

# SimuLED Tutorials



**STR-Group Ltd**  
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# Tutorial 1

SiLENSe 5.10 & SiLENSe Laser Edition 5.10



**Specifying a New Problem in SiLENSe:  
Simulation of InGaN MQW LED Heterostructure**

## Creating a new project for InGaN MQW heterostructure

This tutorial shows how to create a new project similar to 'MQW-example' supplied with the software, specify all necessary input data, run simulations, and prepare input data for SpeCLED. It includes the following steps:

**Step 1:** Choosing material data and creating new project

**Step 2:** Specification of the heterostructure layers

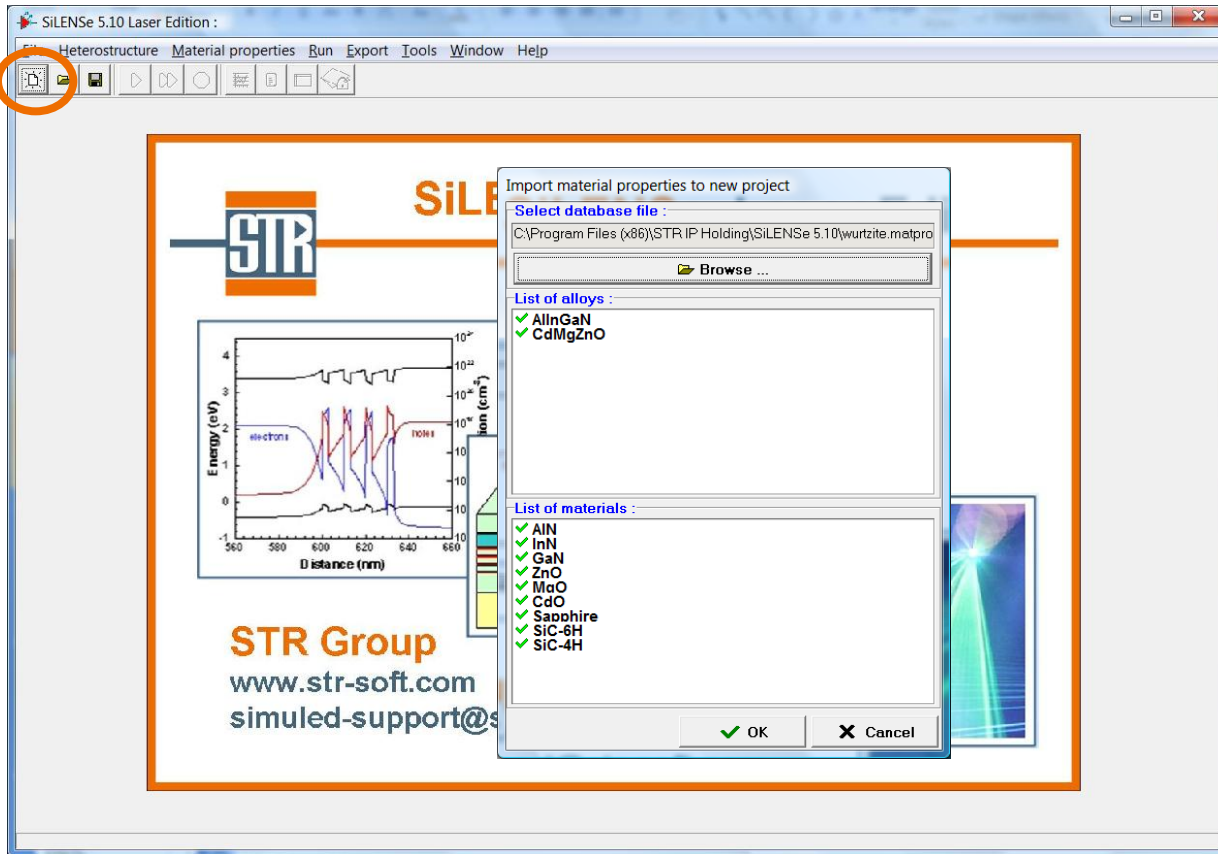
**Step 3:** Specification of global parameters (like temperature)

**Step 4:** Simulation of the band diagram, carrier concentration, carrier transport; inspecting results

**Step 5:** Simulation of carrier energy levels, wave functions, and emission spectrum; inspecting results

**Step 6 (optional):** Preparing input data for SpeCLED

## Step 1: Creating a new project



1. Open SiLENSe and press **New** button from the toolbar.

A modal window appears where the user is prompted to browse a database file (\*.matprop) with materials properties.

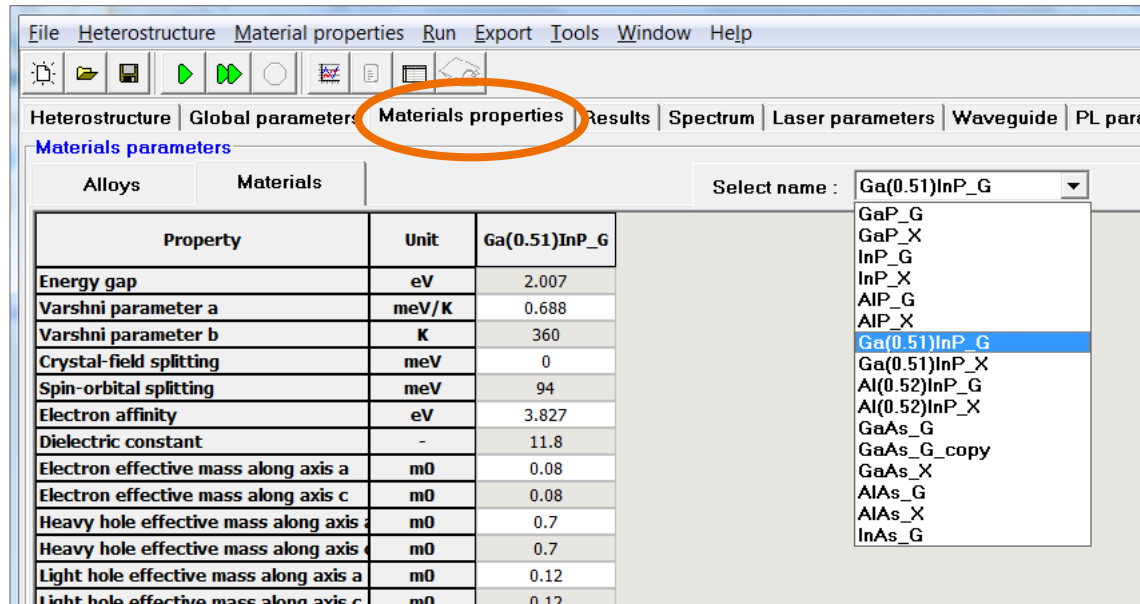
2. Choose **wurtzite** database supplied with SiLENSe. It includes properties of two systems with wurtzite crystal symmetry, namely, AllnGaN and MgZnO.

Lists of available materials and alloys shows data contained in the chosen database file. **Green mark** and **red cross** indicate good and insufficient data.

3. Press **OK** to create the project.

SiLENSe comes with two databases of material properties, **wurtzite** and **zinc\_blende**. The user can edit the data contained in these databases using a separate Properties Editor (**ProEdit.exe**) and create new custom \*.matprop files.

## Step1 (Continued): Materials vs. Alloys in SiLENSe database



The screenshot shows the SiLENSe software interface with the 'Materials properties' tab selected. The 'Materials parameters' section is active, and a dropdown menu is open for selecting a material name. The table below lists the properties for the selected material, Ga(0.51)InP\_G.

Property	Unit	Ga(0.51)InP_G
Energy gap	eV	2.007
Varshni parameter a	meV/K	0.688
Varshni parameter b	K	360
Crystal-field splitting	meV	0
Spin-orbital splitting	meV	94
Electron affinity	eV	3.827
Dielectric constant	-	11.8
Electron effective mass along axis a	m0	0.08
Electron effective mass along axis c	m0	0.08
Heavy hole effective mass along axis a	m0	0.7
Heavy hole effective mass along axis c	m0	0.7
Light hole effective mass along axis a	m0	0.12
Light hole effective mass along axis c	m0	0.12

In specification of materials properties, SiLENSe distinguishes between materials of fixed composition (like GaN, AlN, InN) and their alloys where composition may be continuously varied with one or more degree of freedom (like  $\text{Al}_x\text{Ga}_{1-x}\text{N}$ ,  $\text{In}_x\text{Ga}_{1-x}\text{N}$ ,  $\text{Al}_x\text{In}_y\text{Ga}_{1-x-y}\text{N}$ ) and properties calculated through the respective properties of materials and bowing parameters (both are stored in the respective \*.matprop file).

Note that ternary and quaternary compounds can also be treated by the software as materials when they have fixed composition and properties described in the database explicitly with no option of composition variation and respective adjustments, see the example above, where  $\text{Ga}_{0.51}\text{In}_{0.49}\text{P}$  alloy is specified as a material. Because of its importance it might be useful to specify its properties explicitly. Also, it may be used later as a basic material for AlGaInP alloys lattice matched to GaAs.

## Step1 (Continued): Inspecting material properties

1. Open **Materials Properties** tab for read-only inspection of the properties

3. Select the desired material or alloy from the drop down menu

2. Choose between materials and alloys by switching to the respective tab

Materials parameters

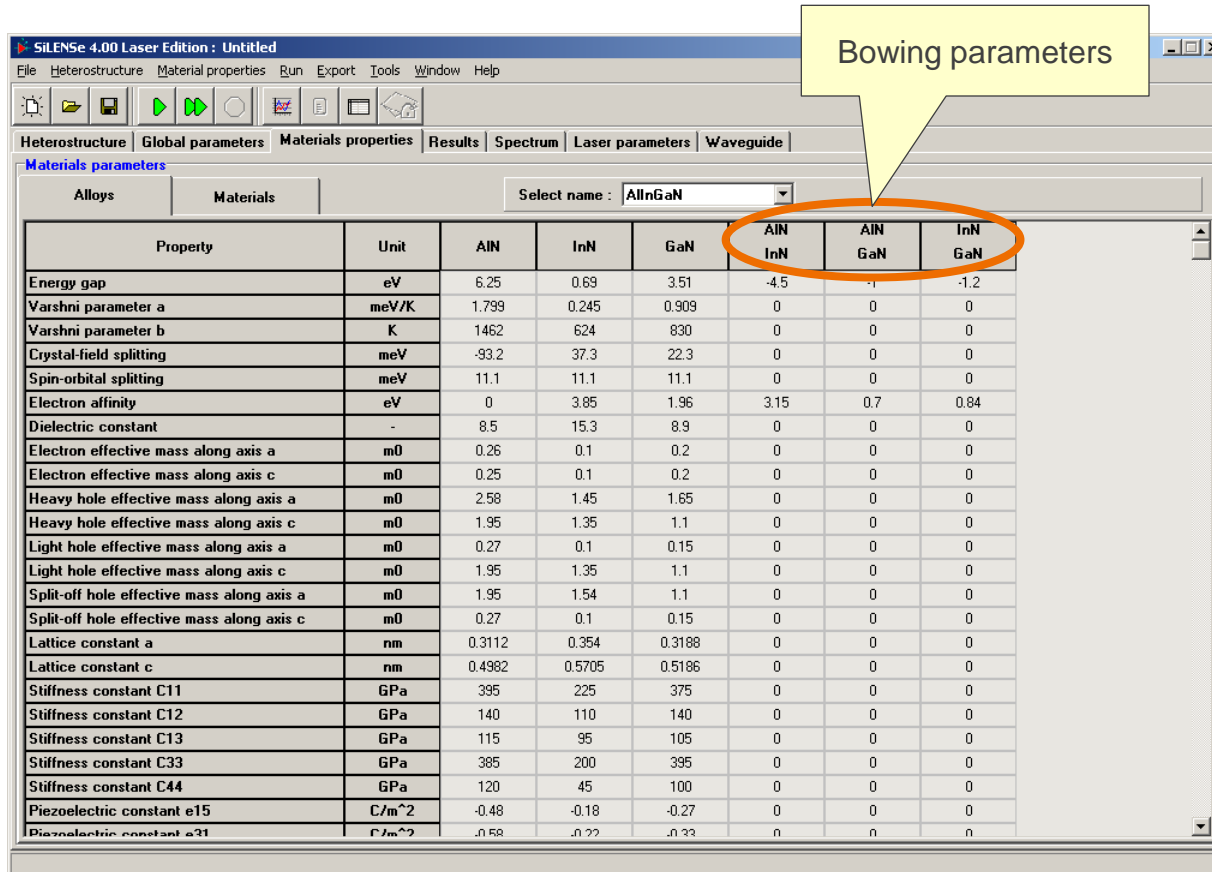
Select name : AlInGaN

Property	Unit	Alloys			Bowling parameters		
		AlN	InN	GaN	AlN InN	AlN GaN	InN GaN
Band gap	eV	6.25	0.63	3.51	-4.5	0	-1.2
Band gap	meV/K	1.799	2.245	0.909	0	0	0
Band gap	K	1462	224	830	0	0	0
Band splitting	meV	-93.2	1.3	22.3	0	0	0
Band splitting	meV	11.1	11.1	11.1	0	0	0
Band splitting	eV	1.96	3.15	0.7	0	0	0
Dielectric constant		8.9	0	0	0	0	0
Electron effective mass a		0.2	0	0	0	0	0
Electron effective mass a		0.2	0	0	0	0	0
Heavy hole effective mass		0.65	0	0	0	0	0
Heavy hole effective mass		1.1	0	0	0	0	0
Light hole effective mass		0.15	0	0	0	0	0
Light hole effective mass along axis c	m0	1.95	1.35	1.1	0	0	0
Split-off hole effective mass along axis a	m0	1.95	1.54	1.1	0	0	0
Split-off hole effective mass along axis c	m0	0.27	0.1	0.15	0	0	0
Lattice constant a	nm	0.3112	0.354	0.3188	0	0	0
Lattice constant c	nm	0.4982	0.5705	0.5186	0	0	0
Stiffness constant C11	GPa	395	225	375	0	0	0
Stiffness constant C12	GPa	140	110	140	0	0	0
Stiffness constant C13	GPa	115	95	105	0	0	0
Stiffness constant C33	GPa	385	200	395	0	0	0
Stiffness constant C44	GPa	120	45	100	0	0	0
Piezoelectric constant e15	C/m <sup>2</sup>	-0.48	-0.18	-0.27	0	0	0
Piezoelectric constant e31	C/m <sup>2</sup>	-0.68	-0.22	-0.23	0	0	0

4. View the properties of selected material or a group of materials forming the alloy

5. For alloys, there will also be a group of columns containing the bowling parameters.

## Step 1 (Continued): Bowing parameters



Bowing parameters

Property	Unit	AlN			InN		GaN
		AlN	InN	GaN	AlN InN	InN GaN	
Energy gap	eV	6.25	0.69	3.51	-4.5	-1	-1.2
Varshni parameter a	meV/K	1.799	0.245	0.909	0	0	0
Varshni parameter b	K	1462	624	830	0	0	0
Crystal-field splitting	meV	-93.2	37.3	22.3	0	0	0
Spin-orbital splitting	meV	11.1	11.1	11.1	0	0	0
Electron affinity	eV	0	3.85	1.96	3.15	0.7	0.84
Dielectric constant	-	8.5	15.3	8.9	0	0	0
Electron effective mass along axis a	m0	0.26	0.1	0.2	0	0	0
Electron effective mass along axis c	m0	0.25	0.1	0.2	0	0	0
Heavy hole effective mass along axis a	m0	2.58	1.45	1.65	0	0	0
Heavy hole effective mass along axis c	m0	1.95	1.35	1.1	0	0	0
Light hole effective mass along axis a	m0	0.27	0.1	0.15	0	0	0
Light hole effective mass along axis c	m0	1.95	1.35	1.1	0	0	0
Split-off hole effective mass along axis a	m0	1.95	1.54	1.1	0	0	0
Split-off hole effective mass along axis c	m0	0.27	0.1	0.15	0	0	0
Lattice constant a	nm	0.3112	0.354	0.3188	0	0	0
Lattice constant c	nm	0.4982	0.5705	0.5186	0	0	0
Stiffness constant C11	GPa	395	225	375	0	0	0
Stiffness constant C12	GPa	140	110	140	0	0	0
Stiffness constant C13	GPa	115	95	105	0	0	0
Stiffness constant C33	GPa	385	200	395	0	0	0
Stiffness constant C44	GPa	120	45	100	0	0	0
Piezoelectric constant e15	C/m <sup>2</sup>	-0.48	-0.18	-0.27	0	0	0
Piezoelectric constant e31	C/m <sup>2</sup>	-0.58	-0.22	-0.33	0	0	0

By default, most properties have zero bowing parameters, that means that linear interpolation is used to calculate the property for alloy of given composition.

Note the sign of the bowing parameters! **Negative bowing means decreasing** of the property compared to the linear interpolation (an opposite definition is often used)

It is assumed that user does not need to change properties during everyday work. Instead, it is recommended to work with the same chosen set of material properties for all simulations for self-consistency of the whole research project. When necessary, editing of materials properties to be done with **Properties Editor** tool **MatProp.exe** (not discussed in this tutorial). One can update materials properties by using **Materials Properties->Import** menu item.

## Step 2: Adding heterostructure layers

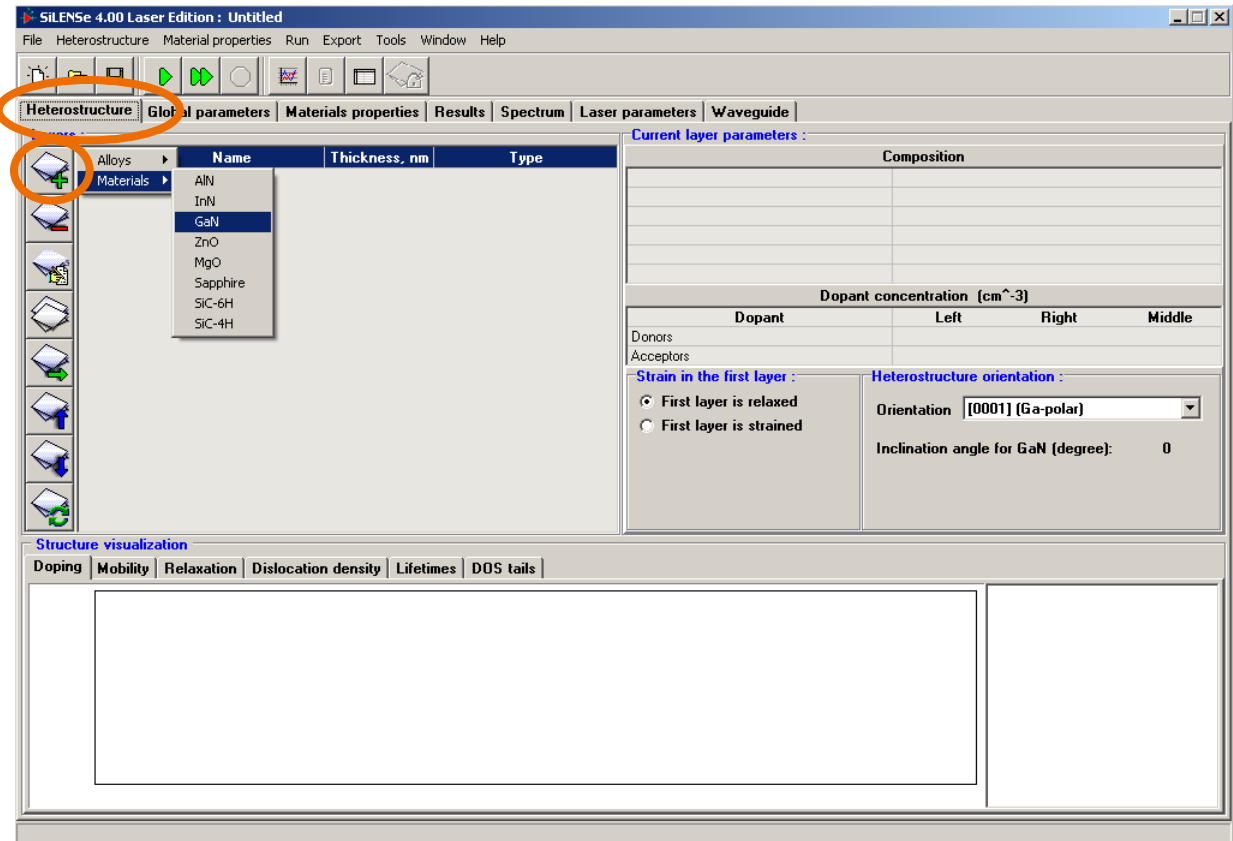
**Heterostructure** tab allows one to specify the heterostructure layers:

1. Press **Add Layer** button to add a new layer.

2. A pop-up menu appears allowing one to choose between **Materials** and **Alloys**. Both items contain submenus with list of available materials and alloys.

3. You can choose either **Materials->GaN** to add GaN layer or, alternatively, **Alloys->AlInGaN**. In the latter case you will also have to specify composition as  $Al_0In_0Ga_1N$ .

Note that later on you can also copy-paste existing layers to create new ones.

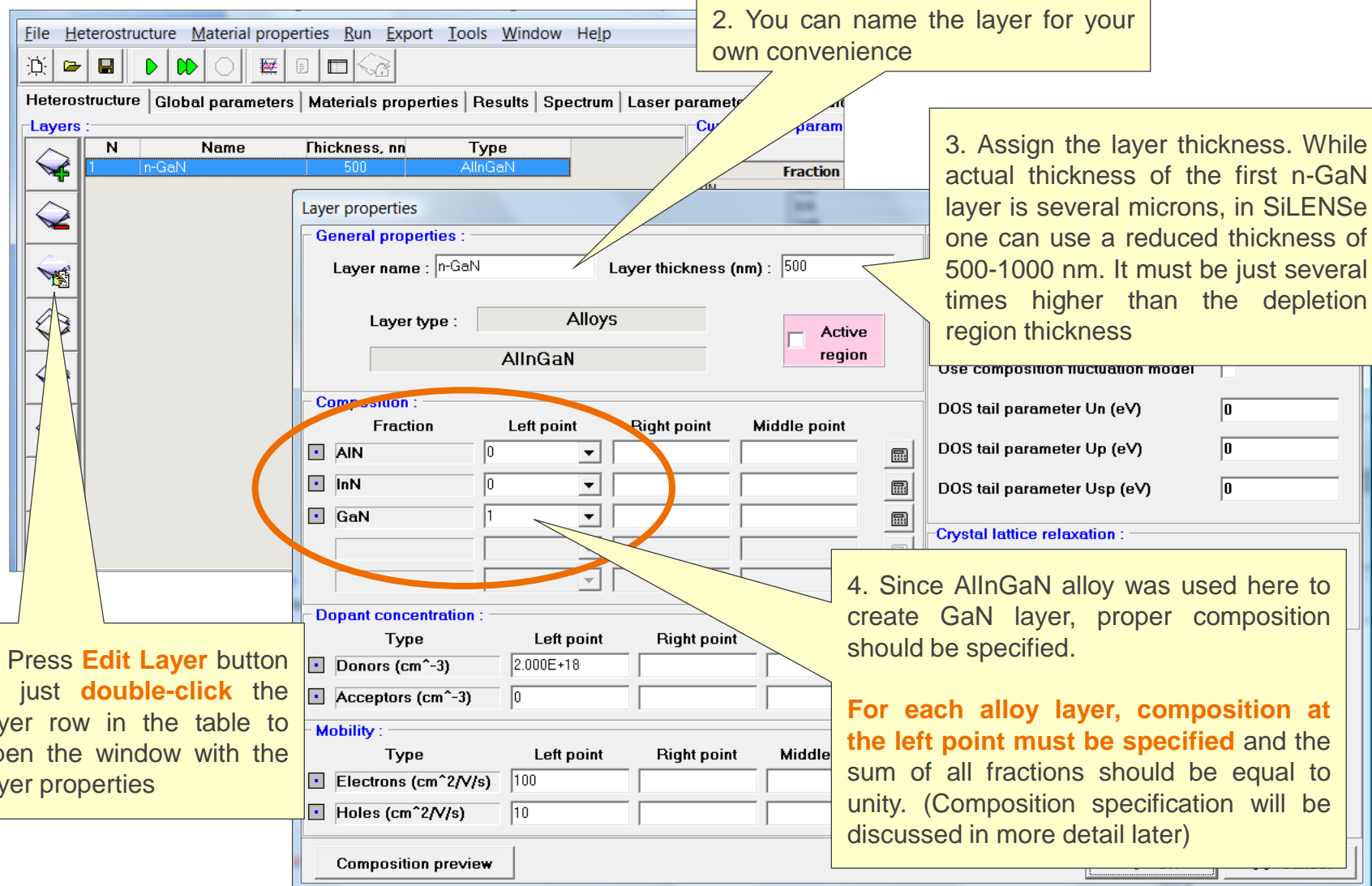


**Heterostructure has to start with n-type layer and end with p-type layer.**

**No nucleation and buffer layers to be specified.**



## Step 2 (Continued): Layer thickness and composition



1. Press **Edit Layer** button or just **double-click** the layer row in the table to open the window with the layer properties

2. You can name the layer for your own convenience

3. Assign the layer thickness. While actual thickness of the first n-GaN layer is several microns, in SiLENSe one can use a reduced thickness of 500-1000 nm. It must be just several times higher than the depletion region thickness

4. Since AlInGaN alloy was used here to create GaN layer, proper composition should be specified.

**For each alloy layer, composition at the left point must be specified** and the sum of all fractions should be equal to unity. (Composition specification will be discussed in more detail later)

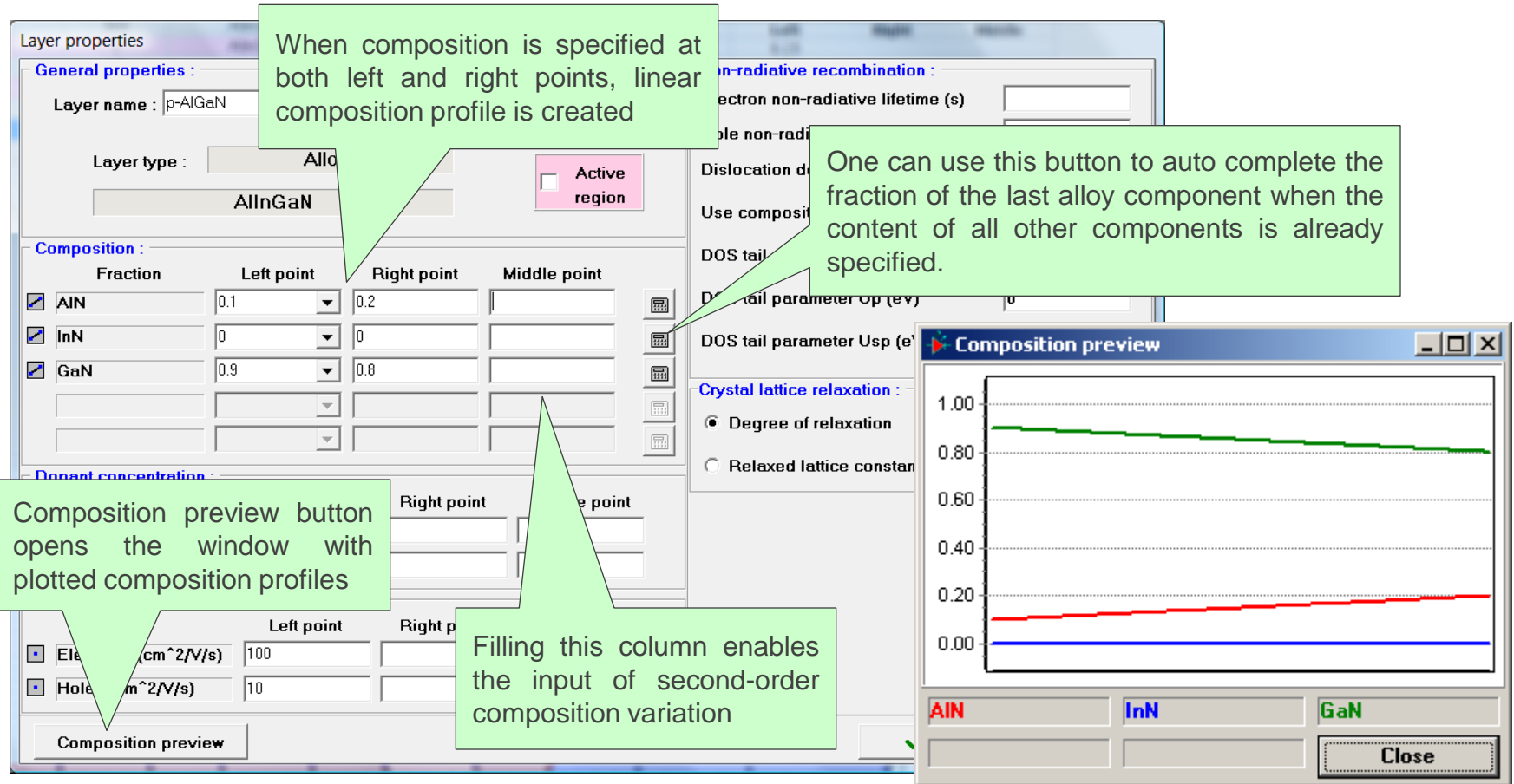
N	Name	Thickness, nm	Type
1	n-GaN	500	AlInGaN

Fraction	Left point	Right point	Middle point
<input checked="" type="checkbox"/> AlN	0		
<input checked="" type="checkbox"/> InN	0		
<input checked="" type="checkbox"/> GaN	1		

Type	Left point	Right point	Middle
<input checked="" type="checkbox"/> Donors (cm <sup>-3</sup> )	2.000E+18		
<input checked="" type="checkbox"/> Acceptors (cm <sup>-3</sup> )	0		

Type	Left point	Right point	Middle
<input checked="" type="checkbox"/> Electrons (cm <sup>2</sup> /V/s)	100		
<input checked="" type="checkbox"/> Holes (cm <sup>2</sup> /V/s)	10		

## Additional information: graded composition



When composition is specified at both left and right points, linear composition profile is created

One can use this button to auto complete the fraction of the last alloy component when the content of all other components is already specified.

Composition preview button opens the window with plotted composition profiles

Filling this column enables the input of second-order composition variation

Layer properties

**General properties :**

Layer name : p-AlGa<sub>0.1</sub>N

Layer type : AllInGa<sub>0.1</sub>N

**Composition :**

Fraction	Left point	Right point	Middle point
<input checked="" type="checkbox"/> AlN	0.1	0.2	
<input checked="" type="checkbox"/> InN	0	0	
<input checked="" type="checkbox"/> GaN	0.9	0.8	

**Donant concentration :**

	Left point	Right point
Electron (cm <sup>-2</sup> /V/s)	100	
Hole (cm <sup>-2</sup> /V/s)	10	

**Composition preview**

Composition preview window showing a graph of composition profiles for AlN (green), InN (red), and GaN (blue) across the layer. The y-axis represents the fraction (0.00 to 1.00) and the x-axis represents the position. The AlN profile starts at 0.1 and decreases to 0.2. The InN profile is constant at 0. The GaN profile starts at 0.9 and increases to 0.8.

Layer composition may be specified by using a **custom function**, defined by user by a script or by a table which can be imported from a text file. To use function, one need pick up the function name in the respective drop-down list. One can edit functions by using **Heterostructure->Functions** menu item. The **auto** menu item means that this component is determined automatically to make total composition equal to 1.

## Step 2 (Continued): Specification of the doping and mobility

**Layer properties**

**General properties :**

Layer name :

Layer type :

Active region

**Composition :**

Fraction	Left point	Right point	Middle point
<input checked="" type="checkbox"/> AlN	0		
<input checked="" type="checkbox"/> InN	0		
<input checked="" type="checkbox"/> GaN	1		

**Dopant concentration :**

Type	Left point	Right point	Middle point
<input checked="" type="checkbox"/> Donors (cm <sup>-3</sup> )	2.000E+18		
<input checked="" type="checkbox"/> Acceptors (cm <sup>-3</sup> )	0		

**Mobility :**

Type	Left point	Right point	Middle point
<input checked="" type="checkbox"/> Electrons (cm <sup>2</sup> /V/s)	100		
<input checked="" type="checkbox"/> Holes (cm <sup>2</sup> /V/s)	10		

**Non-radiative recombination :**

Electron non-radiative lifetime (s)

Hole non-radiative lifetime (s)

Dislocation density (cm<sup>-2</sup>)

Use composition fluctuation model

DOS tail parameter Un (eV)

DOS tail parameter Up (eV)

DOS tail parameter Usp (eV)

**Crystal lattice relaxation :**

Degree of relaxation

Relaxed lattice constant a (nm)

Buttons:

Note that **dopant concentration** means exactly the **concentration of the doping atoms**, NOT the carrier concentration which is calculated by the program! Hole concentration in, for instance, III-nitrides may be ~50 times lower than Mg concentration because of high activation energy.

## Step 2 (Continued): Adding InGaN quantum well layer

1. To add InGaN quantum well layer, press **Add Layer** button and choose **Alloys->AllInGaN**. Double-click new layer to edit it.

2. Mark this layer as **Active region** (it can also be done later, because specification of the active region affects only the spectrum computation)

3. For each alloy layer, **composition at the Left point** must be specified. Here, we consider InGaN QW with 13% Indium content. Sum of all rows has to be unity  
Blank Right point and Middle point columns mean that composition does not vary across the layer

Fraction	Left point	Right point	Middle point
<input checked="" type="checkbox"/> AlN	0		
<input checked="" type="checkbox"/> InN	0.13		
<input checked="" type="checkbox"/> GaN	0.87		

Type	Left point
<input checked="" type="checkbox"/> Donors (cm <sup>-3</sup> )	0
<input checked="" type="checkbox"/> Acceptors (cm <sup>-3</sup> )	0

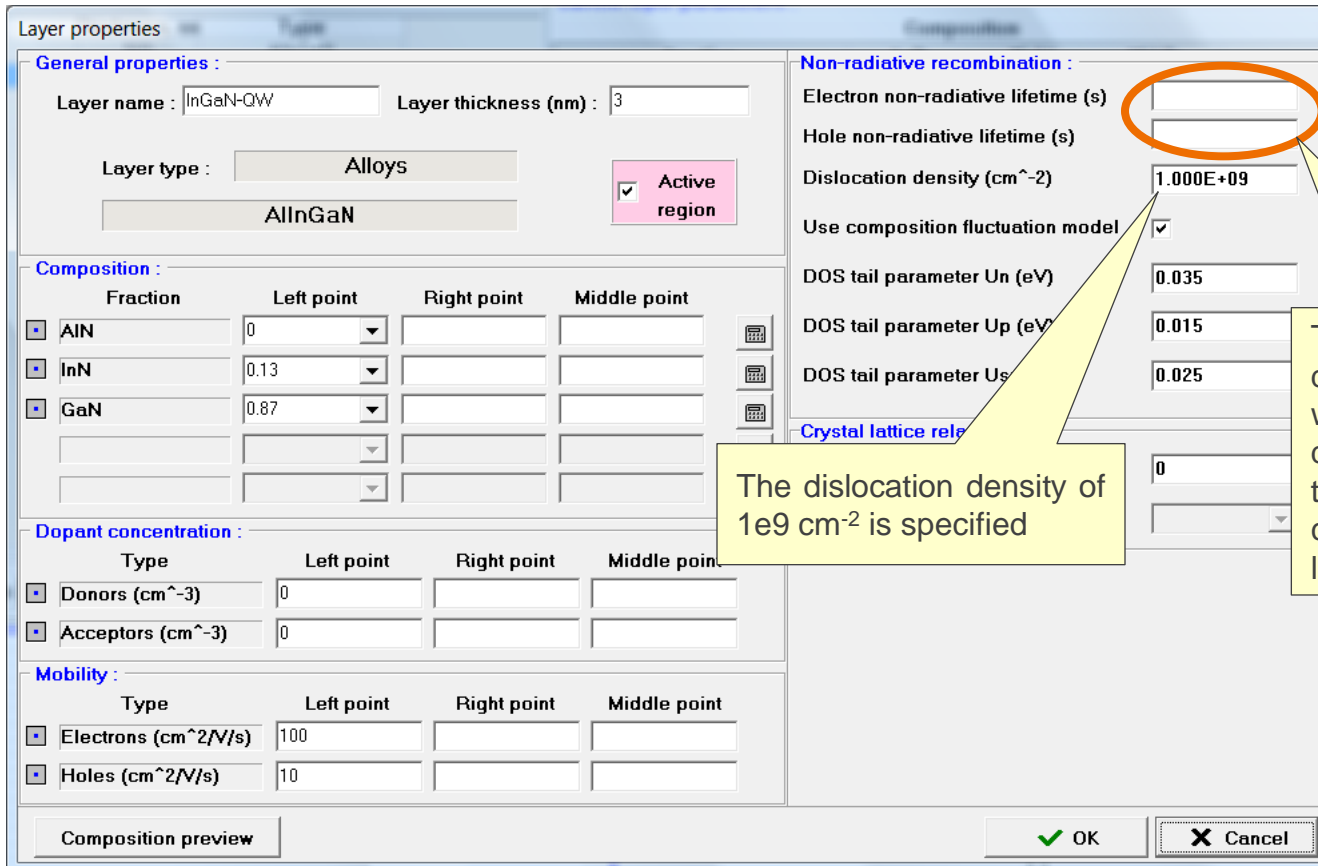
Type	Left point
<input checked="" type="checkbox"/> Electrons (cm <sup>2</sup> /V/s)	100
<input checked="" type="checkbox"/> Holes (cm <sup>2</sup> /V/s)	10

Composition preview

OK Cancel

## Step 2 (Continued): Shockley-Read-Hall recombination

In SiLENSe, there are two ways to specify the rate of non-radiative Shockley-Read-Hall recombination. One is direct specification of the carrier lifetimes due to point defects. The other way is to use an original model which relates the carrier lifetimes with the dislocation density. Both mechanisms contribute to the total non-radiative recombination rate independently, see Theory manual for details.



The screenshot shows the 'Layer properties' dialog box in SiLENSe. The 'General properties' section includes 'Layer name' (InGa<sub>N</sub>-QW), 'Layer thickness (nm)' (3), 'Layer type' (Alloys), and 'AllInGa<sub>N</sub>'. The 'Composition' section shows a table with columns for Fraction, Left point, Right point, and Middle point, with rows for AlN, InN, and GaN. The 'Dopant concentration' section has a table for Donors and Acceptors. The 'Mobility' section has a table for Electrons and Holes. The 'Non-radiative recombination' section includes fields for Electron non-radiative lifetime (s), Hole non-radiative lifetime (s), Dislocation density (cm<sup>-2</sup>) (1.000E+09), Use composition fluctuation model (checked), and DOS tail parameters (Un, Up, Us). The 'Crystal lattice relaxation' section is partially visible. The 'Active region' checkbox is checked. The 'Composition preview' button is at the bottom left, and 'OK' and 'Cancel' buttons are at the bottom right.

Fraction	Left point	Right point	Middle point
<input checked="" type="checkbox"/> AlN	0		
<input checked="" type="checkbox"/> InN	0.13		
<input checked="" type="checkbox"/> GaN	0.87		

Type	Left point	Right point	Middle point
<input checked="" type="checkbox"/> Donors (cm <sup>-3</sup> )	0		
<input checked="" type="checkbox"/> Acceptors (cm <sup>-3</sup> )	0		

Type	Left point	Right point	Middle point
<input checked="" type="checkbox"/> Electrons (cm <sup>2</sup> /V/s)	100		
<input checked="" type="checkbox"/> Holes (cm <sup>2</sup> /V/s)	10		

The dislocation density of 1e9 cm<sup>-2</sup> is specified

These two parameters describe **carrier lifetimes** with respect to point defects. Blank fields mean that this recombination channel is ignored for this layer

## Step 2 (Continued): Composition fluctuation and relaxation

Layer properties

**General properties :**

Layer name :  Layer thickness (nm) :

Layer type :   Active region

**Composition :**

Fraction	Left point	Right point	Middle point
<input checked="" type="checkbox"/> AlN	<input type="text" value="0"/>	<input type="text"/>	<input type="text"/>
<input checked="" type="checkbox"/> InN	<input type="text" value="0.13"/>	<input type="text"/>	<input type="text"/>
<input checked="" type="checkbox"/> GaN	<input type="text" value="0.87"/>	<input type="text"/>	<input type="text"/>
<input type="checkbox"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>
<input type="checkbox"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>

**Dopant concentration :**

Type	Left point	Right point	Middle point
<input checked="" type="checkbox"/> Donors (cm <sup>-3</sup> )	<input type="text" value="0"/>	<input type="text"/>	<input type="text"/>
<input checked="" type="checkbox"/> Acceptors (cm <sup>-3</sup> )	<input type="text" value="0"/>	<input type="text"/>	<input type="text"/>

**Mobility :**

Type	Left point	Right point	Middle point
<input checked="" type="checkbox"/> Electrons (cm <sup>2</sup> /V/s)	<input type="text" value="100"/>	<input type="text"/>	<input type="text"/>
<input checked="" type="checkbox"/> Holes (cm <sup>2</sup> /V/s)	<input type="text"/>	<input type="text"/>	<input type="text"/>

Composition preview

**Non-radiative recombination :**

Electron non-radiative lifetime (s) :

Hole non-radiative lifetime (s) :

Dislocation density (cm<sup>-2</sup>) :

Use composition fluctuation model

DOS tail parameter Un (eV) :

DOS tail parameter Up (eV) :

DOS tail parameter Usp (eV) :

**Crystal lattice relaxation :**

Degree of relaxation :

Relaxed lattice constant a (nm) :

Section **Composition fluctuations** allows the user to input parameters related to Indium composition fluctuations in InGaN material. Default Un and Up parameters are 35 meV and 15 meV, respectively

Zero degree of relaxation means that no relaxation occurs in this layer (by default, heterostructure is assumed to be grown pseudomorphically, i.e. all layers have the same lattice constant)

Alternatively to assigning the relaxation degree at the left interface of the layer, the user can specify the relaxed layer constant a. It may be also specified using a custom function or by tabulated data

## Step 2 (Continued): Copy, paste and move layers

1. To add GaN MQW barrier layer, select n-GaN layer and press **Copy Layer To Buffer** button

2. Select InGaN QW layer and use **Insert Layer From Buffer** button

3. A copy of n-GaN layer appears below the currently selected InGaN QW layer (that is why we have selected QW layer before inserting a copy), you just need to correct the parameters of the new layer

These buttons allow one to move a selected layer up and down

The screenshot shows the SiLENSe software interface. The 'Heterostructure' tab is active, displaying a table of layers. The 'Layers' table is as follows:

N	Name	Thickness, nn	Type
1	n-GaN	500	AllnGaN
2	InGaN-QW	3	AllnGaN
3	n-GaN-barrier	12	AllnGaN
4	InGaN-QW	3	AllnGaN

Below the table, the 'Structure visualization' section shows a plot of carrier concentration (log scale, 1.0E+00 to 1.0E+18) versus position (0 to 503.0 nm). The plot shows a step-like structure with a red line at the bottom and a blue line at the top, indicating the presence of different layers.

## Step 2 (Continued): Creating periodic structures

1. Add one more QW by copying the first one

2. Select two layers, first QW and the barrier

3. Click **Edit Periodic Structure** button

4. A modal window appears where the user is prompted to input the number of periods. Input **3** and press **OK**. To delete the periodic structure, one should input 0 or 1 period

5. Periodic structure will be marked by green color. One can specify several non-overlapping periodic structures. In this case, they will be marked by alternating green and blue colors

N	Name	Thickness, nn	Type
1	n-GaN	500	AllInGaN
2	InGaN-QW	3	AllInGaN
3	n-GaN-barrier	12	AllInGaN
4	InGaN-QW	3	AllInGaN

N	Name	Thickness, nn	Type
1	n-GaN	500	AllInGaN
2×3	InGaN-QW	3	AllInGaN
3×3	n-GaN-barrier	12	AllInGaN
4	InGaN-QW	3	AllInGaN



## Step 2 (Continued): Finalizing the structure

File Heterostructure Material properties Run Export Tools Window Help

Heterostructure | Global parameters | Materials properties | Results | Spectrum | Laser parameters | Waveguide | PL parameters

Layers :

N	Name	Thickness, nm	Type
1	n-GaN	500	AllnGaN
2 × 3	InGaN-QW	3	AllnGaN
3 × 3	n-GaN-barrier	12	AllnGaN
4	InGaN-QW	3	AllnGaN
5	n-GaN-barrier	12	AllnGaN
6	p-AlGaN	60	AllnGaN
7	p-GaN	500	AllnGaN

Current layer parameters :

Fraction	Composition		
	Left	Right	Middle
AlN	0		
InN	0		
GaN	1		

Dopant concentration (cm<sup>-3</sup>)

Donors  
Acceptors

Strain in

First  
 First

1. Add top GaN barrier, p-AlGaN electron blocking layer, and final p-GaN layer following **MQW-example.sls** file supplied with the software. Please note that the top barrier is p-doped because of Mg diffusion from p-side

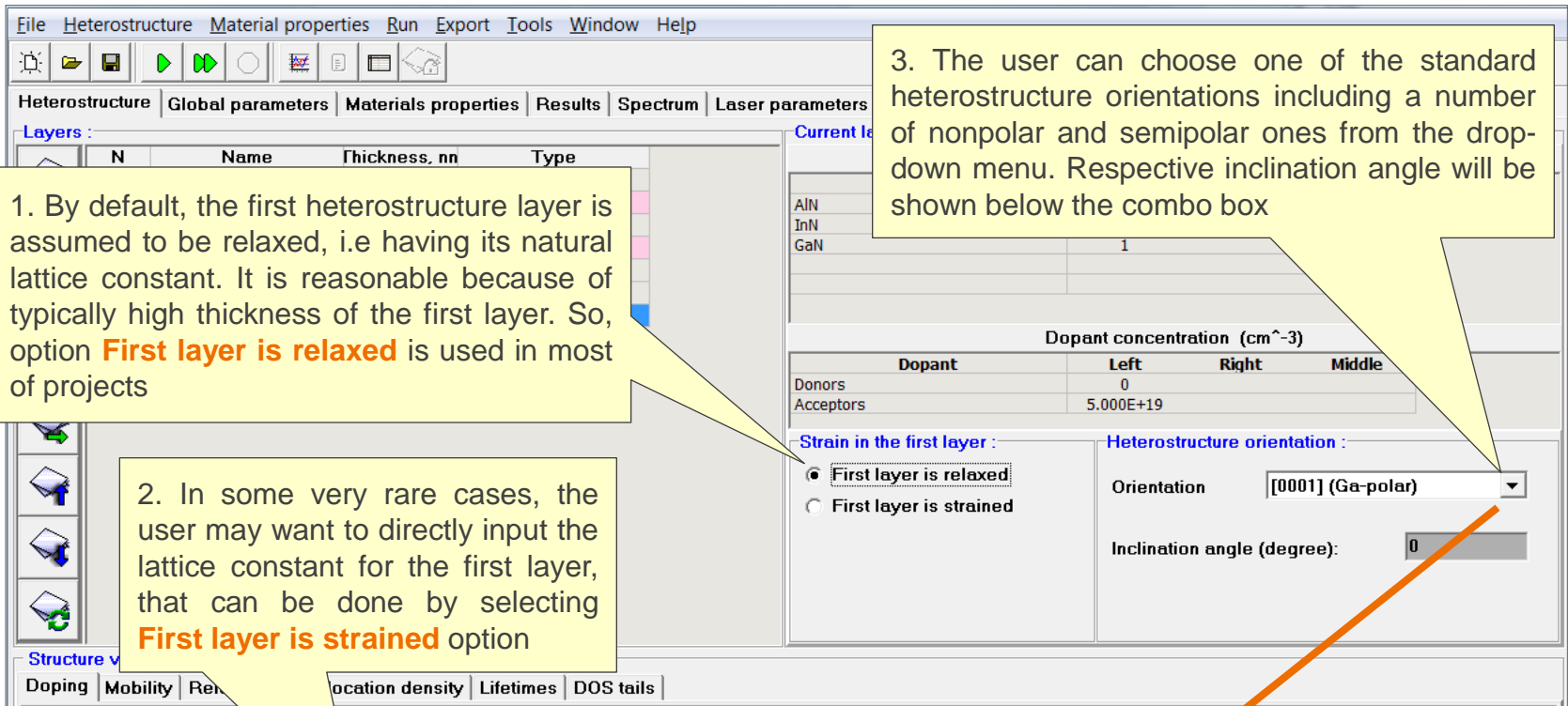
2. Plots in the bottom part of the window allows one to see how key input parameters are varied across the whole heterostructure. Note that in this plot second-order variation of parameters is shown as the linear one

Structure visualization

Doping | Mobility | Relaxation | Dislocation density | Lifetimes | DOS tails

Donors (1/cm<sup>3</sup>)  
 Acceptors (1/cm<sup>3</sup>)

## Step 3: Specification of polarity and lattice constant

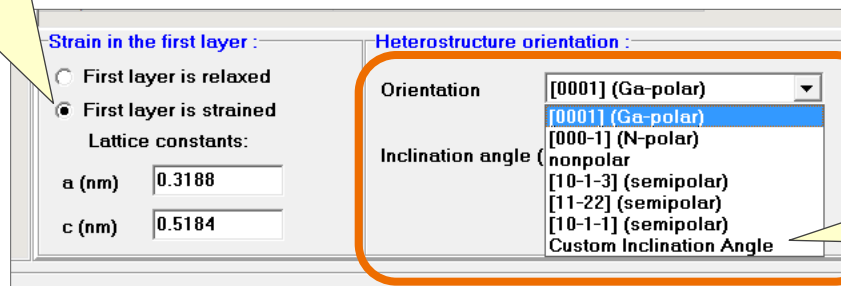


1. By default, the first heterostructure layer is assumed to be relaxed, i.e having its natural lattice constant. It is reasonable because of typically high thickness of the first layer. So, option **First layer is relaxed** is used in most of projects

2. In some very rare cases, the user may want to directly input the lattice constant for the first layer, that can be done by selecting **First layer is strained** option

3. The user can choose one of the standard heterostructure orientations including a number of nonpolar and semipolar ones from the drop-down menu. Respective inclination angle will be shown below the combo box

Dopant concentration (cm <sup>-3</sup> )			
Dopant	Left	Right	Middle
Donors	0		
Acceptors	5.000E+19		



**Strain in the first layer :**

First layer is relaxed

First layer is strained

**Lattice constants:**

a (nm) 0.3188

c (nm) 0.5184

**Heterostructure orientation :**

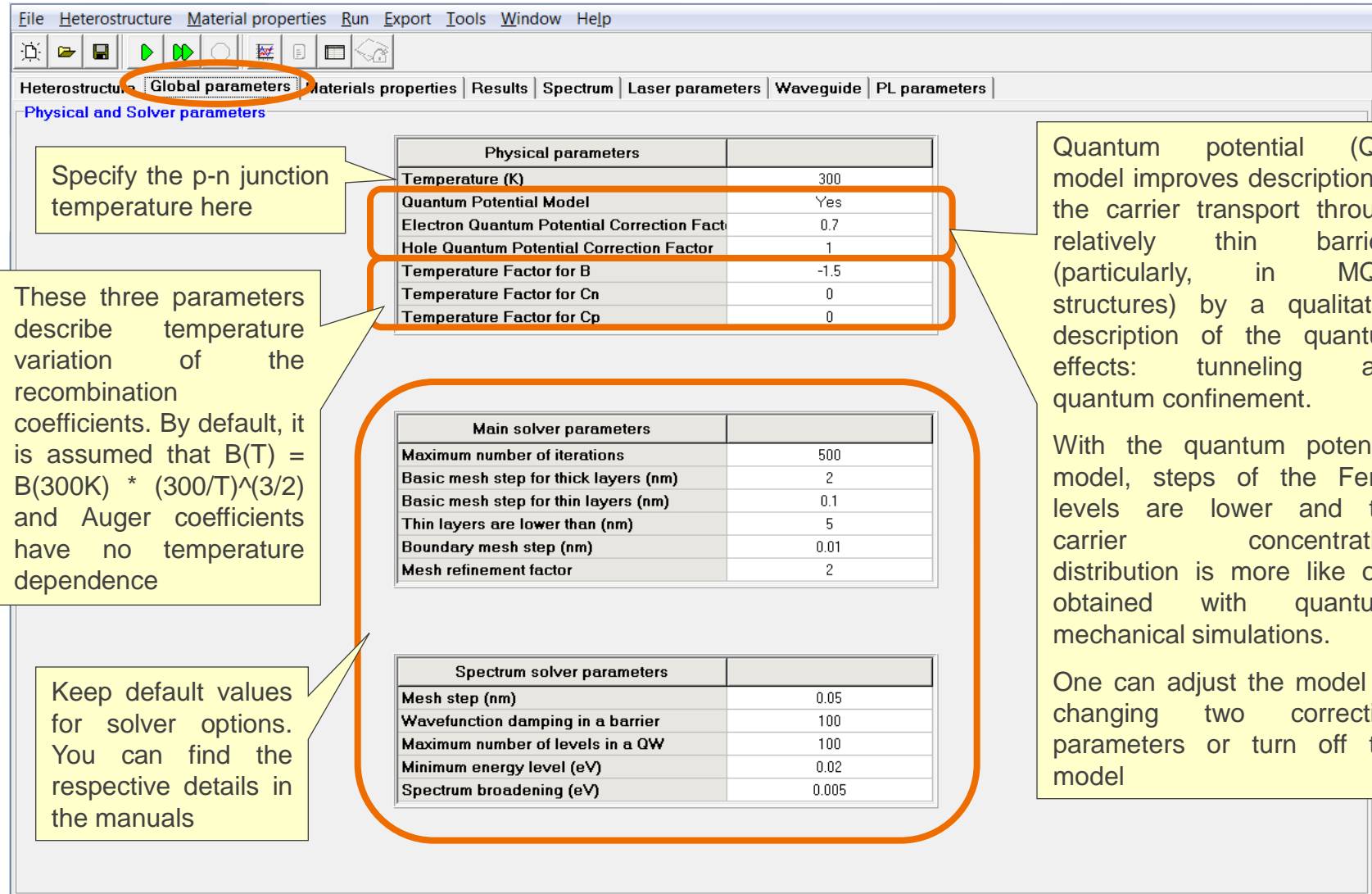
Orientation [0001] (Ga-polar)

Inclination angle ( )

- [0001] (Ga-polar)
- [000-1] (N-polar)
- nonpolar
- [10-1-3] (semipolar)
- [11-22] (semipolar)
- [10-1-1] (semipolar)
- Custom Inclination Angle

4. Choosing **Custom Inclination Angle** in the combo box allows one to specify a custom inclination angle in [0,180] range

## Step 3 (Continued): Temperature and solver options



File Heterostructure Material properties Run Export Tools Window Help

Heterostructure **Global parameters** Materials properties Results Spectrum Laser parameters Waveguide PL parameters

Physical and Solver parameters

Specify the p-n junction temperature here

Physical parameters	
Temperature (K)	300
Quantum Potential Model	Yes
Electron Quantum Potential Correction Factor	0.7
Hole Quantum Potential Correction Factor	1
Temperature Factor for B	-1.5
Temperature Factor for Cn	0
Temperature Factor for Cp	0

These three parameters describe temperature variation of the recombination coefficients. By default, it is assumed that  $B(T) = B(300K) * (300/T)^{(3/2)}$  and Auger coefficients have no temperature dependence

Main solver parameters	
Maximum number of iterations	500
Basic mesh step for thick layers (nm)	2
Basic mesh step for thin layers (nm)	0.1
Thin layers are lower than (nm)	5
Boundary mesh step (nm)	0.01
Mesh refinement factor	2

Keep default values for solver options. You can find the respective details in the manuals

Spectrum solver parameters	
Mesh step (nm)	0.05
Wavefunction damping in a barrier	100
Maximum number of levels in a QW	100
Minimum energy level (eV)	0.02
Spectrum broadening (eV)	0.005

Quantum potential (QP) model improves description of the carrier transport through relatively thin barriers (particularly, in MQW structures) by a qualitative description of the quantum effects: tunneling and quantum confinement.

With the quantum potential model, steps of the Fermi levels are lower and the carrier concentration distribution is more like one obtained with quantum-mechanical simulations.

One can adjust the model by changing two correction parameters or turn off the model

## Step 4: Running the simulation of the band diagram

Run calculations for a single bias

Run series calculations

The screenshot shows the main software window with a menu bar (File, Heterostructure, Materials properties, Run, Export, Tools, Window, Help) and a toolbar. The 'Layers' table is visible, and the 'Series Calculat...' dialog box is open over it.

N	Name	Thickness, nm	Type
1	n-GaN	500	AllnGaN
2	InGa <sub>N</sub> -QW	3	AllnGaN
3	n-GaN-barrier	12	AllnGaN
4	InGa <sub>N</sub> -QW	3	AllnGaN
5	n-GaN-barrier	12	AllnGaN
6	p-AlGa <sub>N</sub>	60	AllnGaN
7	p-GaN	500	AllnGaN

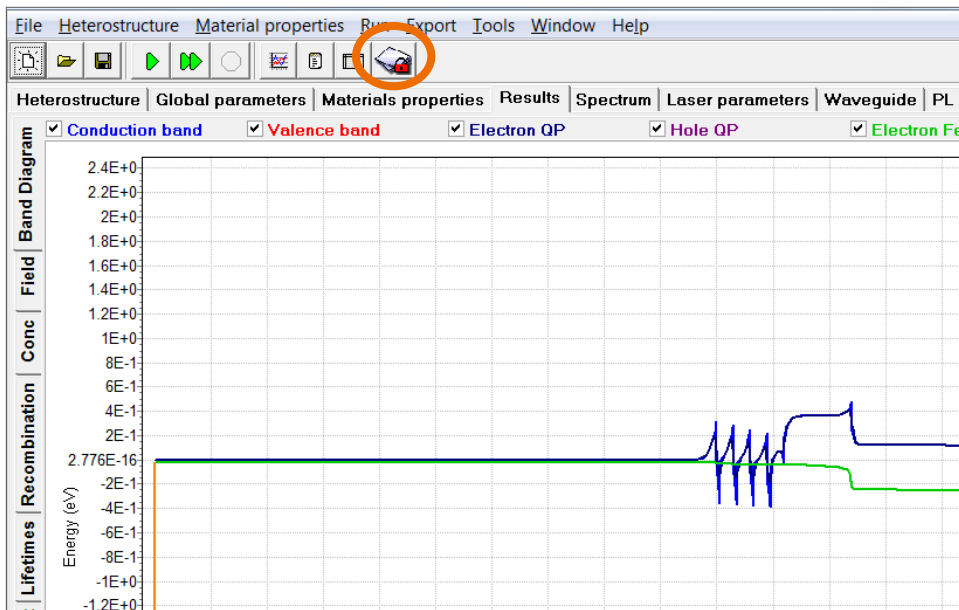
The 'Edit Bias' dialog box has a text input field labeled 'Bias (V)' containing the value '0'. There are 'OK' and 'Cancel' buttons at the bottom.

Enter the desired bias

This 'Edit Bias' dialog box is for series calculations. It contains three input fields: 'Start bias (V)' with '0', 'End bias (V)' with '0', and 'Number of intervals' with '0'. There are 'OK' and 'Cancel' buttons at the bottom.

The 'Run' and 'Cancel' buttons from the 'Series Calculat...' dialog box.

## Step 4 (Continued): Consistency of input data and simulation results, “locking” of the input data



In SiLENSe, all completed results are considered as a part of the project file and saved with it. To keep self-consistency between the input data and results, the project input data are “locked” as at least one result is computed.

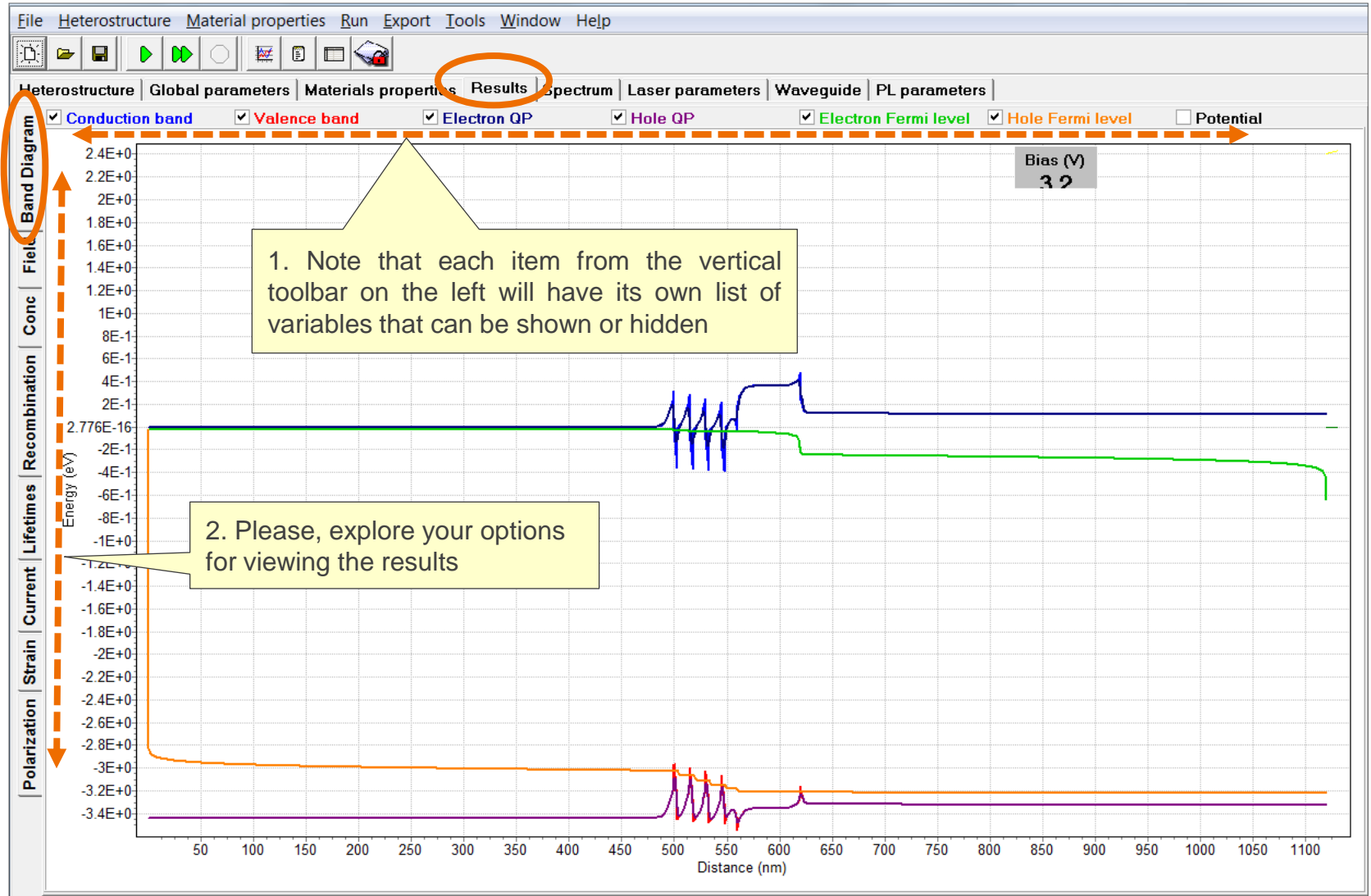
For “locked” project, most of the buttons for editing heterostructure are disabled. Edit Layer button is enabled, while most of the layer properties appear in read-only mode, that is shown by the grey color of the text fields.

The only properties one can change for “locked” project is the Layer name, the Active region flag, and the Usp parameter (since the latter two do not effect the band diagram simulation)

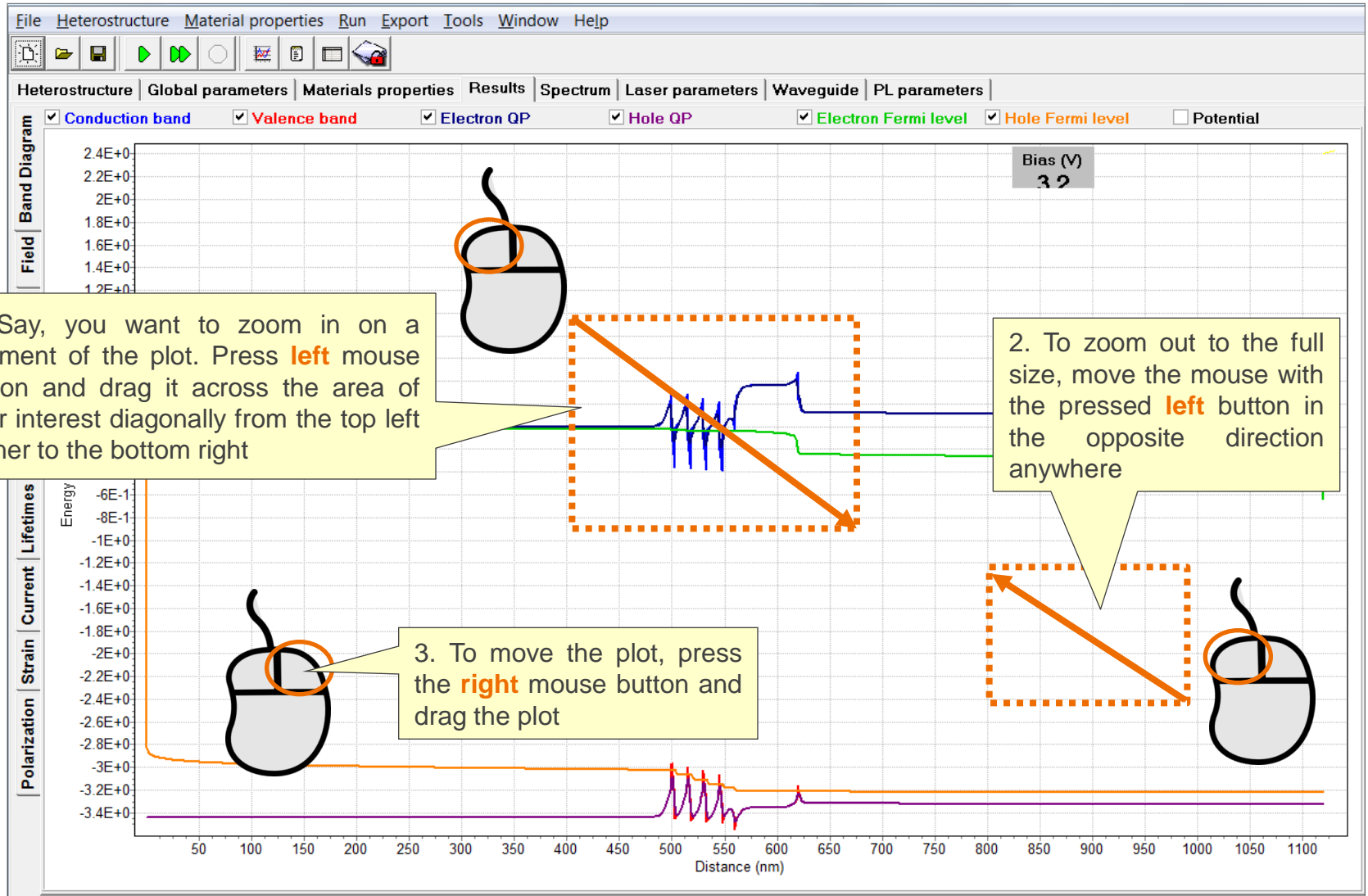
To be able to edit input data, one needs to previously clear all the results by **clicking the lock button** and thus unlock the editing.

These restrictions may look strange at the first glance, but they guarantee that simulation results stored in the project file are always consistent with the input data. So, you do not need to worry about remembering what parameters the results you see correspond to, you can just check them in the project file.

## Step 4 (Continued): Results tab



## Step 4 (Continued): Neat tricks with zooming and moving



## Step 4 (Continued): LED results

The screenshot displays the SiLENSe interface with the 'LED Results' window open. The main window shows a table of results for 11 different bias conditions. A callout box points to the 'Window->LED Results' menu option, stating: 'To view more results (including I-V curve, IQE, spectrum, etc.) you can either go to **Window->LED Results** or press this button'. Another callout points to the 'Export to SpeCLED' button, stating: 'This button computes peak wavelengths for all the listed biases and fills the last column'. A third callout points to the 'Show I-V characteristic' button, stating: 'Show I-V characteristic button provides  $j(U)$  and  $IQE(j)$  plots'. The 'I-V characteristic' window shows a plot of Current density (A/cm<sup>2</sup>) versus Bias (V) on a semi-log scale. The 'LED Results' table includes columns for various parameters, with the 'Peak WL' column highlighted in blue.

N	Bias	J	J rad	J nrad	J SRH	J Auger	J n	J p	J n right	J p left	IQE	IQE QW	Inj eff	m	Peak WL
1	2.5	3.071E-06	7.000E-08	3.001E-06	3.000E-06	1.003E-09	3.071E-06	3.071E-06	2.877E-26	1.092E-29	0.0228	0.0228	0.6482		
2	2.6	4.713E-06	3.129E-06	4.400E-05	4.396E-05	4.195E-08	4.713E-05	4.713E-05	2.576E-12	3.209E-11	0.0664	0.0663	0.5929	1.4164	
3	2.7	0.0001	0.0001	0.0007	0.0007	1.872E-06	0.0008	0.0008	1.401E-10	1.448E-09	0.1701	0.1697	0.6714	1.3643	
4	2.8	0.01	0.0056	0.0130	0.0129	9.964E-05	0.0185	0.0185	7.184E-09	4.393E-08	0.3005	0.2999	0.8511	1.2320	
5	2.9	0.4	0.1990	0.2722	0.2658	0.0064	0.4711	0.4711	3.590E-07	1.013E-06	0.4223	0.4214	0.9312	1.1957	
6	3	8	4.3827	0.1990	0.2658	0.0064	0.4711	0.4711	3.590E-07	1.013E-06	0.4223	0.4214	0.9312	1.1957	
7	3.1	70	38.4757	0.1990	0.2658	0.0064	0.4711	0.4711	3.590E-07	1.013E-06	0.4223	0.4214	0.9312	1.1957	
8	3.2	200	153.4093	0.1990	0.2658	0.0064	0.4711	0.4711	3.590E-07	1.013E-06	0.4223	0.4214	0.9312	1.1957	
9	3.3	500	360.5123	0.1990	0.2658	0.0064	0.4711	0.4711	3.590E-07	1.013E-06	0.4223	0.4214	0.9312	1.1957	
10	3.4	1000	658.4856	0.1990	0.2658	0.0064	0.4711	0.4711	3.590E-07	1.013E-06	0.4223	0.4214	0.9312	1.1957	
11	3.5	2000	1071.915	0.1990	0.2658	0.0064	0.4711	0.4711	3.590E-07	1.013E-06	0.4223	0.4214	0.9312	1.1957	



## Step 4 (Continued): More LED results

There are several ways to export the computed results in ASCII format, try the icons below and the **Export** section of the menu

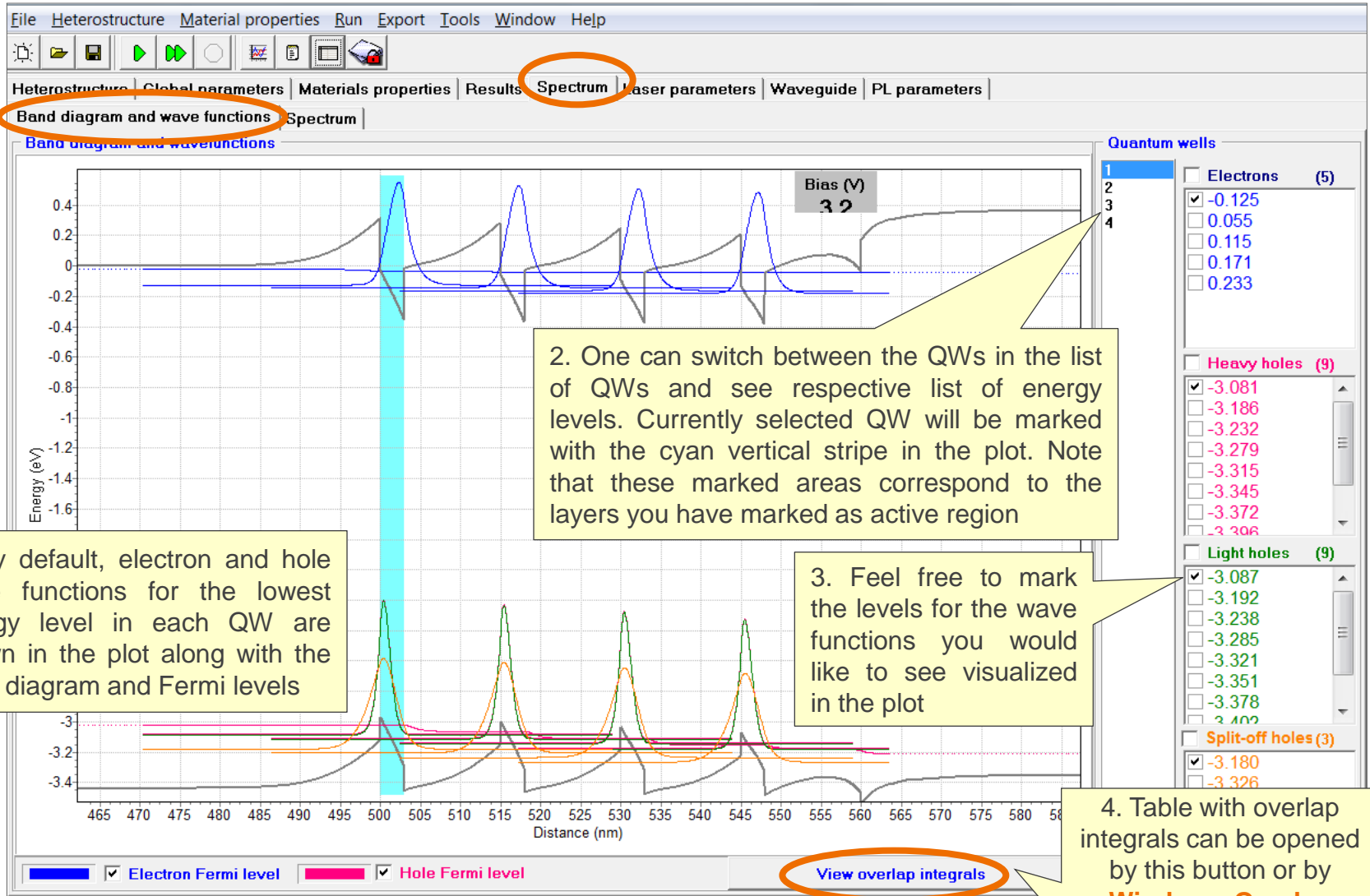
**Export to SpeCLED** button starts export of the results for its further using by SpeCLED (discussed below in details)

The screenshot shows the 'LED Results' window with a table of 11 rows and 16 columns. The first row is highlighted in blue. The toolbar includes an 'Export to SpeCLED' button. A 'Close' button is visible in the bottom right corner.

N	Bias	J	J rad	Jnrad	J SRH	J Auger	J n	J p	Jn right	Jp left	IQE	IQE QW	Inj eff	m	Peak WL
<input checked="" type="checkbox"/>	1	2.5	3.071E-06	7.000E-08	0.001E-06	3.000E-06	1.003E-09	3.071E-06	3.071E-06	2.877E-26	1.092E-29	0.0228	0.0228	0.6482	
<input checked="" type="checkbox"/>	2	2.6	4.713E-05	3.129E-06	0.001E-05	4.396E-05	4.195E-08	4.713E-05	4.713E-05	2.576E-12	3.209E-11	0.0664	0.0663	0.5929	1.4164
<input checked="" type="checkbox"/>	3	2.7	0.0008	0.0001	0.0007	1.872E-06	0.0008	0.0008	0.0008	1.401E-10	1.448E-09	0.1701	0.1697	0.6714	1.3643
<input checked="" type="checkbox"/>	4	2.8	0.0185	0.0056	0.0129	9.964E-05	0.0185	0.0185	7.184E-09	4.393E-08	0.3005	0.2999	0.8511	1.2320	
<input checked="" type="checkbox"/>	5	2.9	0.4711	0.1990	0.2658	0.0064	0.4711	0.4711	3.590E-07	1.013E-06	0.4223	0.4214	0.9312	1.1957	
<input checked="" type="checkbox"/>	6	3	8.4021	4.3827	3.6067	0.4126	8.4021	8.4021	1.376E-05	2.080E-05	0.5216	0.5202	0.9662	1.3426	
<input checked="" type="checkbox"/>	7	3.1	70.2334	38.4757	3.9613	8.7955	70.2330	70.2329	0.0005	0.0004	0.5478	0.5453	0.9704	1.8217	
<input checked="" type="checkbox"/>	8	3.2	286.0739	153.4093	4.112	59.7364	286.0701	286.0607	0.0132	0.0038	0.5363	0.5320	0.9686	2.7543	
<input checked="" type="checkbox"/>	9	3.3	698.3882	360.5123	4.36	190.3475	698.3679	698.0184	0.3698	0.0203	0.5162	0.5100	0.9662	4.3340	
<input checked="" type="checkbox"/>	10	3.4	1336.5880	658.4858	4.6	424.3949	1336.5080	1328.1730	8.4159	0.0807	0.4927	0.4844	0.9554	5.9593	
<input checked="" type="checkbox"/>	11	3.5	2410.0070	1071.9150	4.9	807.7733	2409.6980	2291.0500	118.9566	0.3090	0.4448	0.4351	0.8939	6.5617	

To compute wave functions and **spectrum**, select the row in the table that contains the desired bias (it will get highlighted blue) and press the button that **looks like spectrum**. Once the computations are complete, **Spectrum** tab is opened, see the next slide

## Step 5: Energy levels, wave functions, spectrum



Spectrum

Band diagram and wave functions

2. One can switch between the QWs in the list of QWs and see respective list of energy levels. Currently selected QW will be marked with the cyan vertical stripe in the plot. Note that these marked areas correspond to the layers you have marked as active region

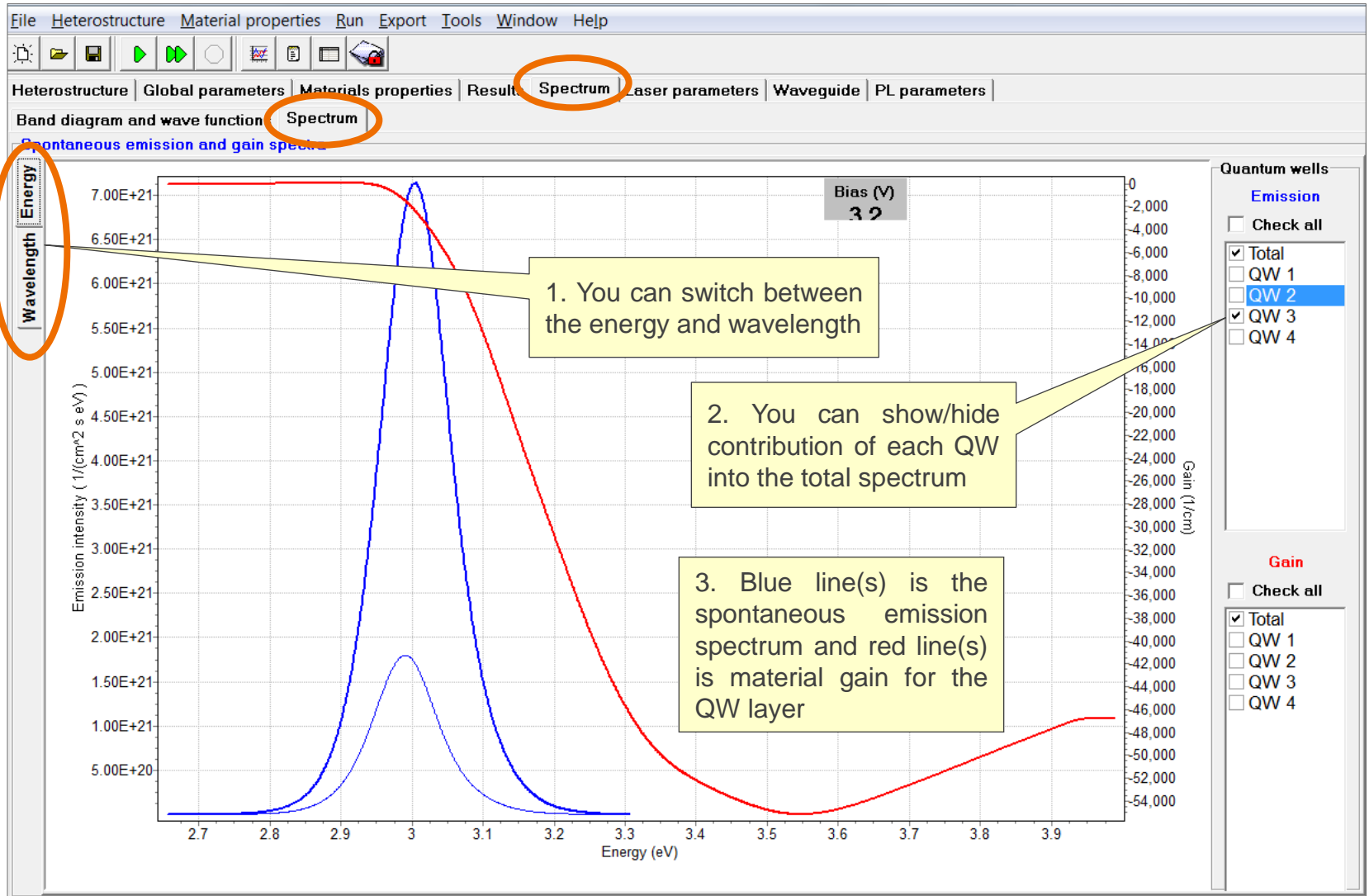
1. By default, electron and hole wave functions for the lowest energy level in each QW are shown in the plot along with the band diagram and Fermi levels

3. Feel free to mark the levels for the wave functions you would like to see visualized in the plot

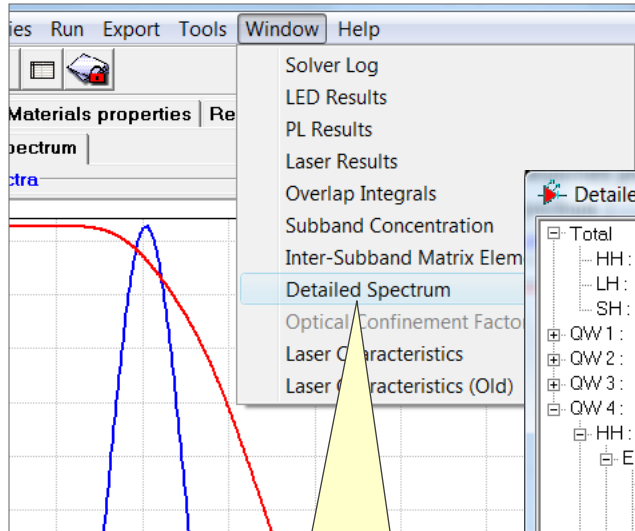
4. Table with overlap integrals can be opened by this button or by **Window->Overlap Integrals** menu item

View overlap integrals

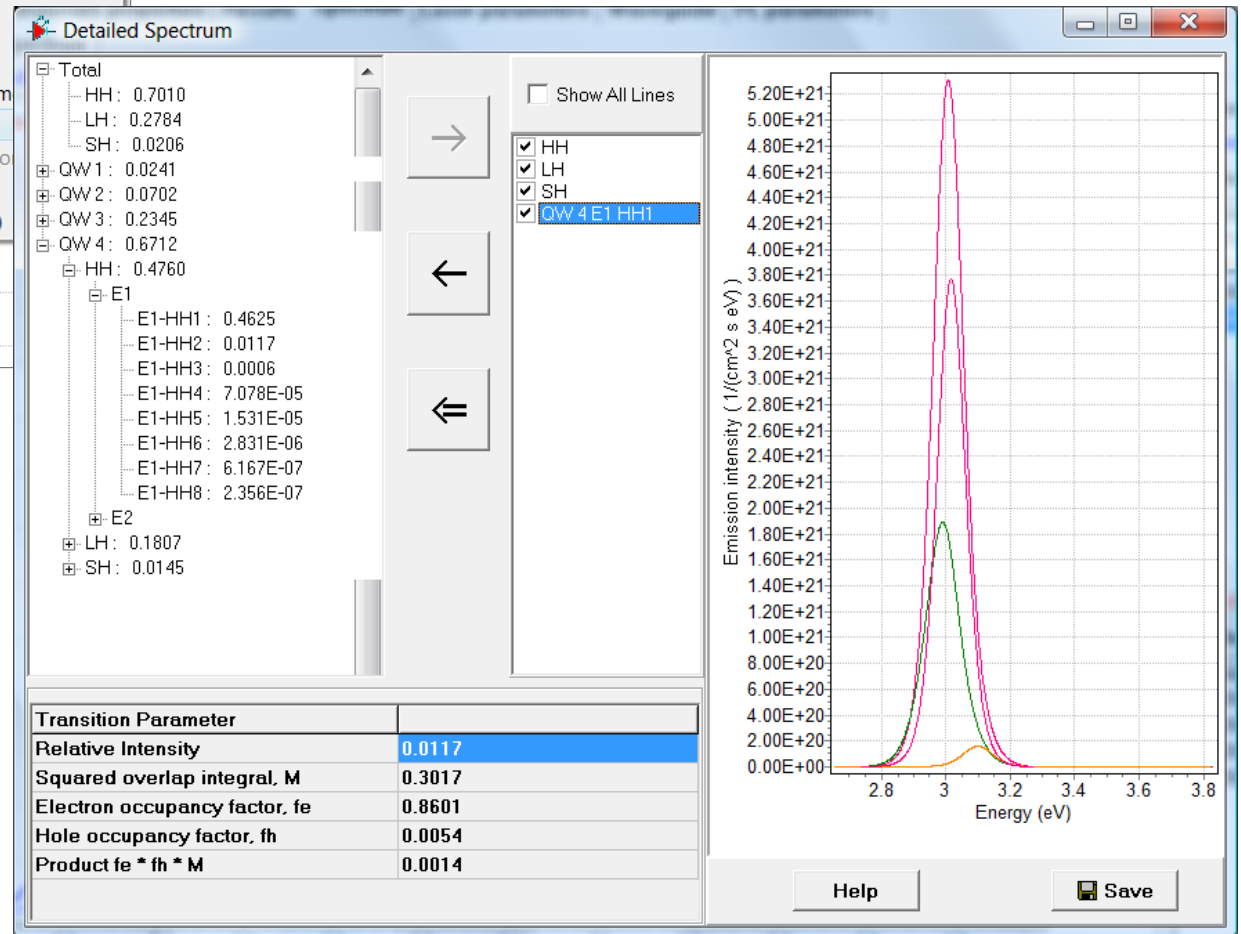
## Step 5 (Continued): Emission and gain spectrum



## Step 5 (Continued): Detailed spectrum



**Window -> Detailed Spectrum** menu item opens the window with complete information on spectrum resolved by QW and energy level



## Step 6: Preparing input data for SpeCLED

The screenshot shows the SiLENSe 4.00 Laser Edition interface. A 'List of Results' dialog box is open, displaying a table of simulation results. The table has columns for N, Bias, J, J rad, J nrad, J n, J p, J n right, J p left, and IQE. All rows are selected with checkboxes. A callout points to the 'Export to SpeCLED' button, and another callout points to the selected rows. A third callout provides a list of bias values used in the simulation.

N	Bias	J	J rad	J nrad	J n	J p	J n right	J p left	IQE
1	2.5	1.978E-06	4.436E-07	1.535E-06	1.978E-06	1.978E-06	1.978E-14	7.383E-16	0.2242
2	2.6	3.405E-05	7.757E-06	2.629E-05	3.405E-05	3.405E-05	3.405E-14	1.957E-14	0.2278
3	2.7	0.0006	0.0001	0.0004	0.0006	0.0006	6.000E-14	2.999E-13	0.2099
4	2.8	0.0077	0.0017	0.0060	0.0077	0.0077	7.000E-14	3.999E-13	0.1999
5	2.9	0.0623	0.0170	0.0453	0.0623	0.0623	6.000E-14	4.999E-13	0.1899
6	3	0.2422	0.0802	0.1620	0.2422	0.2422	2.400E-13	1.999E-12	0.1799
7	3.1	0.6544	0.2468	0.4076	0.6544	0.6544	6.500E-13	6.999E-12	0.1699
8	3.2	1.5632	0.6463	0.9168	1.5632	1.5631	3.581E-05	6.848E-08	0.4135
9	3.3	3.9022	1.735	2.167	3.9022	3.902	0.0002	1.429E-06	0.4446
10	3.4	9.6874	4.5245	5.1619	9.6874	9.6865	0.0009	1.971E-05	0.4671
11	3.5	27.609	11.414	14.414	27.609	27.609	0.0027	2.761E-04	0.4799

1. Run series computations to cover typical range of the local bias variation. The step may be high at low bias, and has to be lower for high bias. Something like this: U= 0.5, 1.0, 1.5, 2.5, 2.6, 2.7, 2.8, 2.9, 3.0, 3.05, 3.1, 3.15, ..., 3.95, 4 V.

2. Select the results you want to export for SpeCLED (usually, all the results)

3. Press **Export to SpeCLED** button which opens a modal window (next page)

## Step 6 (Continued): Preparing input data for SpeCLED

The screenshot shows the SiLENSe 4.00 Laser Edition software interface. The 'List of Results' table is visible, showing parameters for various simulation runs. The 'Export to SpeCLED' dialog box is open, showing a list of bias voltages from 2.5 to 3.9 V. The 'RUN spectra' button is highlighted with a green checkmark, and the 'Export' button is also highlighted.

N	Bias	J	J rad	J nrad	J n	J p	J n right	J p left	IQE
1	2.5	1.978E-06	4.436E-07	1.535E-06	1.978E-06	1.978E-06	6.710E-14	7.383E-16	0.2242
2	2.6	3.405E-05	7.757E-06	2.629E-05	3.405E-05	3.405E-05	4.700E-12	1.957E-14	0.2278
3	2.7	0.0006	0.0001	0.0004	0.0006	0.0006	2.371E-10	2.142E-13	0.2099
4	2.8	0.0077	0.0017	0.0060	0.0077	0.0077	9.306E-09	1.890E-12	0.2176
5	2.9	0.0623	0.0170	0.0453	0.0623	0.0623	1.982E-07	1.884E-11	0.2731
6	3	0.2422	0.0802	0.1620	0.2422	0.2422	1.679E-06	2.475E-10	0.3312
7	3.1	0.6544	0.2468	0.4076	0.6544	0.6544	8.257E-06	8.286E-09	0.3772
8	3.2								
9	3.3								
10	3.4								
11	3.5								

3. To run **SpeCLED** simulations with account for self-heating effects, one needs to repeat the described steps for a certain temperature range with a step of 10-50K (for instance,  $T = 300, 320, 340, 360, 380, 400, 420, 440, 460, 480, 500$  K)

1. Press **RUN Spectra** button. The program will automatically compute emission spectrum for all results

2. Press **Export** button (it appears enabled when spectrum computations are complete) and save data to an \*.sct file used for data exchange between SiLENSe and SpeCLED



**End of Tutorial 1**

# Tutorial 2

SiLENSe 5.10 & SiLENSe Laser Edition 5.10



**Using SiLENSe for Modeling of Lasers:  
Simulation of InGaN MQW UV laser diode**



## Features specific to laser diodes

File Heterostructure Material properties Run Export Tools Window Help

Heterostructure | Global parameters | Materials properties | Results | Spectrum | **Laser parameters** | **Waveguide** | PL parameters

Layers :

N	Name	Thickness, nm	Type
1	n-GaN	700	AllInGaN
2	n-InGaN	100	AllInGaN
3	n-AlGaN-emitter	800	AllInGaN
4	n-AlGaN-WG		
5 x 4	n-InGaN		
6 x 4	n-InAlGaN-barrier		
7	n-InGaN		
8	p-AlGaN-BL		
9	p-AlGaN-WG		
10	p-AlGaN-emitter		
11	p-GaN-contact		

Current injection parameters :

Composition	Left	Right	Middle
	0		
	0		
	1		

Carrier concentration (cm<sup>-3</sup>)

	Left	Right	Middle
DOE+18			
10			

Structure orientation :

Orientation: [0001] (Ga-polar)

Incidence angle (degree): 0

This tutorial describes simulation of laser diodes. Most of the input data specification is similar to LED simulation discussed in the previous tutorial. Let us skip options common for simulation of LEDs and LDs and focus on features specific to laser diodes:

1. Computation of waveguide modes
2. Computation of threshold characteristics

Options specific for simulation of LDs are located under two tabs: **Laser parameters** and **Waveguide**

Structure visualization

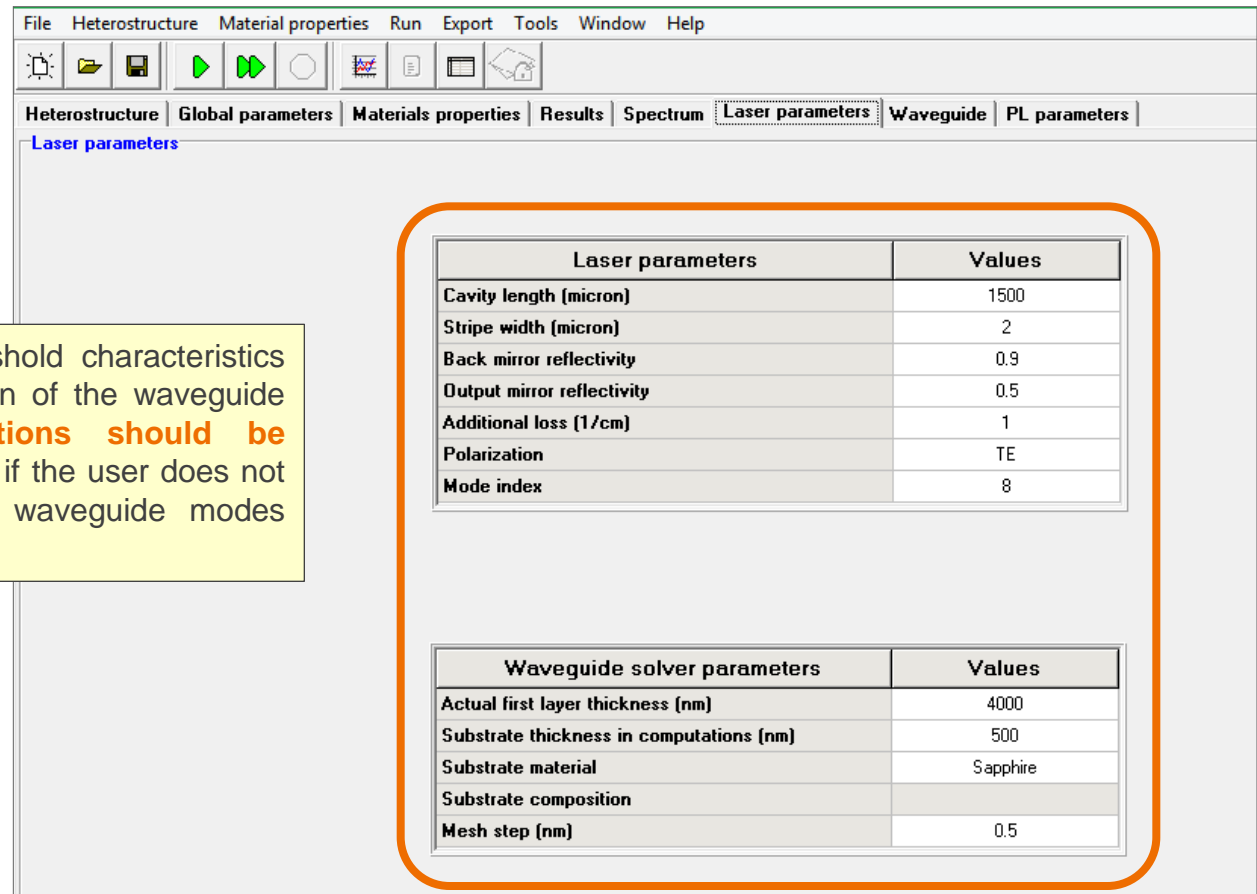
Doping | Mobility | Relaxation | Dislocation density | Lifetimes | DOS tails

Legend:

- Donors (1/cm<sup>3</sup>)
- Acceptors (1/cm<sup>3</sup>)

## Specifying options specific for LDs

Computation of the waveguide modes is done independently from computation of the band diagram. However, it also uses the **Heterostructure** and **Materials properties** input data. Laser parameters tab contains a number of additional input data for simulation of LDs. They are split into two sections specific to computation of the waveguide modes and to computation of the threshold characteristics, respectively.



Laser parameters	Values
Cavity length (micron)	1500
Stripe width (micron)	2
Back mirror reflectivity	0.9
Output mirror reflectivity	0.5
Additional loss (1/cm)	1
Polarization	TE
Mode index	8

Waveguide solver parameters	Values
Actual first layer thickness (nm)	4000
Substrate thickness in computations (nm)	500
Substrate material	Sapphire
Substrate composition	
Mesh step (nm)	0.5

Computation of the threshold characteristics implicitly calls computation of the waveguide modes, so **both sections should be specified correctly** even if the user does not run computation of the waveguide modes directly!

## Specifying parameters for computation of waveguide modes

The screenshot shows the software interface with the 'Laser parameters' and 'Waveguide solver parameters' tabs selected. The 'Laser parameters' table is as follows:

Laser parameters	Values
Cavity length (micron)	1500
Stripe width (micron)	2
Back mirror reflectivity	0.9
Output mirror reflectivity	0.5
Additional loss (1/cm)	1
Propagation mode	TE
Order	8

The 'Waveguide solver parameters' table is as follows:

Waveguide solver parameters	Values
Actual first layer thickness (nm)	4000
Substrate thickness in computations (nm)	500
Substrate material	Sapphire
Substrate composition	
Mesh step (nm)	0.5

Unlike the carrier transport in LEDs, waveguide modes may depend on the substrate. As you might remember, some reduced thickness is specified for the first and last layers at the stage of the heterostructure modeling, because remote parts of homogeneous bulk n-region do not affect p-n junction and the light generation. However, whole **first layer and even substrate may be important for computation of the waveguide modes**

Actual first layer thickness allow to specify real thickness of the first layer. (Not the reduced one that was used in the heterostructure tab)

Substrate usually has a thickness ~100 times higher than the heterostructure. However, confined modes exponentially decay in the substrate. Substrate thickness in computations should be at least 2-3 decay lengths

To choose the substrate material, click in the respective input field. A drop-down list will appear. If the material you choose is an allow, specification of composition will be required

This close-up shows the 'Substrate material' dropdown menu with the following options:

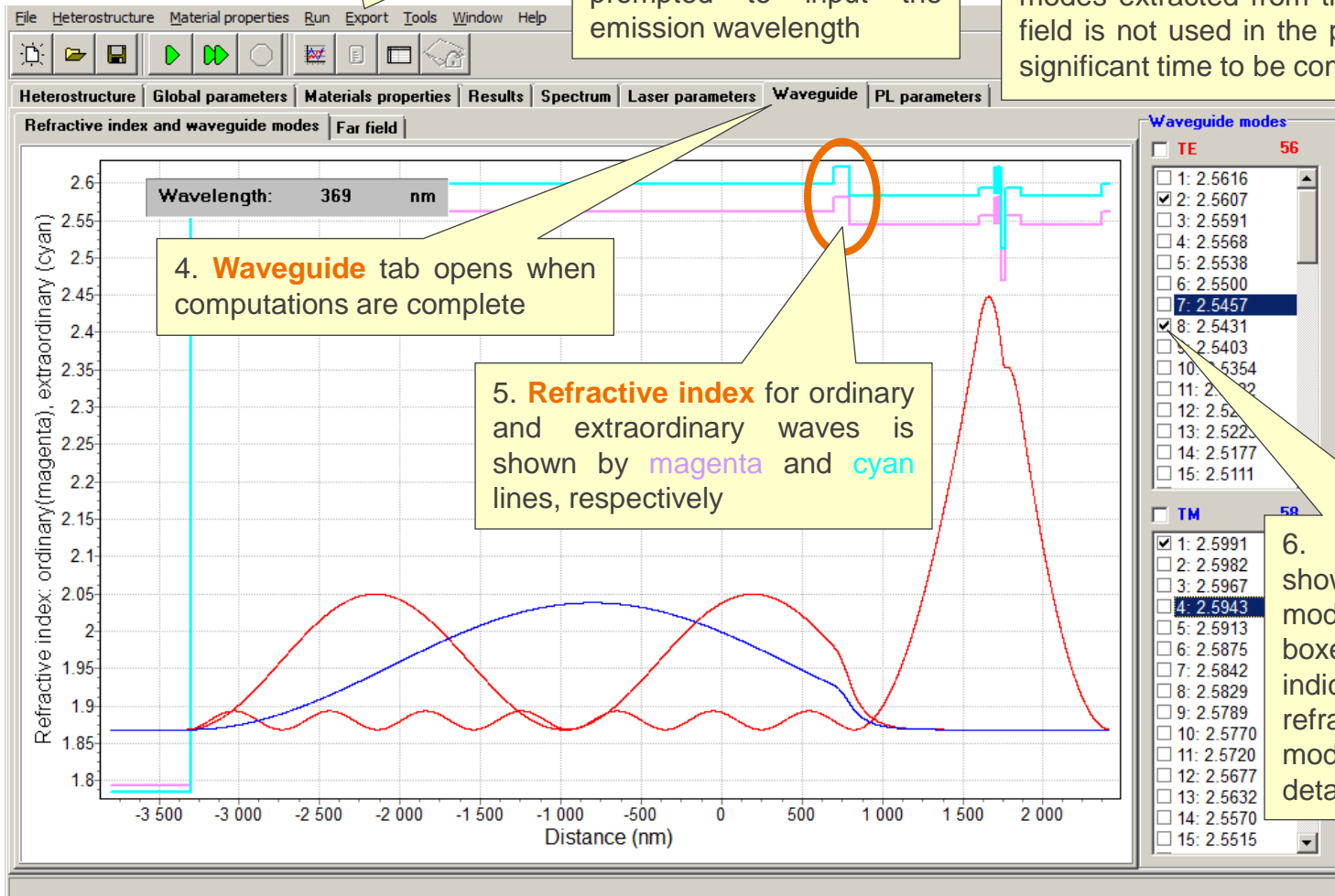
- Sapphire
- CdMgZnO
- AlN
- InN
- GaN
- ZnO
- MgO
- CdO
- Sapphire

## Computation of waveguide modes

1. Use **Run -> Waveguide Modes** to launch computations from the menu

2. A modal window appears where the user is prompted to input the emission wavelength

3. Next, the user is asked if he/she wants to compute far-field distribution of the modes extracted from the laser edge (far-field is not used in the program, but takes significant time to be computed)

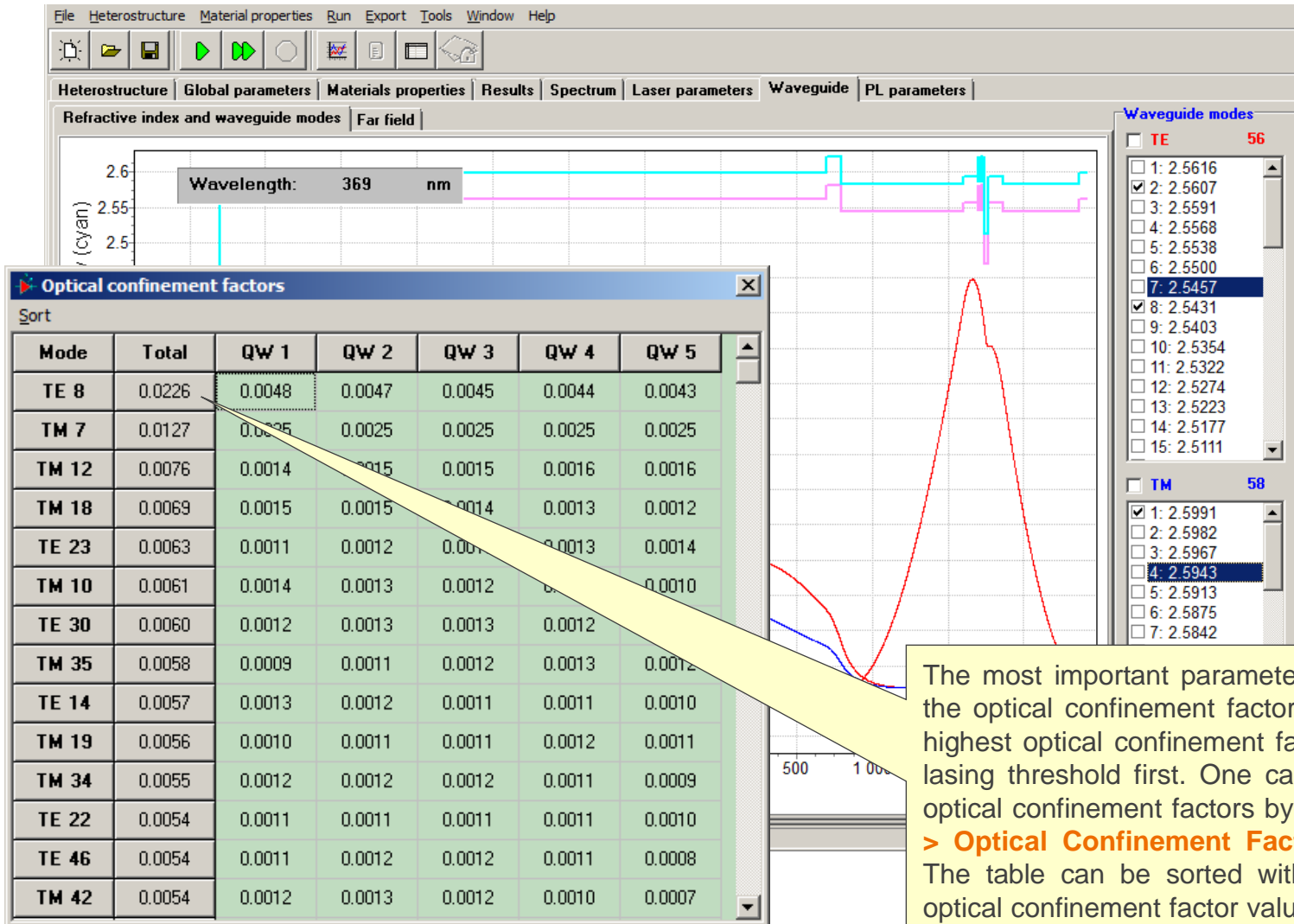


4. **Waveguide** tab opens when computations are complete

5. **Refractive index** for ordinary and extraordinary waves is shown by **magenta** and **cyan** lines, respectively

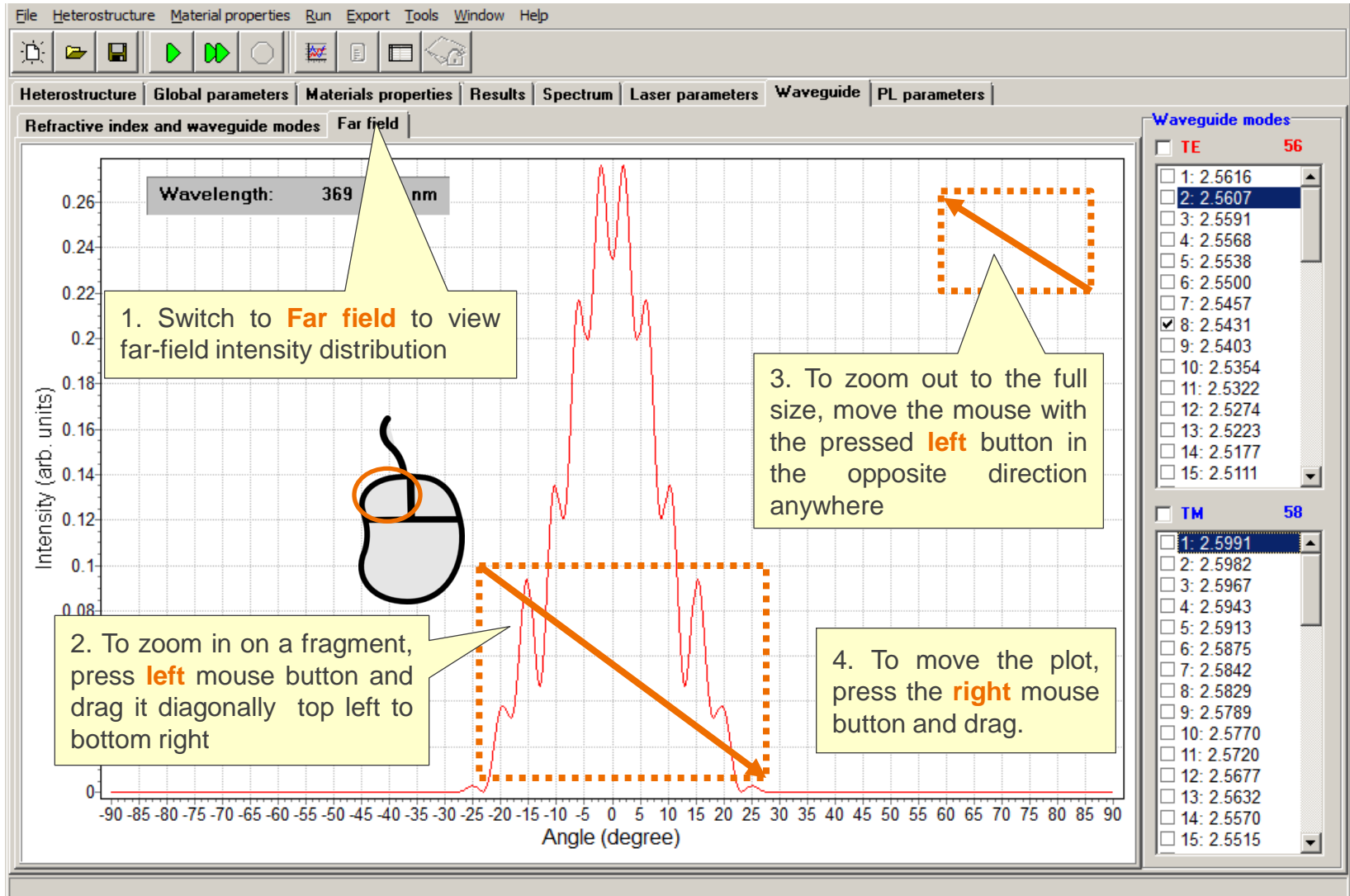
6. The user can show/hide individual modes by the check boxes. The value indicates "effective refractive index" of the mode (see manual for details)

## Viewing the confinement factors



The most important parameter of the mode is the optical confinement factor. The mode with highest optical confinement factor reaches the lasing threshold first. One can see a table of optical confinement factors by using **Window -> Optical Confinement Factors** menu item. The table can be sorted with respect to the optical confinement factor value to help find the mode which will provide laser generation

## Viewing the far-field intensity distribution



## Parameters for computation of threshold characteristics and laser output power beyond the threshold

1. Go back to **Laser parameters** tab

5. Computations of the threshold characteristics are done with respect to a certain waveguide mode. You need to specify the **polarization (TE or TM)** and **Mode index** of the mode having highest optical confinement factor (see before how to find such a mode)

6. Solver settings for self-consistent calculation of the stimulated recombination rate.

7. Options for using imported data on gain instead of ones taken from spectrum calculation. Rarely used option.

2. Specify **dimensions** of the cavity and **reflectivities** of mirrors

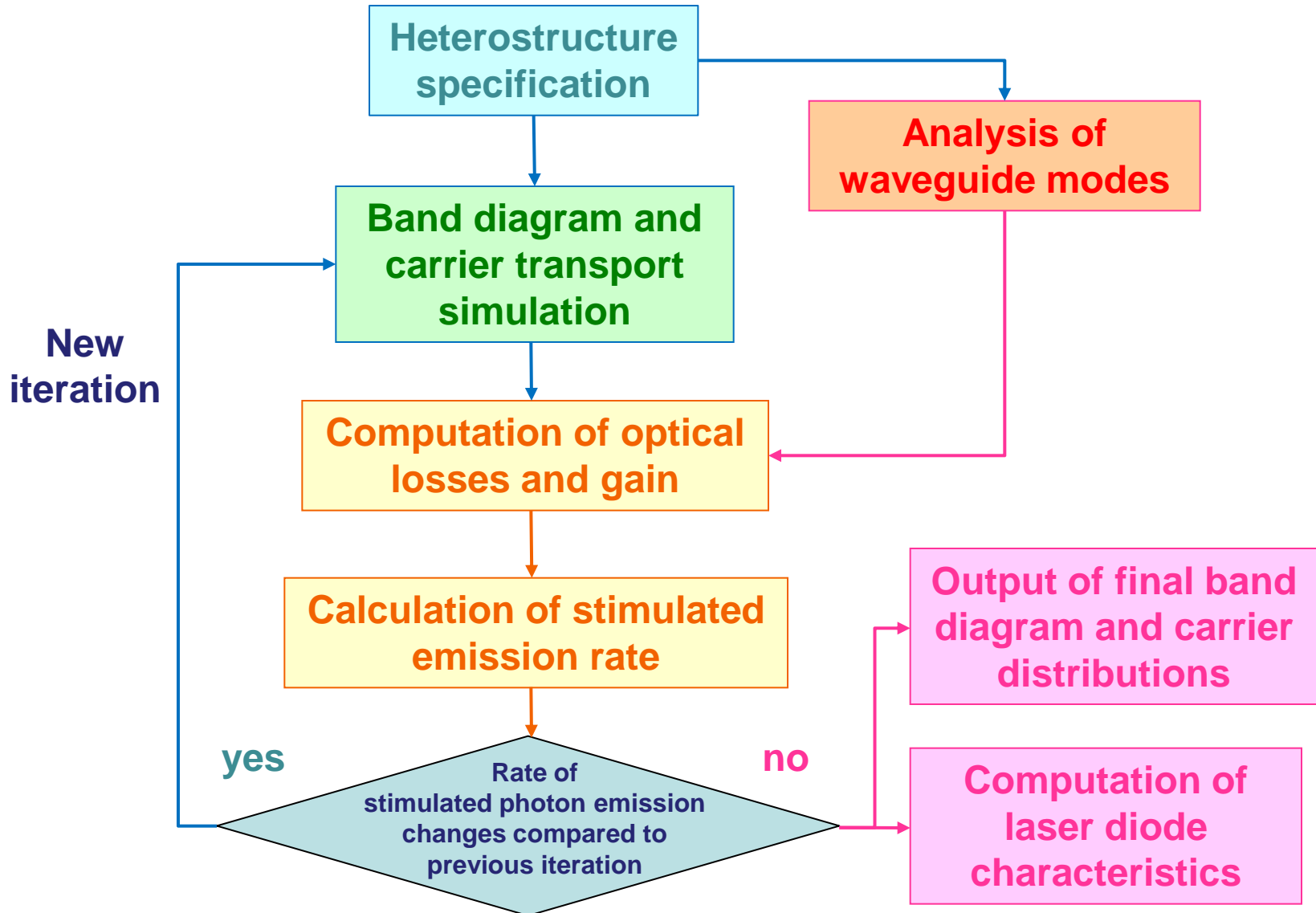
4. Software automatically computes optical loss due to free-carrier absorption and loss at the mirrors. **Additional loss** is a fitting parameter added to the total optical loss

Laser parameters		Values
Cavity length (micron)		1500
Stripe width (micron)		2
Back mirror reflectivity		0.9
Output mirror reflectivity		0.5
Additional loss (1/cm)		1
Polarization		TE
Mode index		8
Initial Step (in units of $\mu\text{rad}$ )		0.05
Gain Fitting Accuracy (1/cm)		0.1
Use Imported Gain Data		No
Peak Gain vs Current Density Function		
Peak Gain Wavelength vs Current Density Function		
Use Absorption From Material Data		No

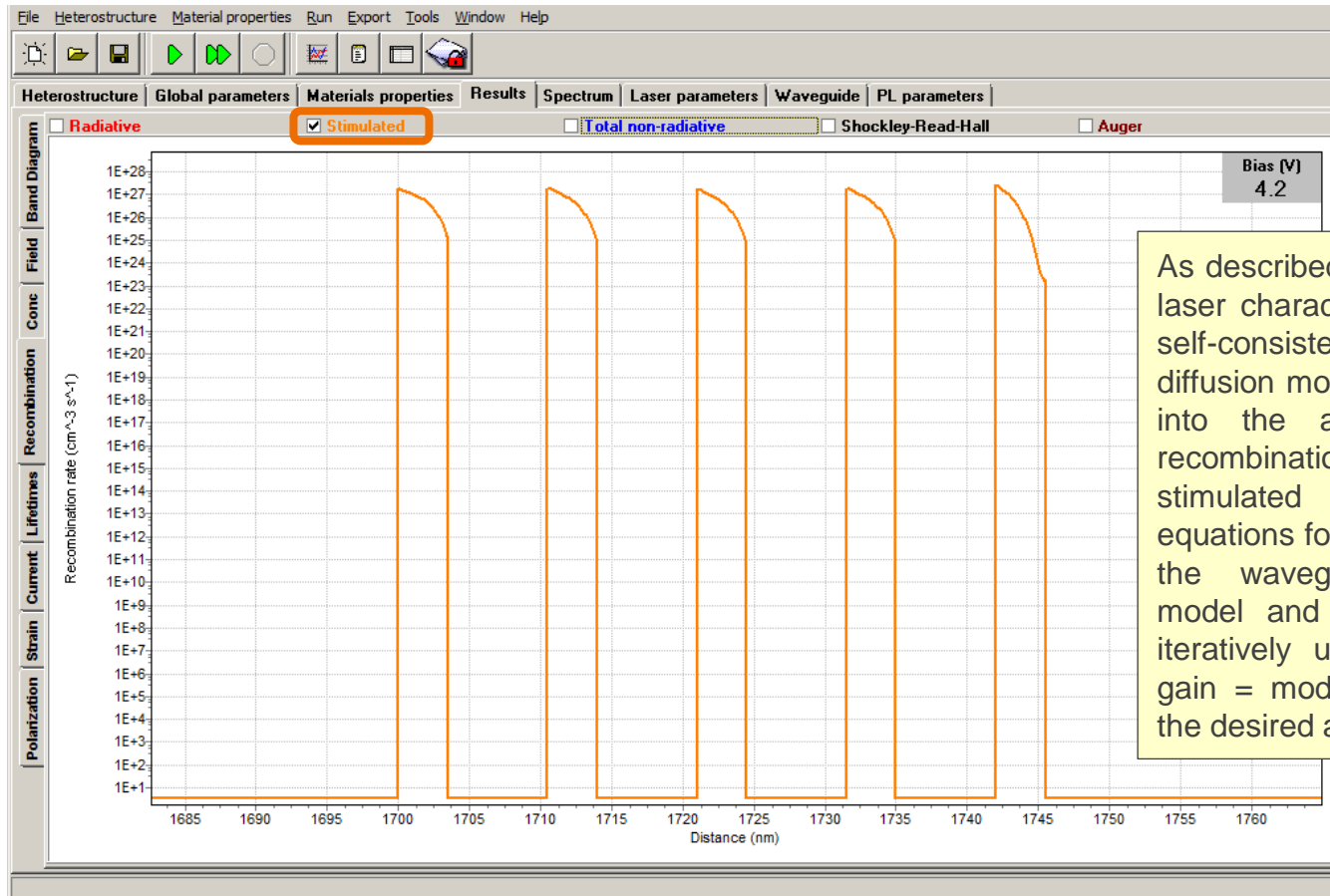
Waveguide solver parameters		Values
Actual first layer thickness (nm)		4000
Substrate thickness in computations (nm)		500
Substrate material		Sapphire
Substrate composition		
Mesh step (nm)		0.5

## Computation flow in self-consistent laser model





## Computation of laser characteristics

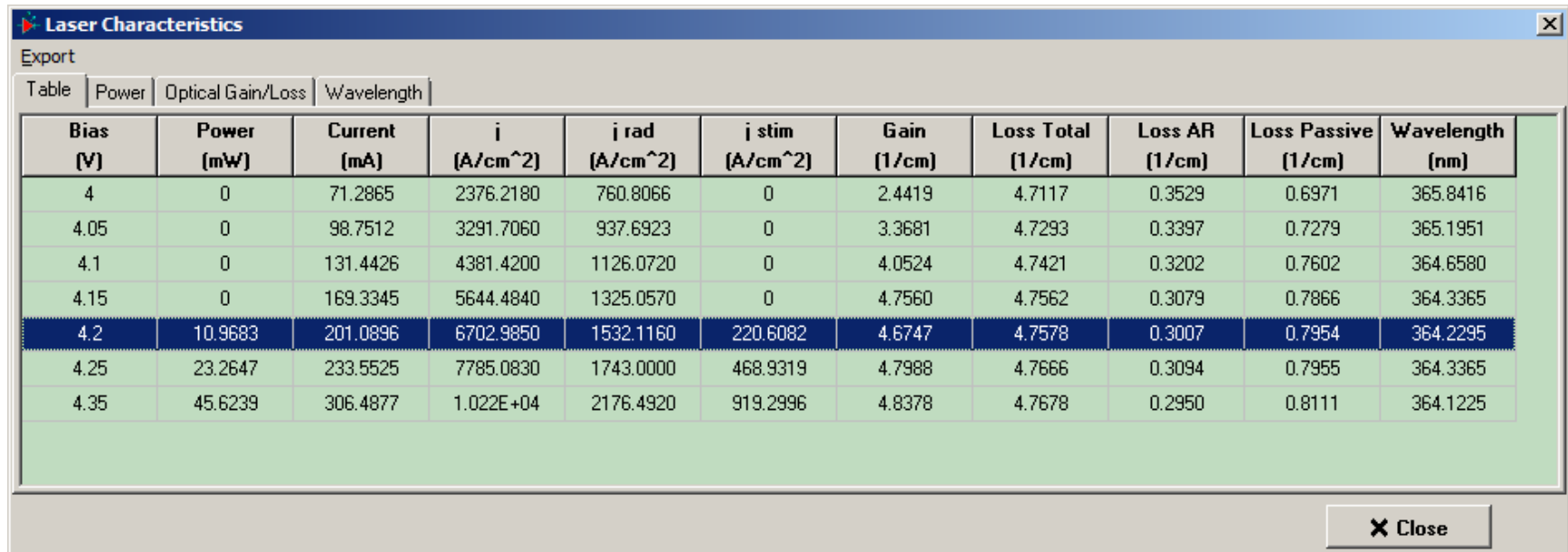


As described in the previous slide, the laser characteristics are computed by self-consistent solution of the drift-diffusion model for the carrier injection into the active region and their recombination there (including stimulated recombination) and rate equations for the number of photons in the waveguide. So, drift-diffusion model and laser model are solved iteratively until the condition “modal gain = modal losses” is fulfilled with the desired accuracy.

Use **Run -> Single Calculation With Laser** or **Run -> Single Calculation With Laser** menu item and specify a bias or a set of biases similarly it is done for LED calculations (see the previous tutorial).

Drift-diffusion calculations look very similar to LED calculation. The only difference is that stimulated recombination is accounted for in the QW layers.

## Viewing computed laser characteristics



The screenshot shows a software window titled "Laser Characteristics" with an "Export" menu. Below the menu is a table with columns for Bias (V), Power (mW), Current (mA), j (A/cm<sup>2</sup>), j rad (A/cm<sup>2</sup>), j stim (A/cm<sup>2</sup>), Gain (1/cm), Loss Total (1/cm), Loss AR (1/cm), Loss Passive (1/cm), and Wavelength (nm). The table contains 11 rows of data, with the row for 4.2V bias highlighted in blue.

Bias (V)	Power (mW)	Current (mA)	j (A/cm <sup>2</sup> )	j rad (A/cm <sup>2</sup> )	j stim (A/cm <sup>2</sup> )	Gain (1/cm)	Loss Total (1/cm)	Loss AR (1/cm)	Loss Passive (1/cm)	Wavelength (nm)
4	0	71.2865	2376.2180	760.8066	0	2.4419	4.7117	0.3529	0.6971	365.8416
4.05	0	98.7512	3291.7060	937.6923	0	3.3681	4.7293	0.3397	0.7279	365.1951
4.1	0	131.4426	4381.4200	1126.0720	0	4.0524	4.7421	0.3202	0.7602	364.6580
4.15	0	169.3345	5644.4840	1325.0570	0	4.7560	4.7562	0.3079	0.7866	364.3365
4.2	10.9683	201.0896	6702.9850	1532.1160	220.6082	4.6747	4.7578	0.3007	0.7954	364.2295
4.25	23.2647	233.5525	7785.0830	1743.0000	468.9319	4.7988	4.7666	0.3094	0.7955	364.3365
4.35	45.6239	306.4877	1.022E+04	2176.4920	919.2996	4.8378	4.7678	0.2950	0.8111	364.1225

**Laser Characteristics** window appears after the end of computations

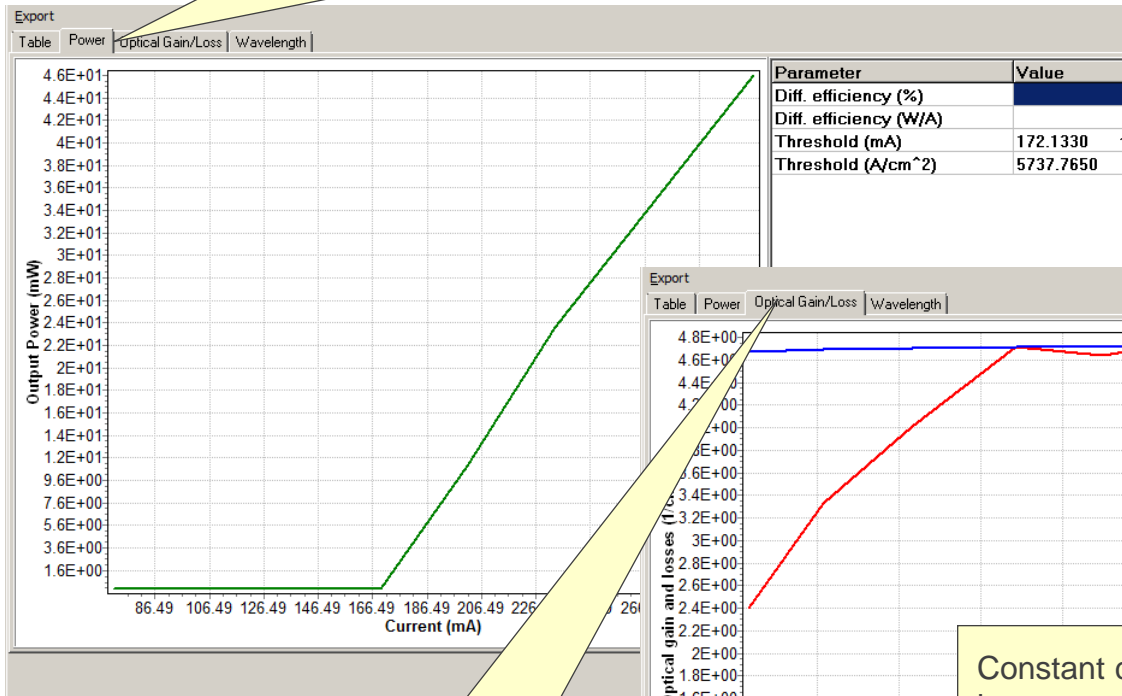
(later one can open it by using **Window -> Laser Characteristics** menu item)

First tab of the window contains a table. From the “Power” column, one can see that threshold is somewhere between 4.15V and 4.2V bias or between 170 mA and 200 mA current, respectively. If necessary, one can split this interval by several bias point by running additional laser computations. Use **Export** menu to store the table as a text file. Other tabs of the window contains a number of plots and some additional values.

Similarly to LED results, the band diagram, carrier concentrations, etc. are stored in the project file. One can see them by using **Laser Results** window (**Window -> Laser Results** menu item). It works very similar to **LED Results** window described in the previous tutorial.

## Viewing the results for threshold characteristics

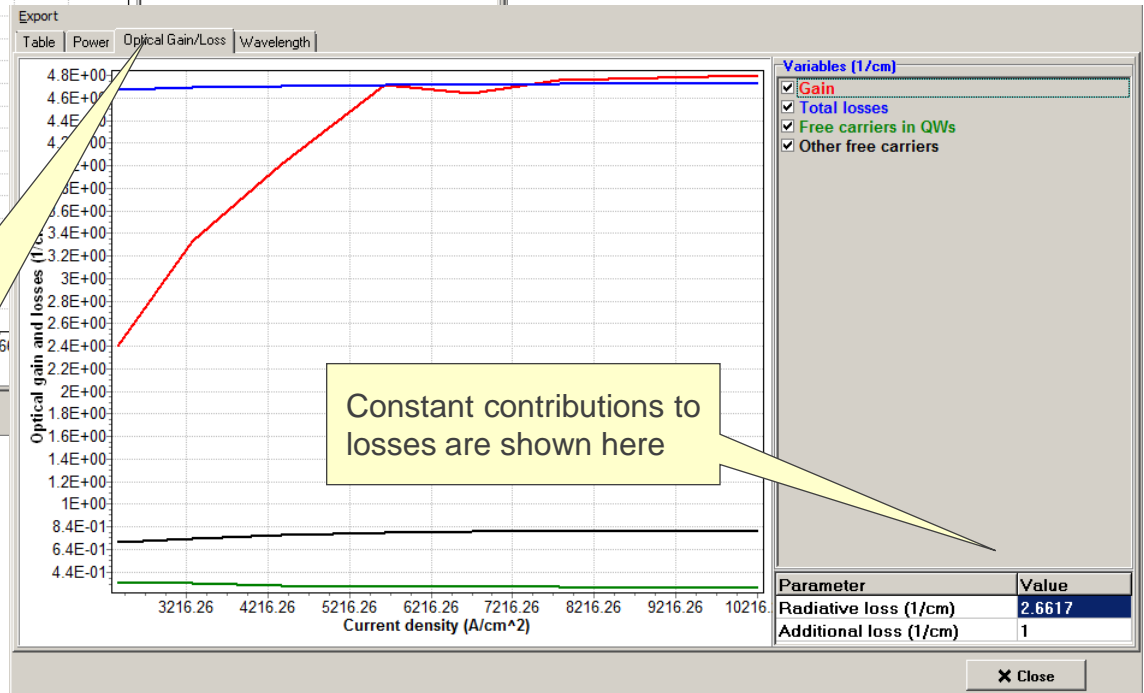
**Power** tab contains a plot of the output power as a function of current (note that SiLENSe always assumes the linear power increase above the threshold)



**Threshold current** and the respective current density are shown here

Parameter	Value
Diff. efficiency (%)	
Diff. efficiency (W/A)	
Threshold (mA)	172.1330
Threshold (A/cm <sup>2</sup> )	5737.7650

**Optical Gain/Loss** tab shows variation of the gain and loss as a function of current density



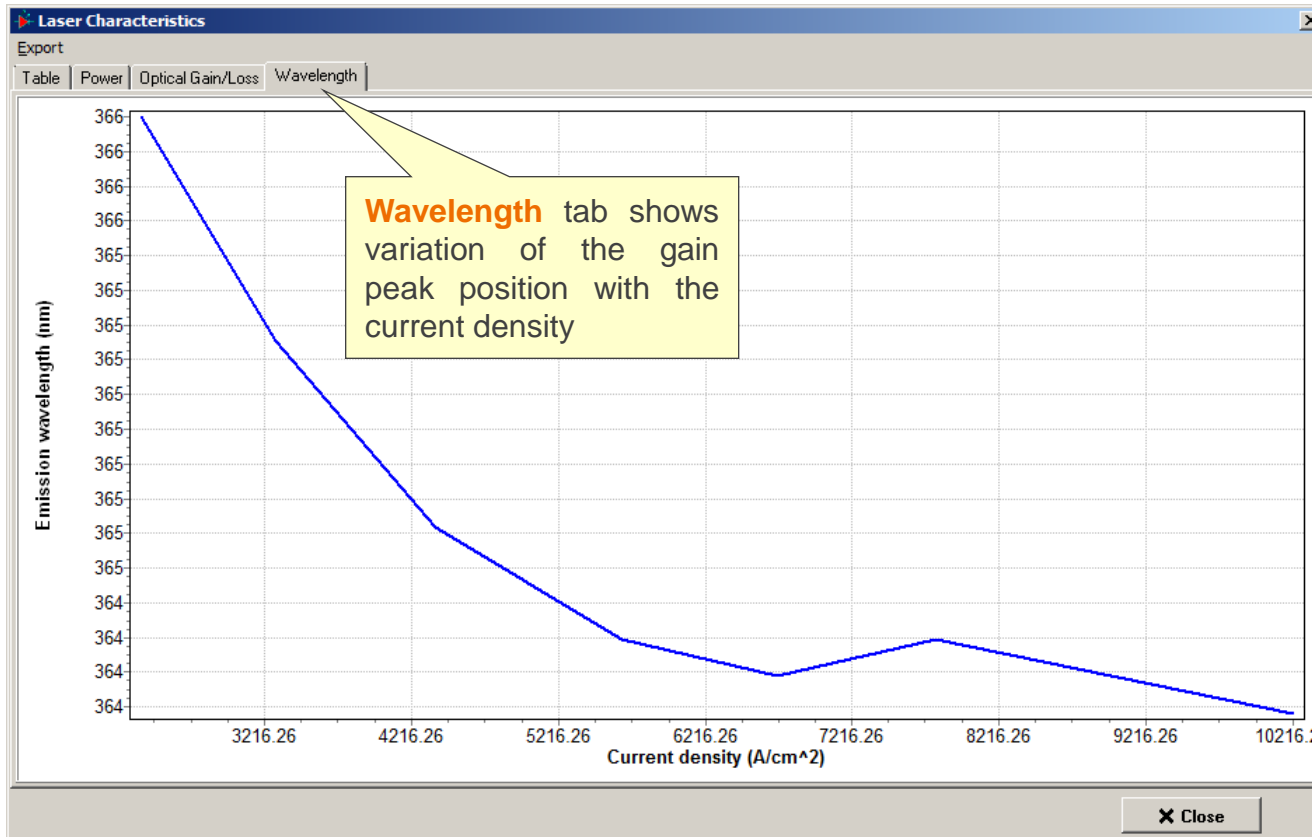
Constant contributions to losses are shown here

- Variables (1/cm)**
- Gain
  - Total losses
  - Free carriers in QWs
  - Other free carriers

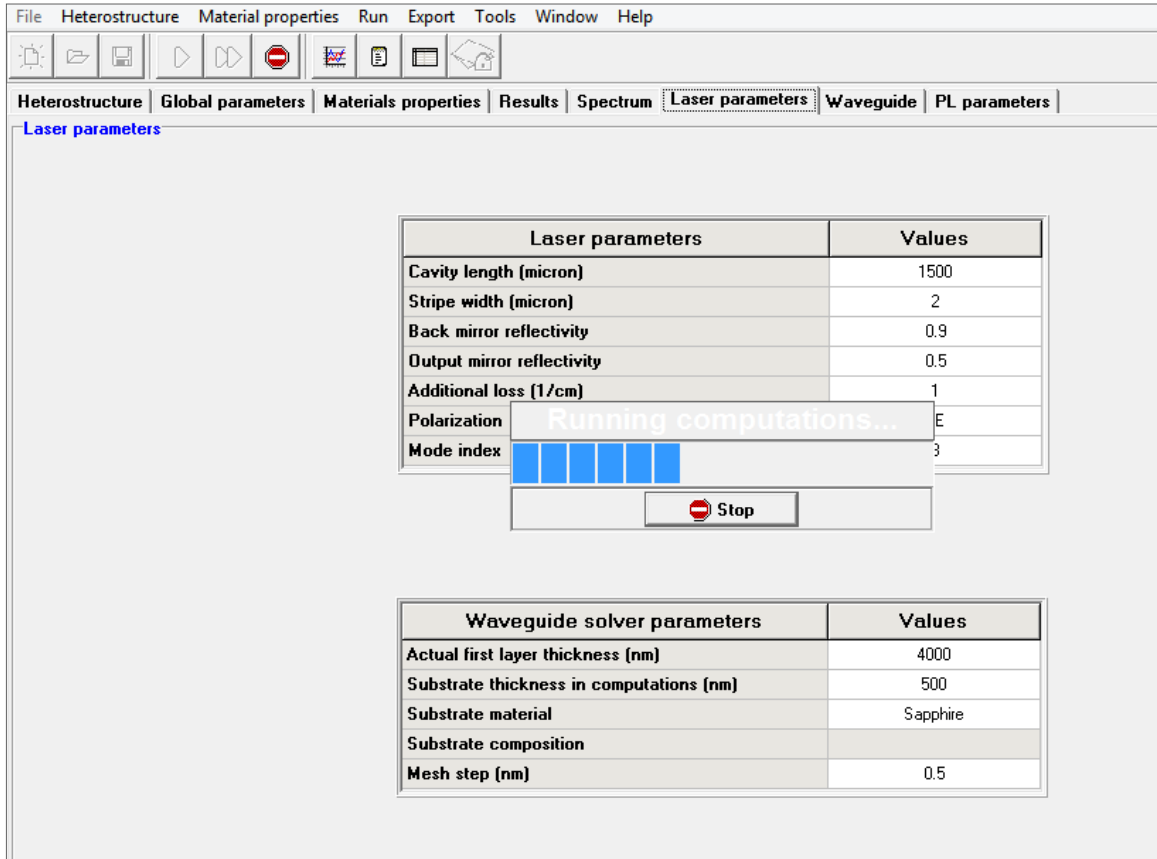
Parameter	Value
Radiative loss (1/cm)	2.6617
Additional loss (1/cm)	1

Close

## Viewing the results (Continued)



## Computation of threshold characteristics (old model)



The screenshot shows the 'Laser parameters' and 'Waveguide solver parameters' sections of the simulation software. A 'Running computations...' dialog box is overlaid on the laser parameters table.

Laser parameters		Values
Cavity length (micron)		1500
Stripe width (micron)		2
Back mirror reflectivity		0.9
Output mirror reflectivity		0.5
Additional loss (1/cm)		1
Polarization		E
Mode index		3

Running computations...

Stop

Waveguide solver parameters		Values
Actual first layer thickness (nm)		4000
Substrate thickness in computations (nm)		500
Substrate material		Sapphire
Substrate composition		
Mesh step (nm)		0.5

Old model for computations of threshold characteristics uses LED results of band diagram computation. In this simplified model, where is no self-consistent account of the stimulated recombination rate in the drift-diffusion model.

1. First, one needs to run computation of the band diagram and current density for a bias/current range covering the threshold bias/current.

2. Then use **Run->Laser Characteristics (Old)** menu item. During computations, the program seeks for the threshold by doing following tasks for each bias

- Computes gain spectrum and finds its maximum
- Computes the waveguide modes at the wavelength of max gain
- Computes modal gain
- Computes optical losses
- Compares gain and loss

Simulation results for the old laser model are similar to that for the model with self-consistent treatment of the stimulated recombination. The only difference is that laser output power beyond the threshold is extrapolated linearly by using differential quantum efficiency estimated from the threshold characteristics.