panel, respectively. The corresponding currents are shown in the Current Calculator tool described above. As in that tool, the '**Number**

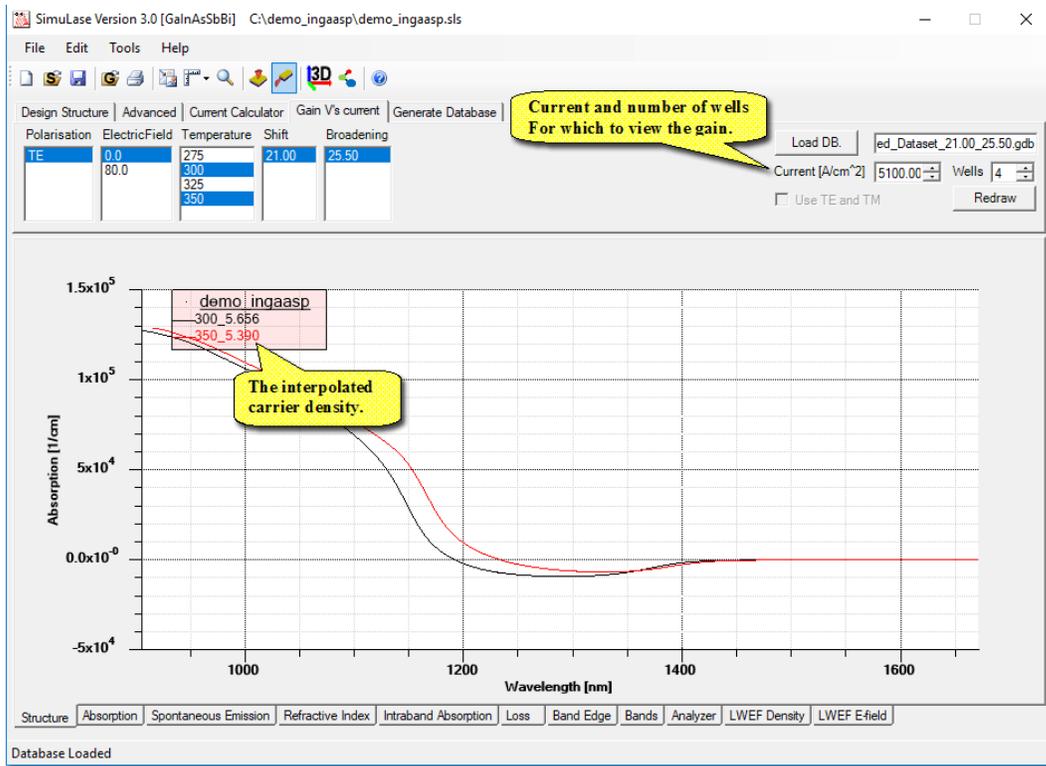


Figure 17: Gain vs. Current tool.

**of Wells'** is the number of repeats of the active structure for which the Gain Database has been set up. The '**Current**' is divided by this number in order to obtain the current density corresponding to the loss values as included in the Gain Database. The displayed spectra are the ones as interpolated from the Gain Database, properly rescaled according to this number of repeats - assuming that the optical confinement factor scales linearly with the number of repeats. If the box '**Combine TE TM losses**' is checked, the radiative loss current is calculated by combining the TE and TM loss currents using  $J_{rad} = 2/3 J_{TE,rad} + 1/3 J_{TM,rad}$ . Otherwise,  $J_{rad} = J_{TE,rad}$  and/or  $J_{rad} = J_{TM,rad}$  is used depending on which polarization(s) has been chosen through the selector field '**Polarization**'.

## 8 Tools for Top-Emitters

**SimuLase™** offers some tools that are most useful for analyzing top emitting structures. They can be accessed by clicking on the icon  in the top panel.

### 8.1 Reflection-Transmission

The '**Reflection-Transmission**'-tool allows to import GainDatabase data for the absorption/gain and carrier induced refractive index change for the calculation of the longitudinal (propagating) mode as well as the reflection and transmission spectra. It also allows to import experimentally measured reflection or transmission spectra and compare them to the theoretical results. This tool is particularly helpful for designing vertically emitting devices like VECSELs (see the main manual for a detailed example).

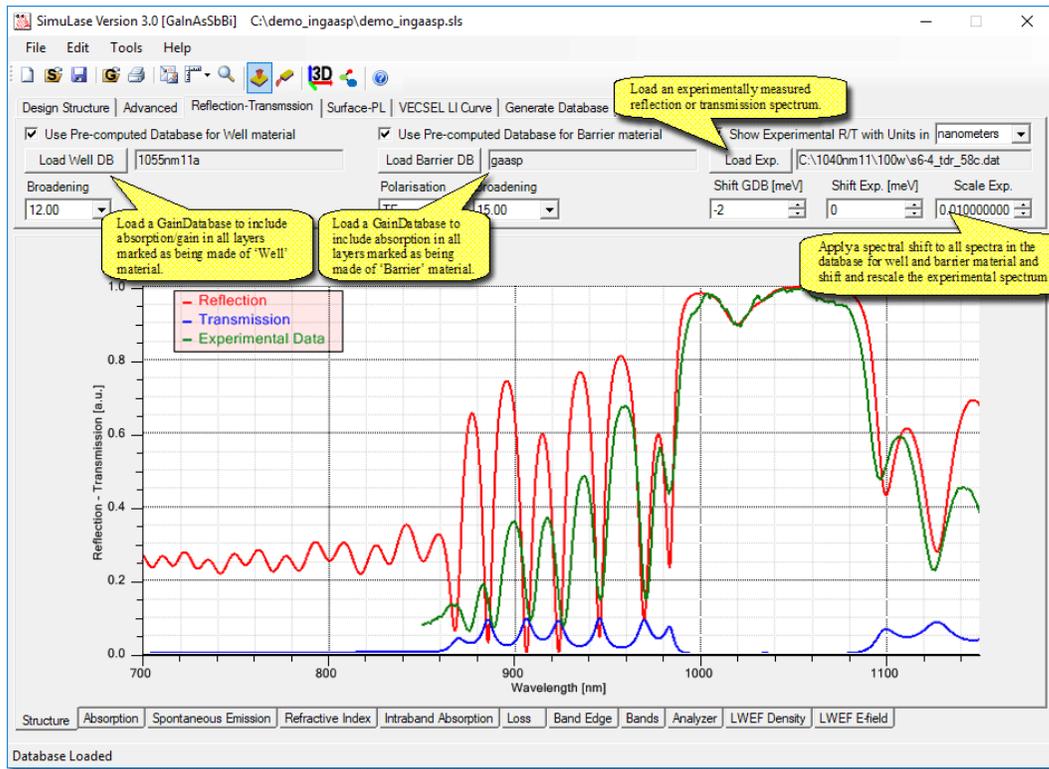


Figure 18: 'Reflection-Transmission' panel for an example of a VECSEL operating at  $1040\text{ nm}$ . The structure has a thin metallization layer on the back which reduces the transmission to a low level.

If a database is loaded for the wells or barriers, absorption/gain is added as imaginary part to the refractive index of the corresponding layers which are identified by selecting the corresponding option 'Type' on the 'Design Structure' panel. The carrier induced refractive index changes are added to the real part of the refractive index. For the absorption/gain in the well layers the carrier density and temperature are set on the 'Advanced'-options panel. Since the barrier layers are usually much wider than the wells, the corresponding carrier densities are usually very small. Thus, for the barrier layers the absorption for the lowest carrier density in the corresponding GainDatabase is used. For this density the carrier induced refractive index change is assumed to be zero.

The tool also allows to shift all spectra in the GainDatabase by a certain amount. This allows to quickly account for small deviations between the nominal structural layout that has been assumed when setting up the well-GainDatabase and actually grown structures without having to re-calculate the database. The experimentally measured data can be rescaled and shifted in order to find a fit to the theory.

## 8.2 Surface-PL

The 'Surface-PL'-tool allows to calculate the PL that is emitted vertically from the surface of a structure and to compare it to experimentally measured data. The surface-PL is calculated using the filter function approach where it is given by the product of the pure material PL as it is contained in the GainDatabases and a filter function that describes the modifications of the PL on its way from the well(s) to the surface due to reflections and interferences at the layer

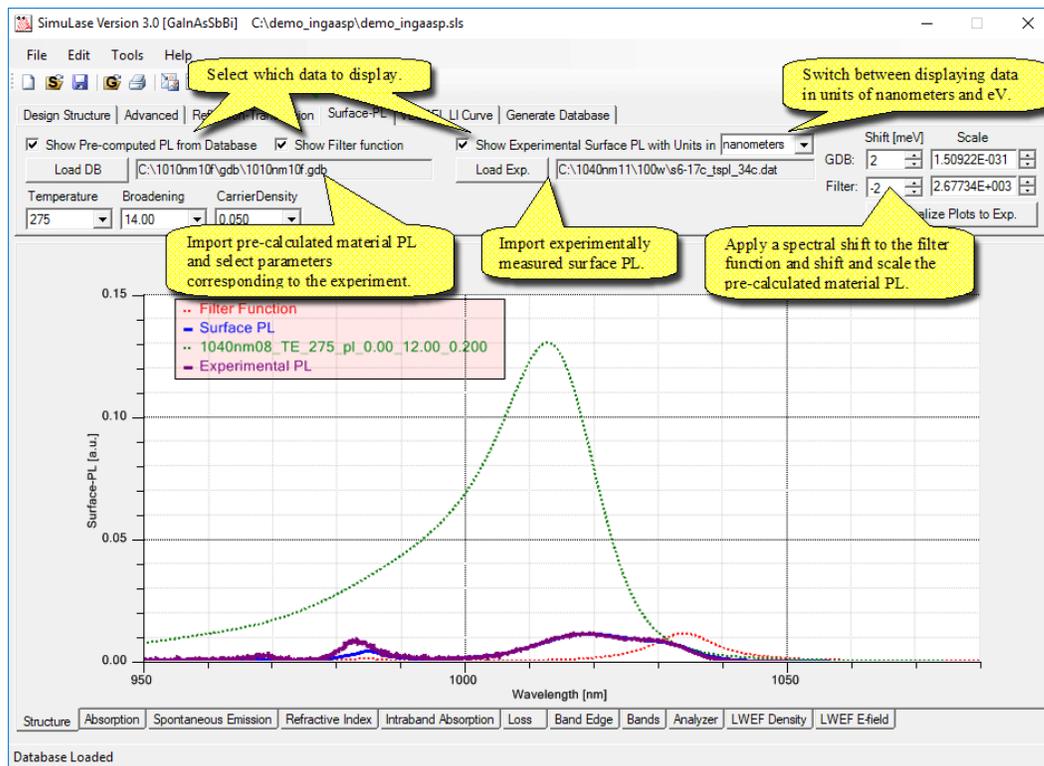


Figure 19: 'Surface-PL' panel for an example of a VECSEL operating at 1040 nm.

interfaces. Especially in V(E)CSELS, these modifications can be very significant and lead to significant changes from the pure material PL that would be measured in the absence of the interfaces or from the edge of the device.

The filter function is calculated for the structure that is currently set up in the 'Design Structure' tool and is updated whenever changes are made to the structure. It is calculated for the temperature and carrier density as specified on the 'Advanced' panel. The experimental PL has to be provided in two column ASCII data files where the first column gives the transition energy in [eV] or the wavelength in [nm] and the second column is the measured PL in arbitrary units.

The material PL from the GainDatabase and the filter function can be shifted and the material PL can be rescaled in order to find a best fit between theory and experiment.

### 8.3 VECSEL LI Curve

The 'VECSEL LI Curve'-tool allows to calculate the operating characteristics of V(E)CSELS. Based on a one-dimensional rate equation model it calculates the input-output power characteristics and other essential characteristics like lasing wavelengths and intrinsic temperatures.

The calculations are done for the structure currently present in the 'Design Structure' window. They require a GainDatabase for the quantum wells of the structure. This has to be loaded through the corresponding option on the 'Reflection-Transmission'-panel. The database for the barriers is not taken into account even if one is loaded through the same panel. The choices for the polarization, inhomogeneous broadening and the shift of the database ('Shift GDB') are also taken over from the Reflection-Transmission panel.

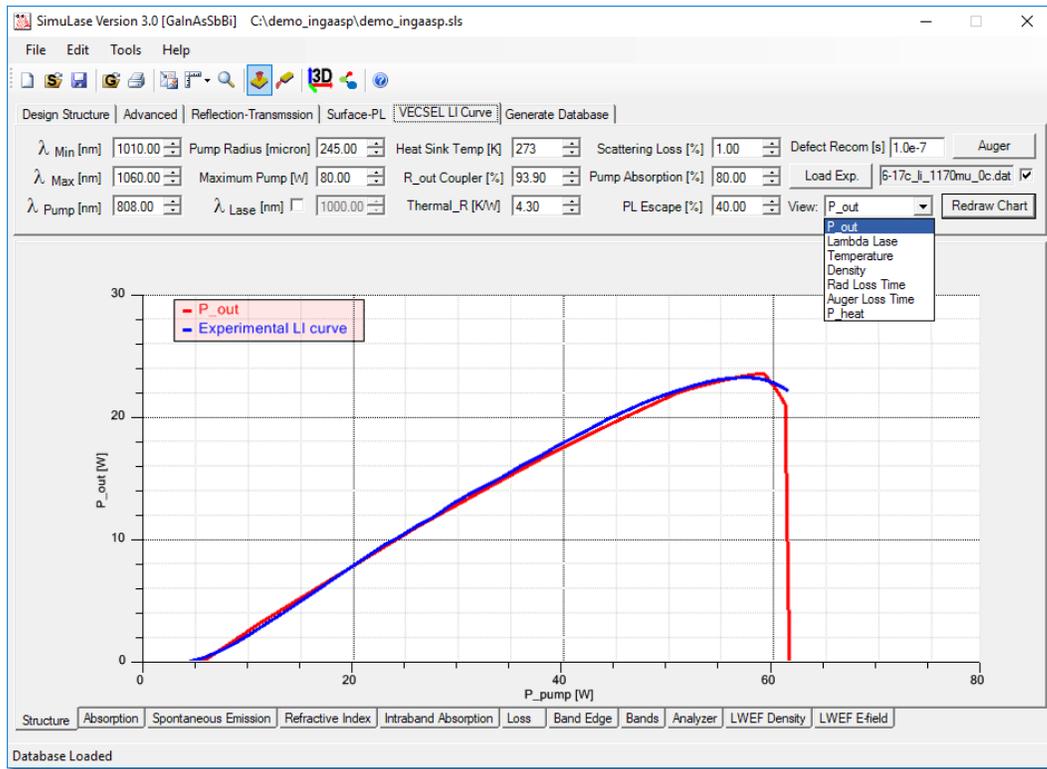


Figure 20: Overview of the 'VECSEL LI Curve' panel with a set up for the example of an VECSEL for 1040nm that is discussed in the examples section of the main manual.

Although the calculation time is only a few seconds, it can be reduced further by changing the values for  $\lambda_{\text{Min,Max}}$  from their default settings in order to reduce the spectral range that is taken into account in the calculation. The lasing wavelength can be fixed using the option  $\lambda_{\text{Lase}}$  in order to simulate devices in which the lasing wavelength is kept pump-independent using, e.g., an etalon in the external cavity.

Heating is simulated using a thermal conductivity ('Thermal\_R'). Incomplete pump absorption is taken into account through the variable 'Pump Absorption' that specifies what fraction of the pump is absorbed in the active region. It is assumed that the rest of the pump energy goes into heating of the device. The variable 'PL Escape' specifies the percentage of spontaneous emission emitted from the active region that is not absorbed in un-pumped regions outside the pump spot but escapes the device. It is assumed that the fraction of the spontaneous emission that does not escape is re-absorbed and contributes to heating. In general, the correct value for this parameter has to be calculated using ray-tracing software or a comparable model. However, the results are typically not very sensitive to this parameter. The maximum output power changes about 10% when varying this parameter between zero and 100%. The influence on the threshold or slope efficiency is even less.

Experimental data can be imported into the plots. The data has to be in two column ASCII format with the first column giving the net pump power in [W] and the second one giving e.g. the output power in [W] or lasing wavelength in [nm].