SimuLED Tutorials. Part I

STR Group Inc
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Part I

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Tutorial 1

SiLENSe 6.3 & SiLENSe Laser Edition 6.3

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

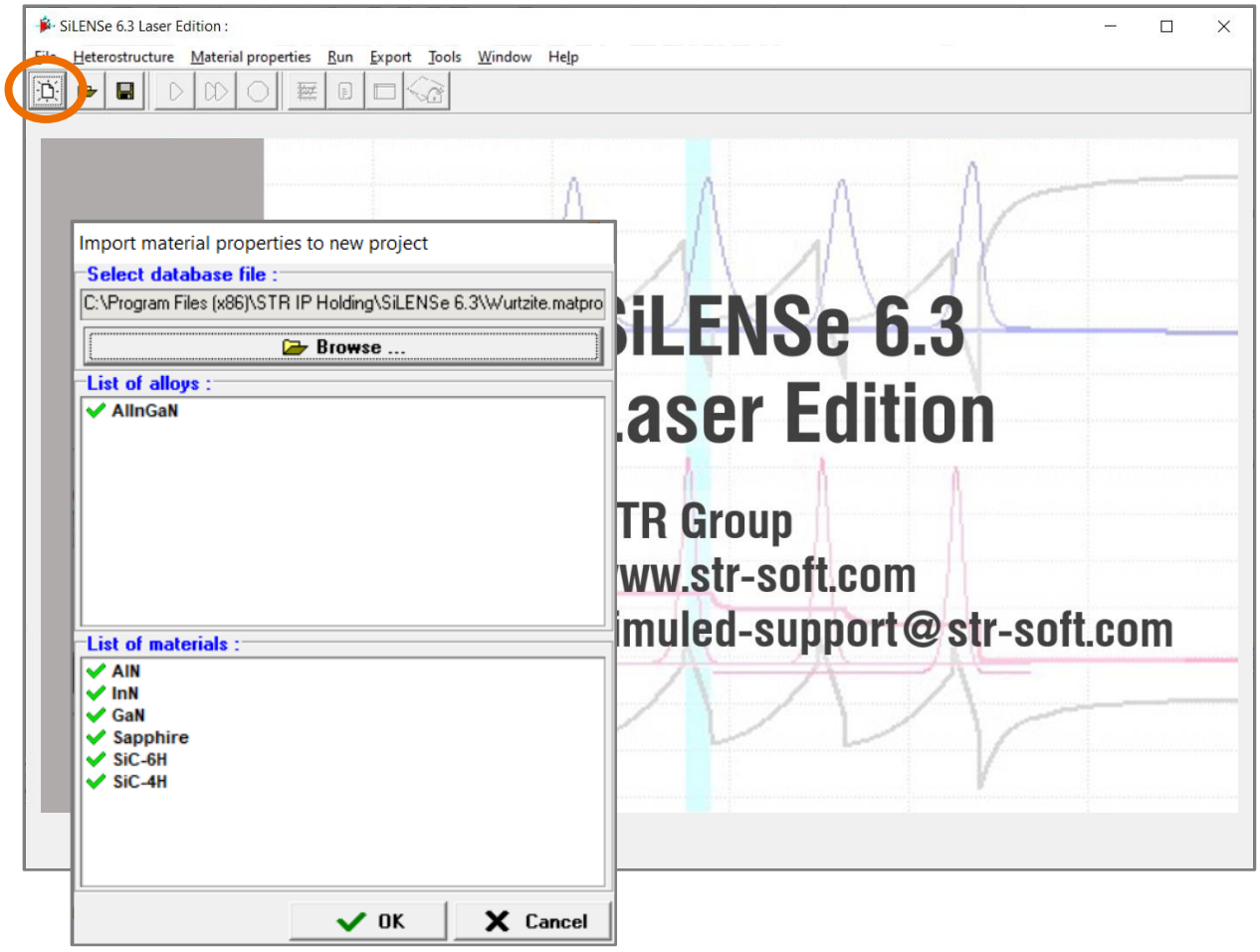
Step 3: Specification of global parameters (like temperature)

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

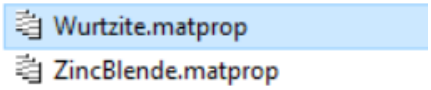
Step 6 (optional): Preparing input data for SpeCLED

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.



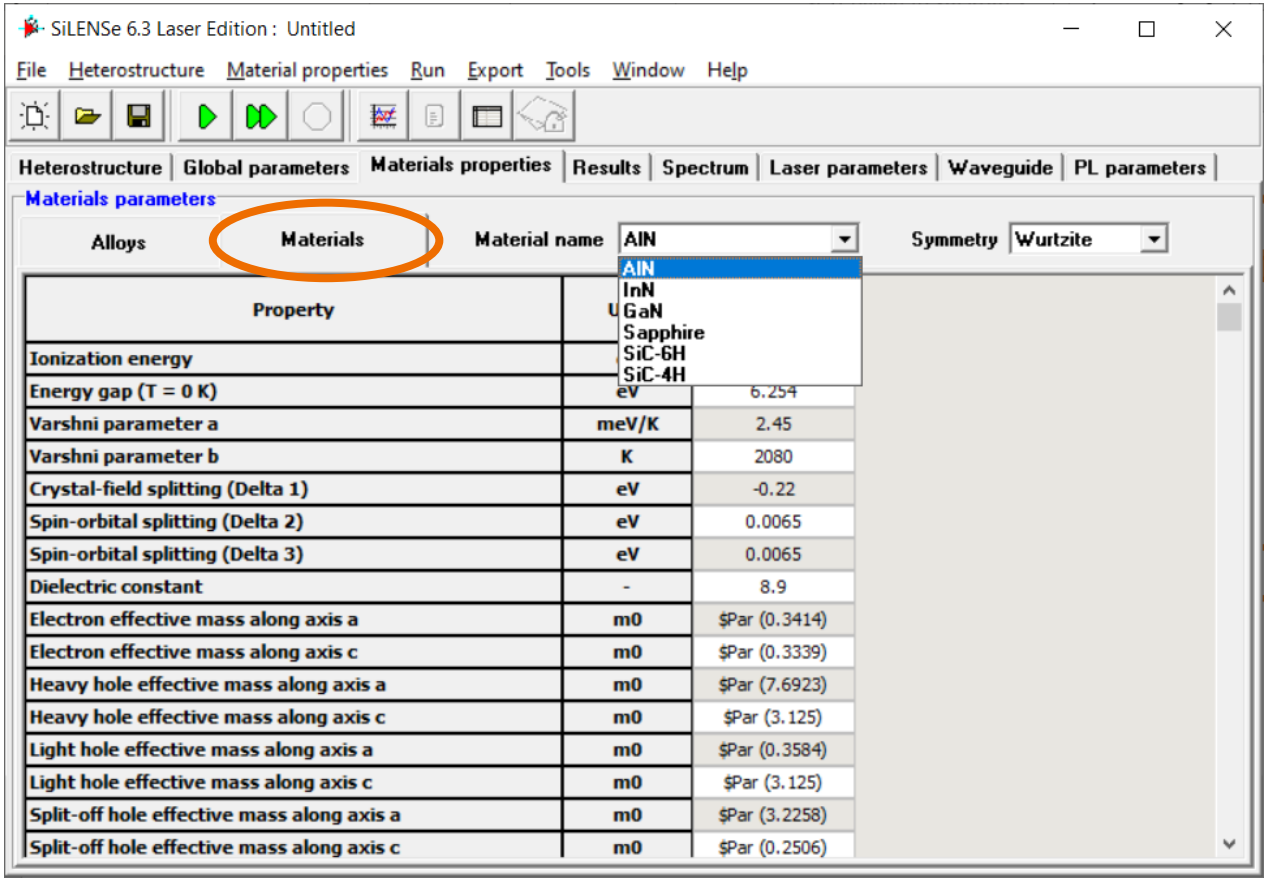
2. Choose **wurtzite** database supplied with SiLENSe. It includes properties of AlInGaN alloy and 3 materials which can be used as a substrate (sapphire, SiC-6H, and SiC-4H).

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 **ZincBlende.** 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



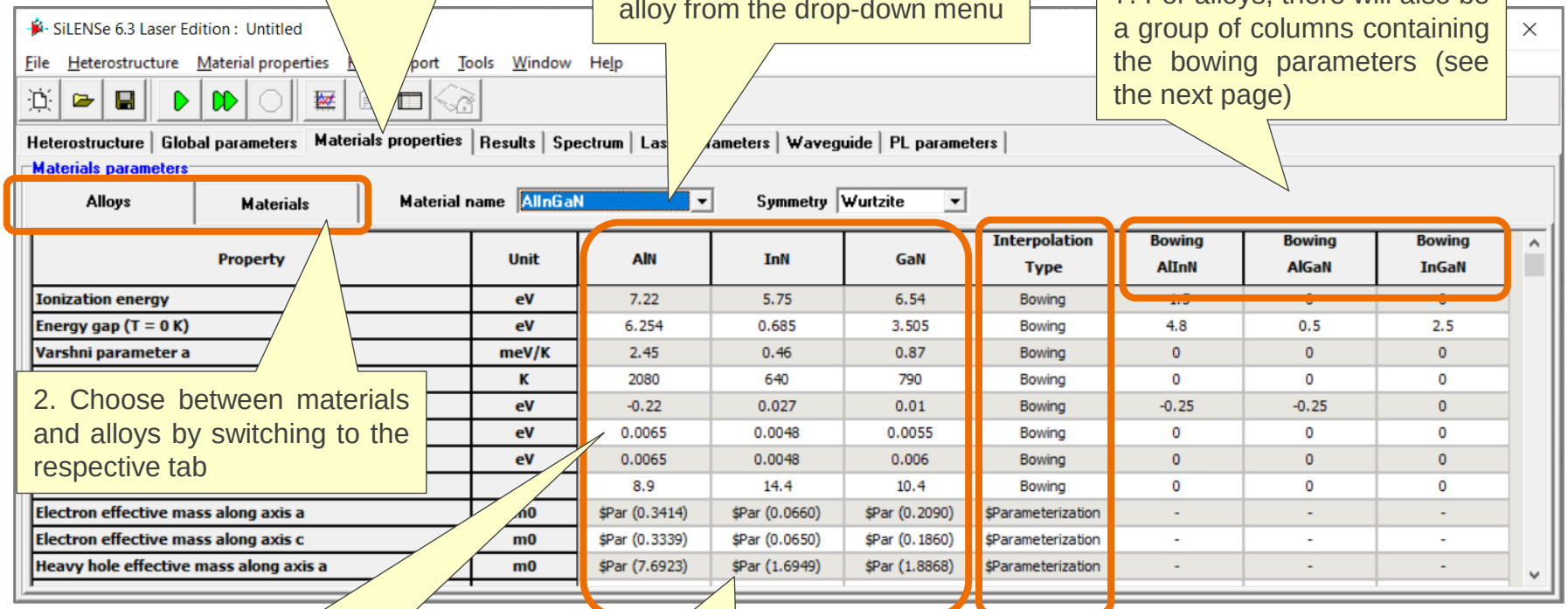
In specification of materials properties, SiLENSe distinguishes between materials of fixed composition (like GaN, AlN, and InN) and their alloys where composition may be continuously varied with one or more degree of freedom (like $Al_xGa_{1-x}N$, $In_xGa_{1-x}N$, $Al_xIn_yGa_{1-x-y}N$). There are 3 options to specify how properties of an alloy are calculated for a certain composition: (i) linear interpolation + bowing, (ii) built-in parameterization, and (iii) custom user-defined function.

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

7. For alloys, there will also be a group of columns containing the bowing parameters (see the next page)



Property	Unit	AlN	InN	GaN	Interpolation Type	Bowing AlInN	Bowing AlGaN	Bowing InGaN
Ionization energy	eV	7.22	5.75	6.54	Bowing	1.5	0	0
Energy gap (T = 0 K)	eV	6.254	0.685	3.505	Bowing	4.8	0.5	2.5
Varshni parameter a	meV/K	2.45	0.46	0.87	Bowing	0	0	0
	K	2080	640	790	Bowing	0	0	0
	eV	-0.22	0.027	0.01	Bowing	-0.25	-0.25	0
	eV	0.0065	0.0048	0.0055	Bowing	0	0	0
	eV	0.0065	0.0048	0.006	Bowing	0	0	0
		8.9	14.4	10.4	Bowing	0	0	0
Electron effective mass along axis a	m0	$Par (0.3414)	$Par (0.0660)	$Par (0.2090)	$Parameterization	-	-	-
Electron effective mass along axis c	m0	$Par (0.3339)	$Par (0.0650)	$Par (0.1860)	$Parameterization	-	-	-
Heavy hole effective mass along axis a	m0	$Par (7.6923)	$Par (1.6949)	$Par (1.8868)	$Parameterization	-	-	-

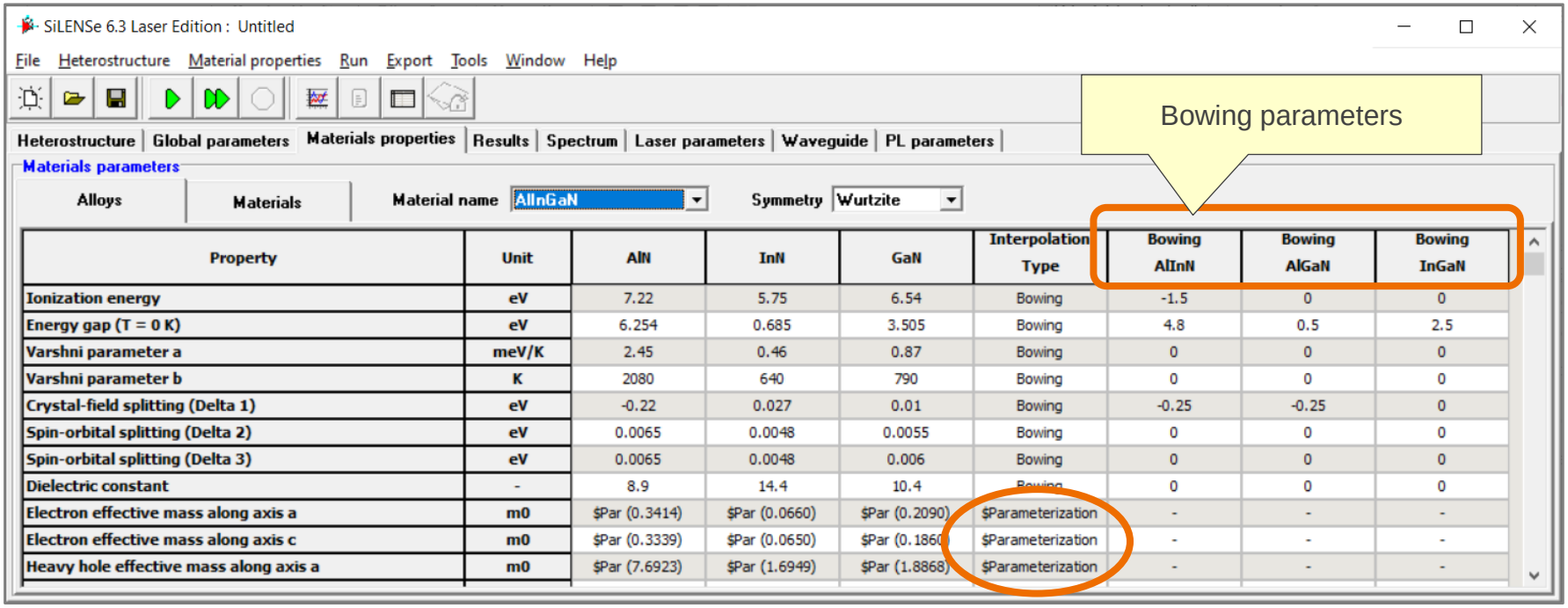
2. Choose between materials and alloys by switching to the respective tab

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

5. **$Par** (parameterization) marks the characteristics derived from some other material properties via theoretical expression. The resulting value is shown in the brackets

6. This column shows how properties of the alloy are calculated (see comment on previous slide)

Step 1 (Continued): Bowing parameters and parameterization



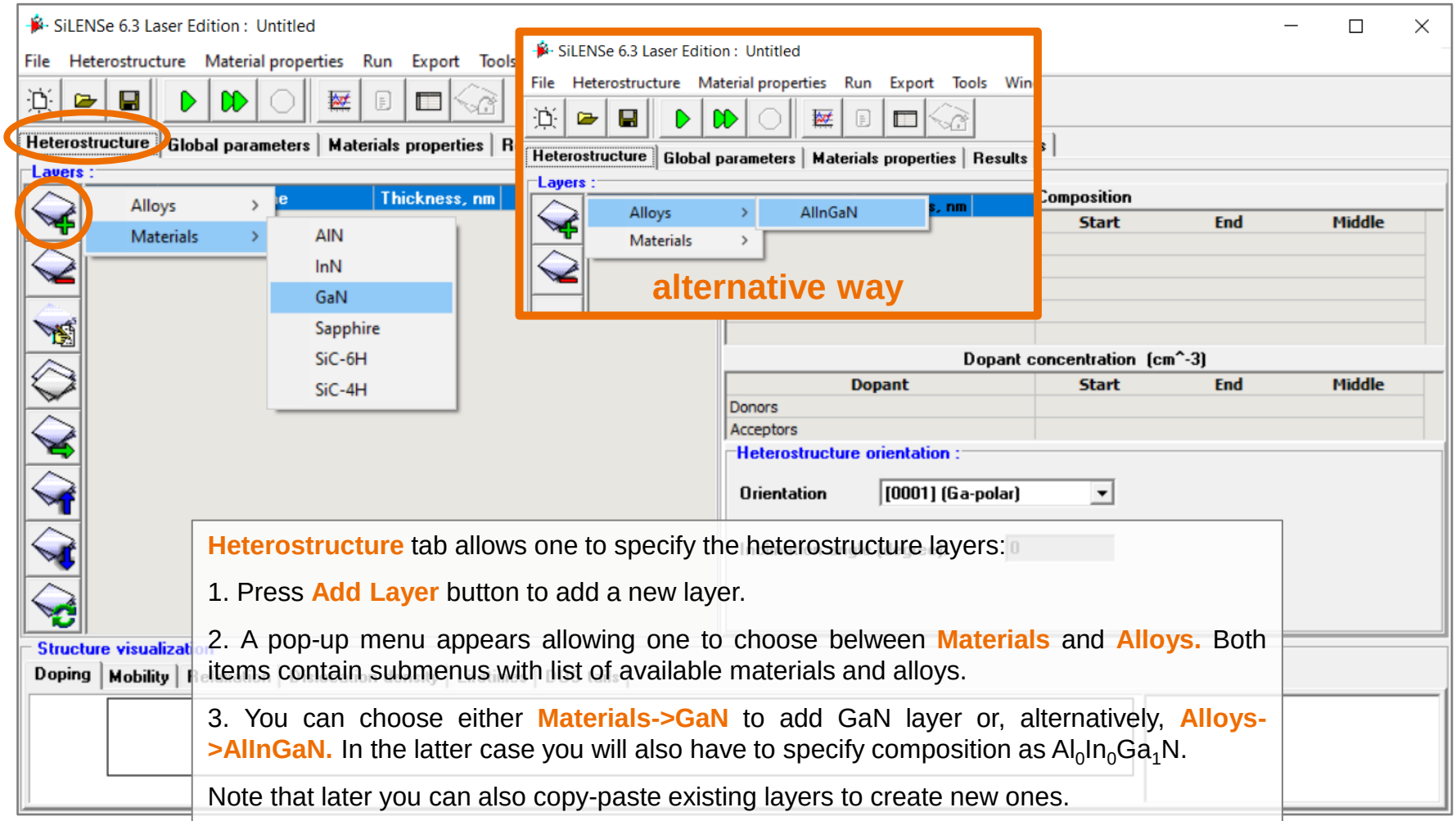
Property	Unit	AlN	InN	GaN	Interpolation Type	Bowing AlInN	Bowing AlGaN	Bowing InGaN
Ionization energy	eV	7.22	5.75	6.54	Bowing	-1.5	0	0
Energy gap (T = 0 K)	eV	6.254	0.685	3.505	Bowing	4.8	0.5	2.5
Varshni parameter a	meV/K	2.45	0.46	0.87	Bowing	0	0	0
Varshni parameter b	K	2080	640	790	Bowing	0	0	0
Crystal-field splitting (Delta 1)	eV	-0.22	0.027	0.01	Bowing	-0.25	-0.25	0
Spin-orbital splitting (Delta 2)	eV	0.0065	0.0048	0.0055	Bowing	0	0	0
Spin-orbital splitting (Delta 3)	eV	0.0065	0.0048	0.006	Bowing	0	0	0
Dielectric constant	-	8.9	14.4	10.4	Bowing	0	0	0
Electron effective mass along axis a	m0	$Par (0.3414)	$Par (0.0660)	$Par (0.2090)	$Parameterization	-	-	-
Electron effective mass along axis c	m0	$Par (0.3339)	$Par (0.0650)	$Par (0.1860)	$Parameterization	-	-	-
Heavy hole effective mass along axis a	m0	$Par (7.6923)	$Par (1.6949)	$Par (1.8868)	$Parameterization	-	-	-

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

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 (**PropEdit.exe**) which is not discussed in this tutorial. One can update materials properties by using **Materials Properties->Import** menu item.

Parameterization interpolation type for alloy means that the property is calculated in two steps: (i) parameters (i.e. some other material properties) involved in the parametrization equation are calculated according to the alloy composion and then (ii) the property is calculated with the equation and values of parameters calculated at step (i).

Step 2: Adding heterostructure layers



Heterostructure tab allows one to specify the heterostructure layers:

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

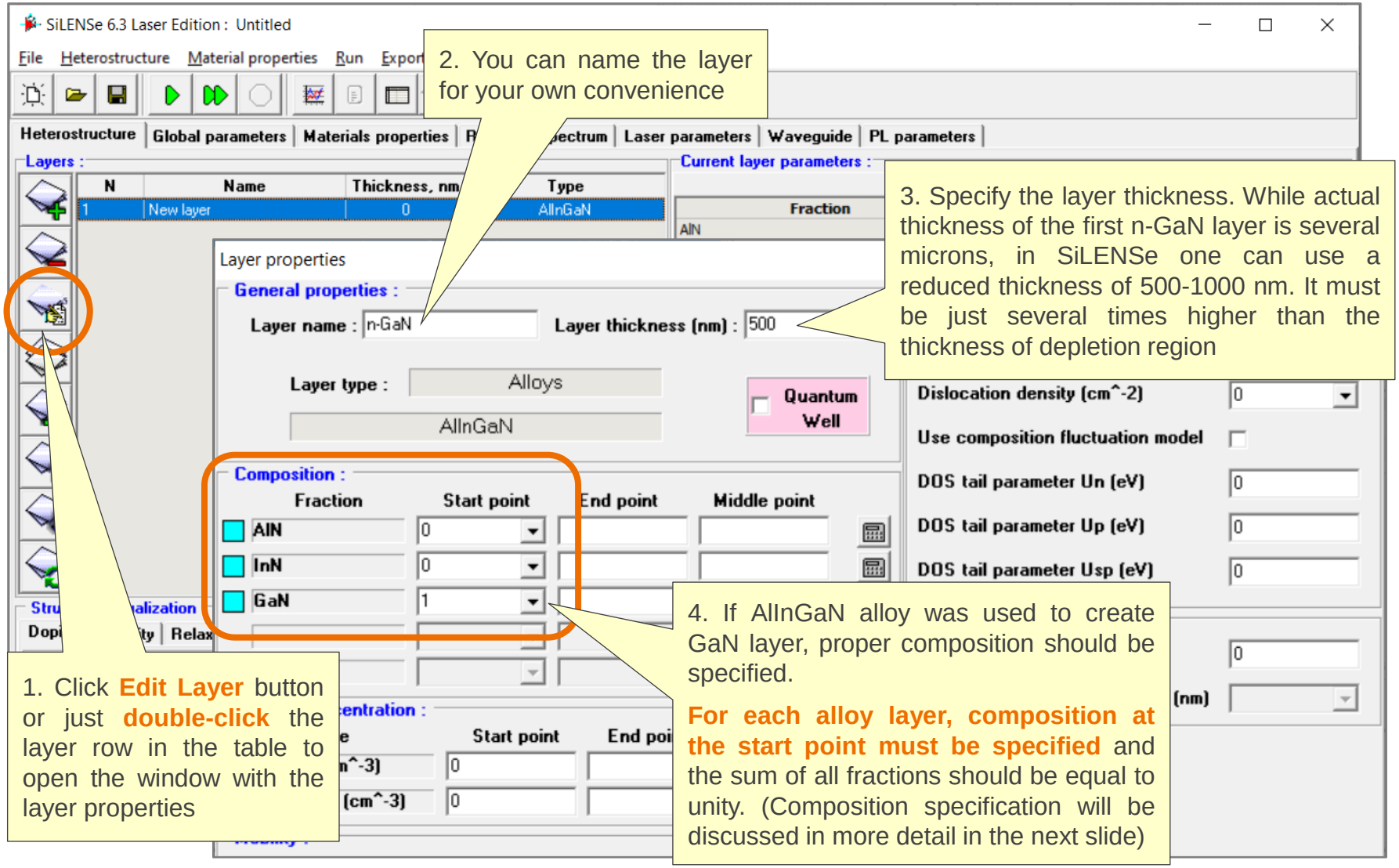
2. A pop-up menu appears allowing one to choose belween **Materials** and **Alloys.** Both items contain submenus with list of available materials and alloys.

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 $Al_0In_0Ga_1N$.

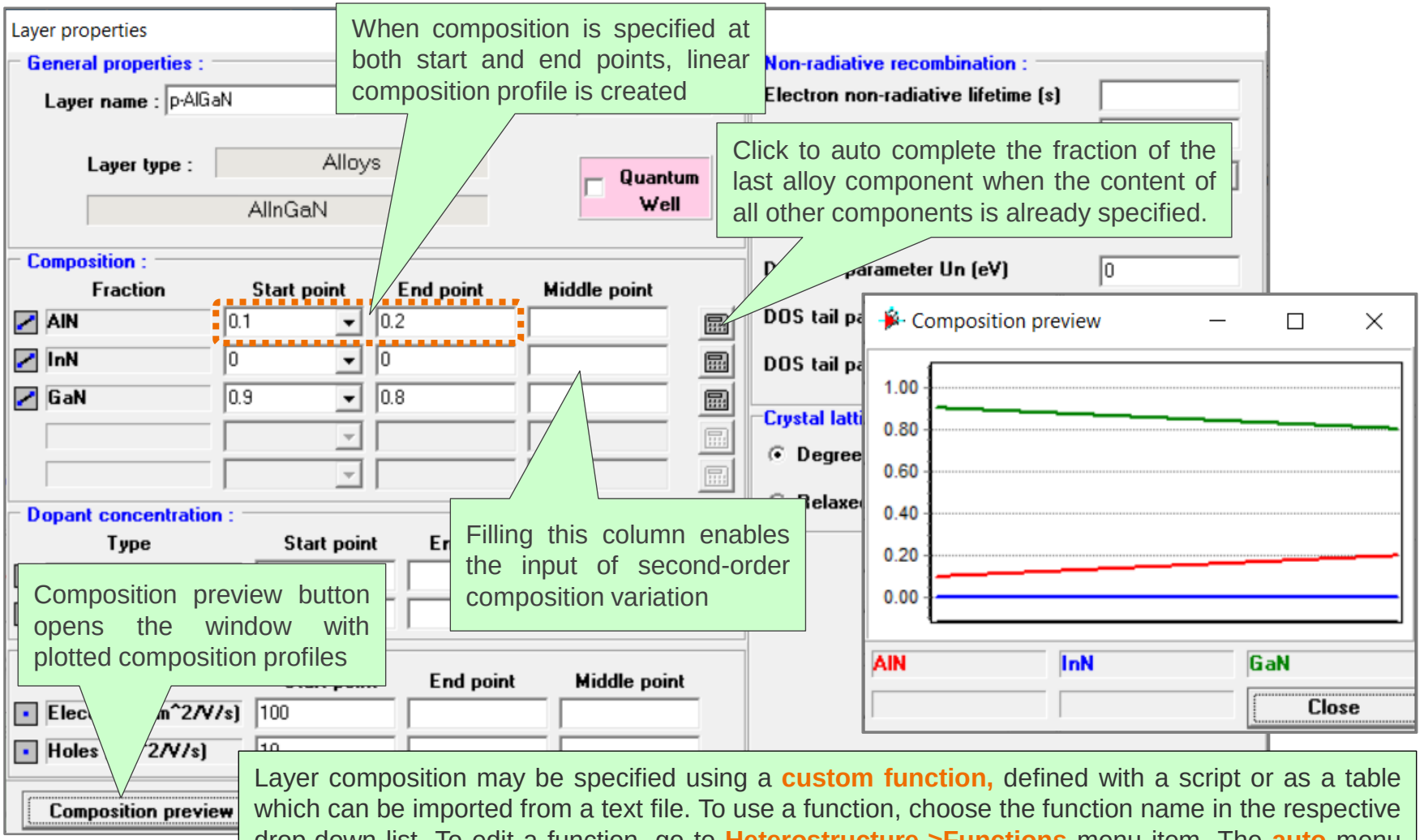
Note that later you can also copy-paste existing layers to create new ones.

Heterostructure has to **start with n-type layer and end with p-type layer.** Nucleation and buffer layers should not be included.

Step 2 (Continued): Layer thickness and composition

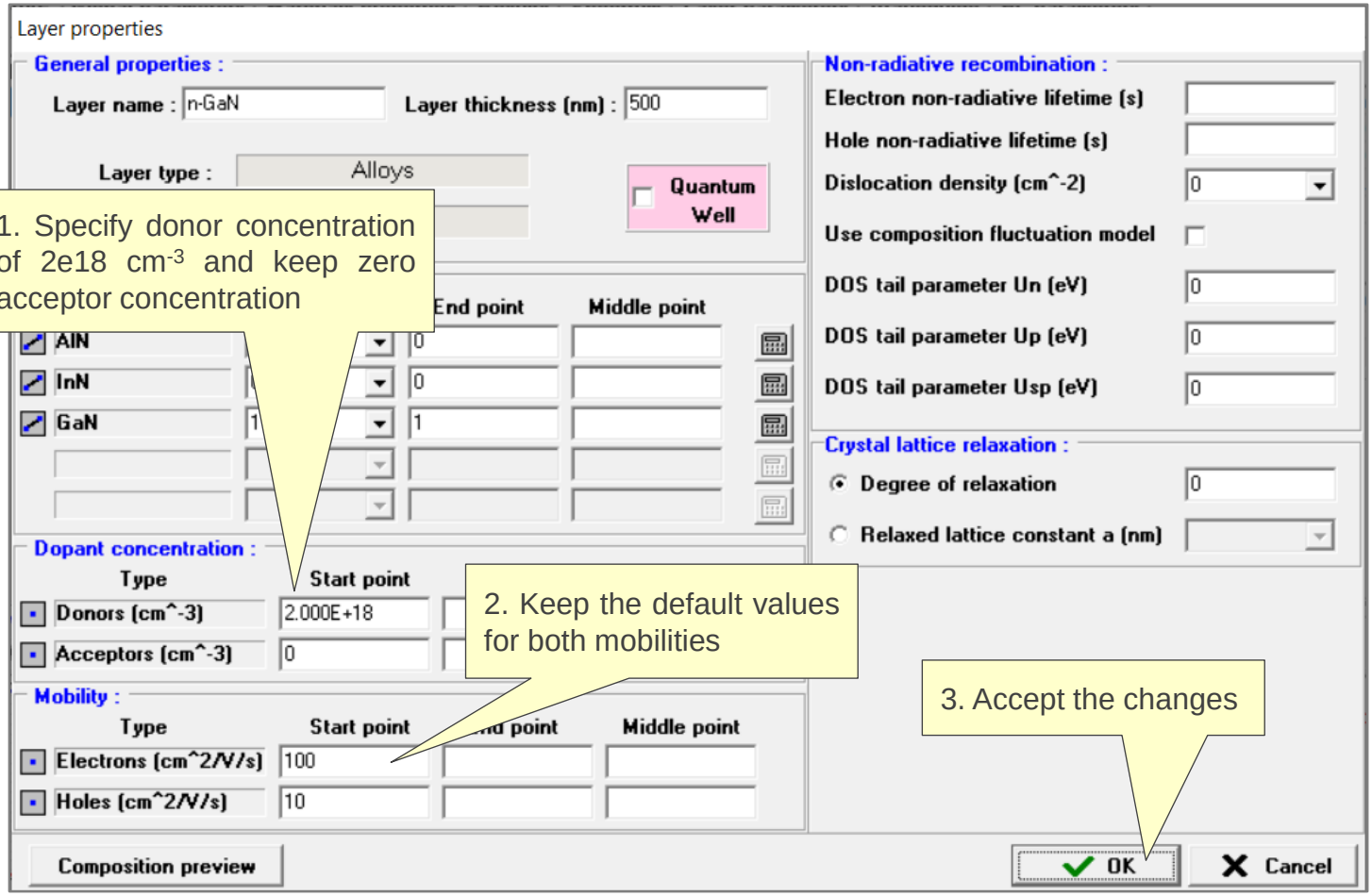


Additional information: graded composition



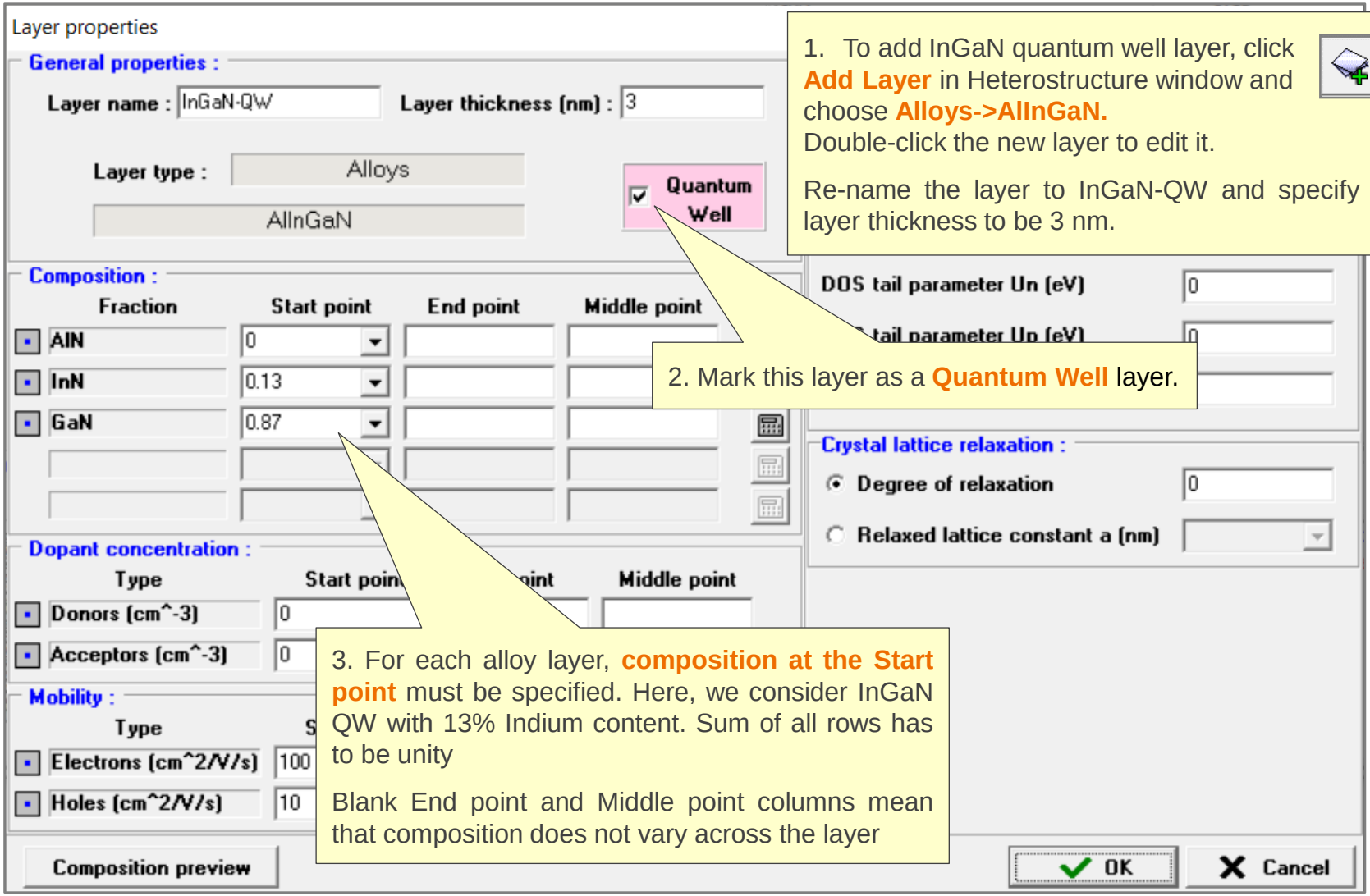
Layer composition may be specified using a **custom function,** defined with a script or as a table which can be imported from a text file. To use a function, choose the function name in the respective drop-down list. To edit a function, go to **Heterostructure->Functions** menu item. The **auto** menu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

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



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, click **Add Layer** in Heterostructure window and choose **Alloys->AlInGaN.**
Double-click the new layer to edit it.

Re-name the layer to InGaN-QW and specify the layer thickness to be 3 nm.

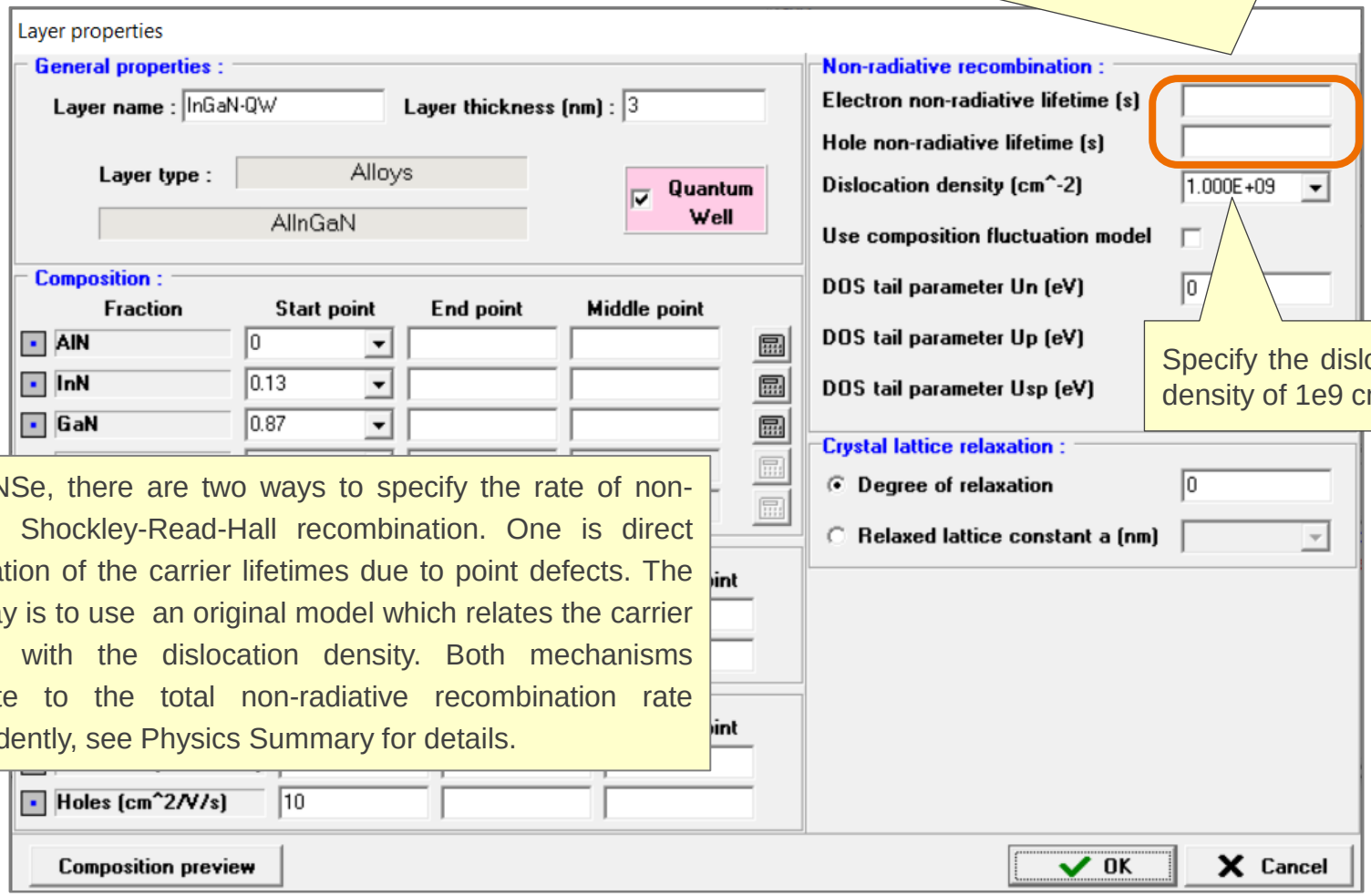
2. Mark this layer as a **Quantum Well** layer.

3. For each alloy layer, **composition at the Start point** must be specified. Here, we consider InGaN QW with 13% Indium content. Sum of all rows has to be unity

Blank End point and Middle point columns mean that composition does not vary across the layer

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

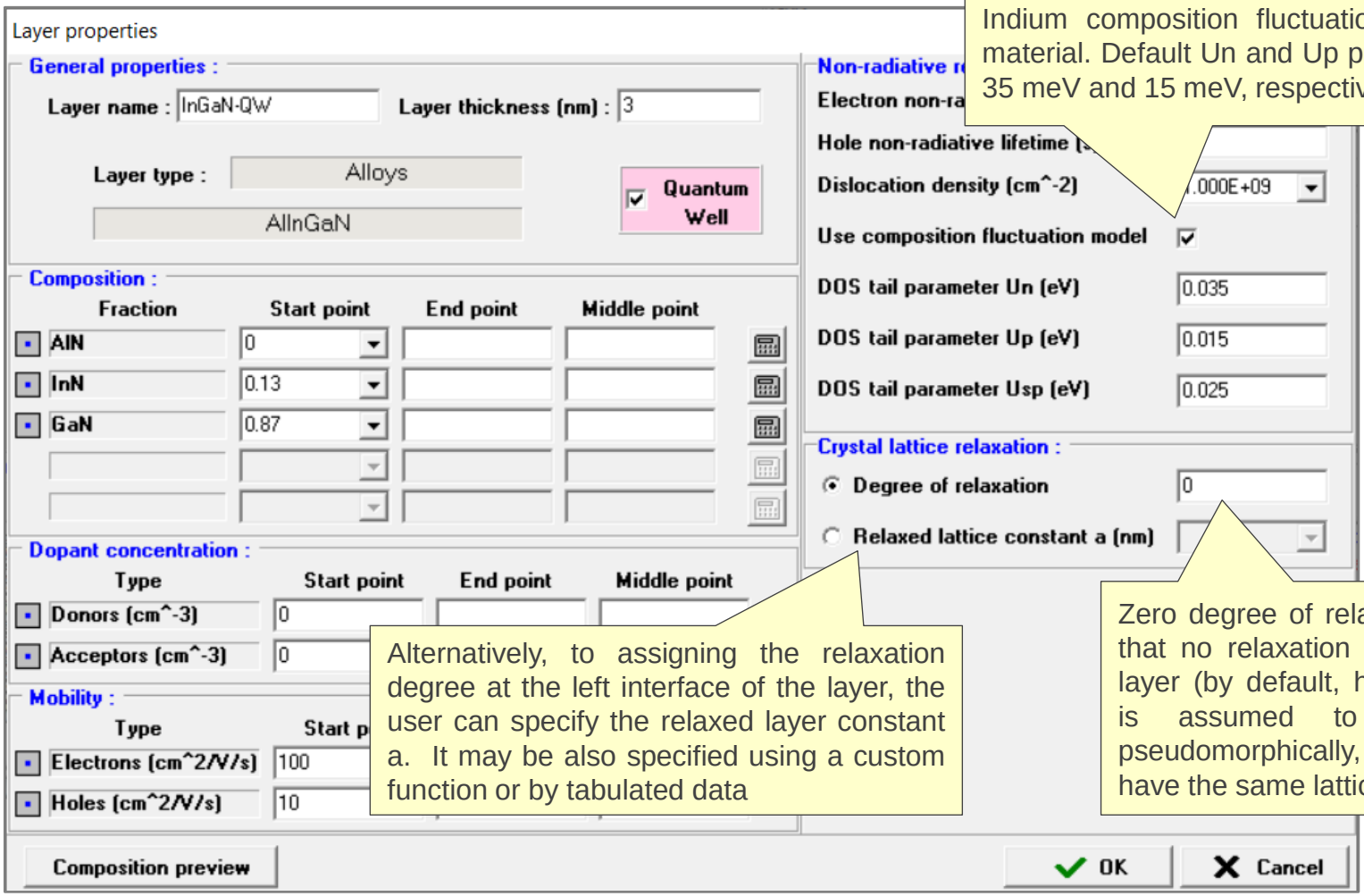
These two parameters describe **carrier lifetimes** with respect to point defects. Blank fields mean that this recombination channel is ignored for this layer



Specify the dislocation density of 1e9 cm^{-2}

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 Physics Summary for details.

Step 2 (Continued): Composition fluctuation and relaxation



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

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

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)

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

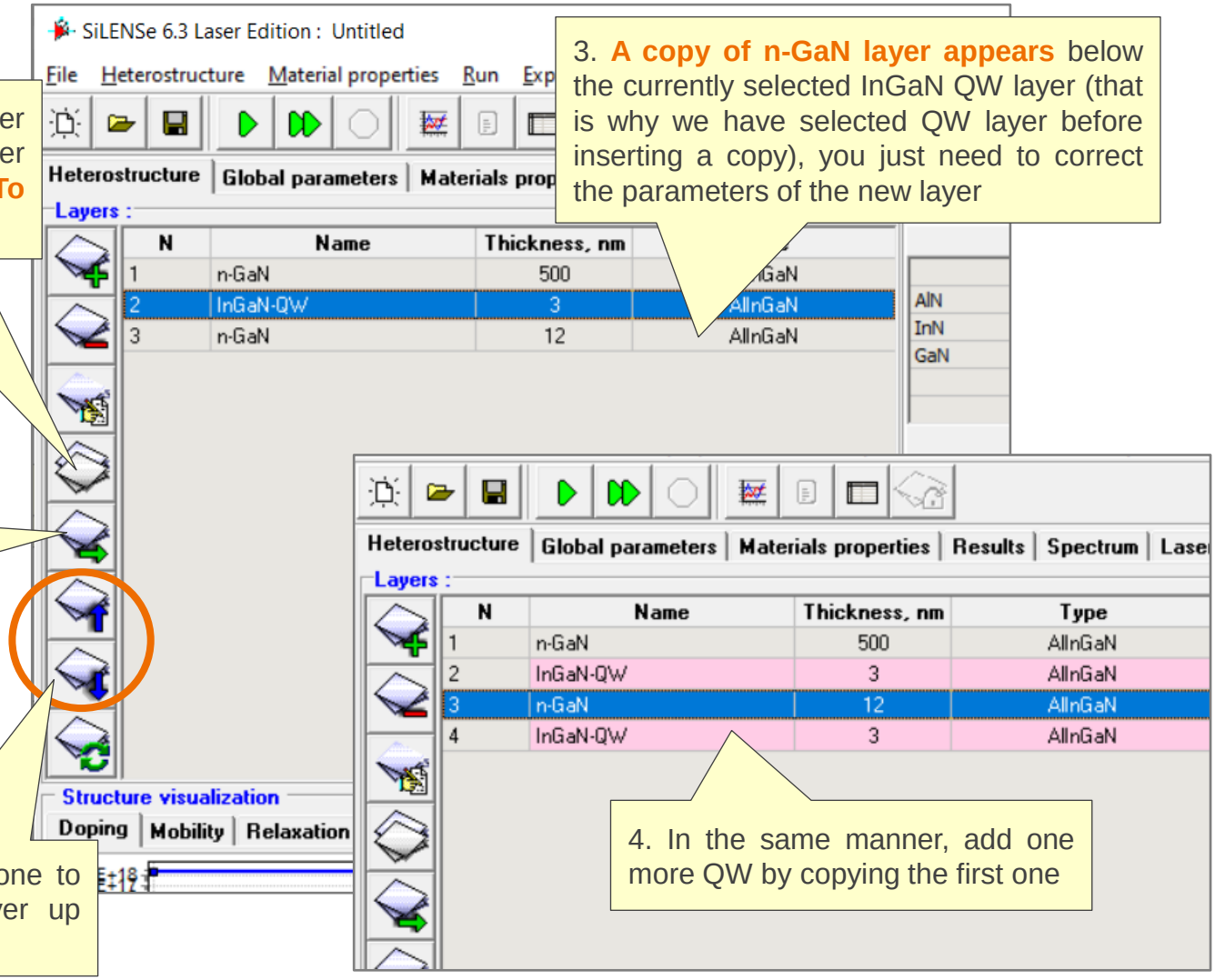
1. To add GaN MQW barrier layer, select n-GaN layer and click **Copy Layer To Buffer** button

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

4. In the same manner, add one more QW by copying the first one

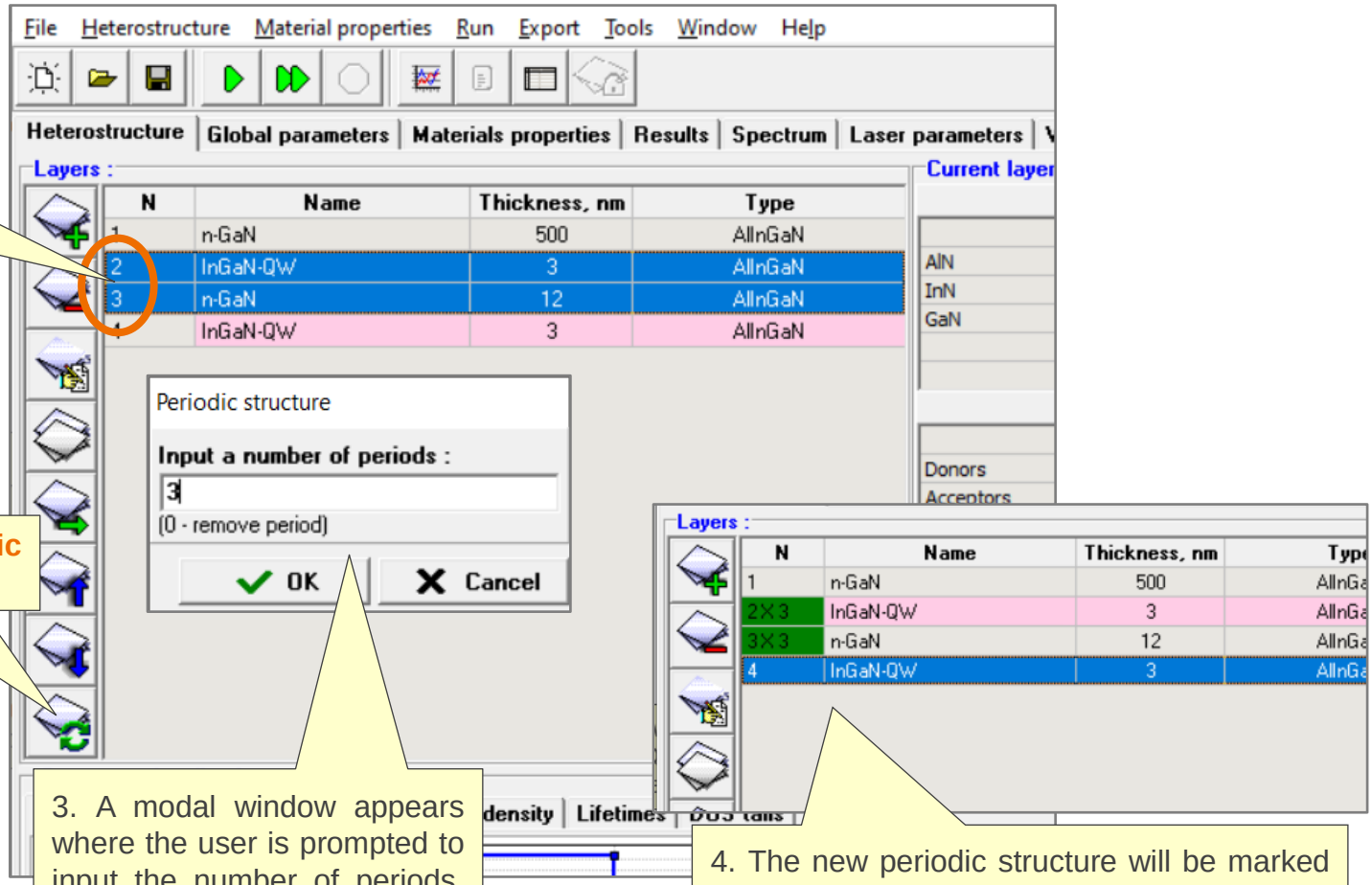
These buttons allow one to move a selected layer up and down



Step 2 (Continued): Creating periodic structures

1. Select two layers, first QW and the barrier

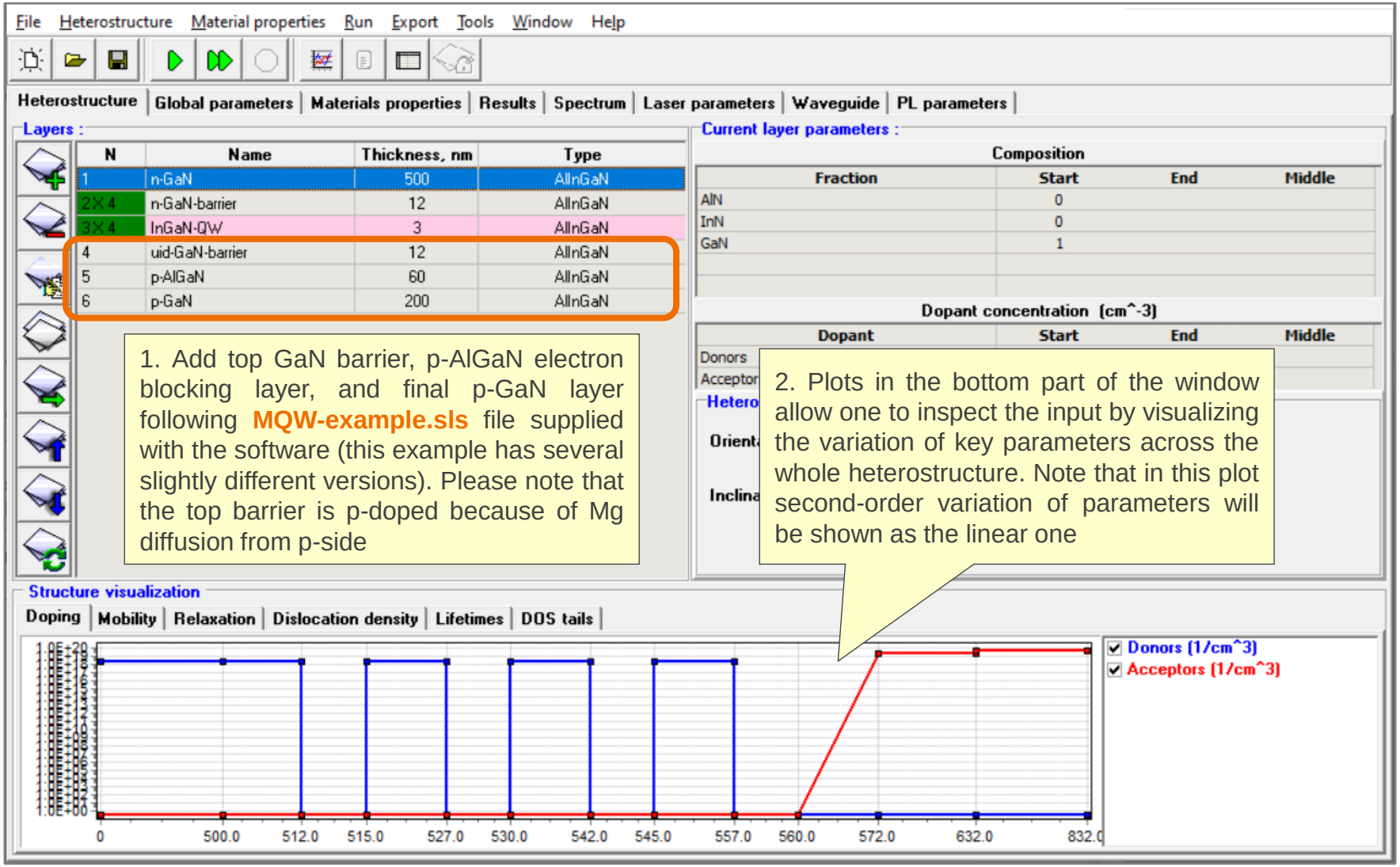
2. Click **Edit Periodic Structure** button



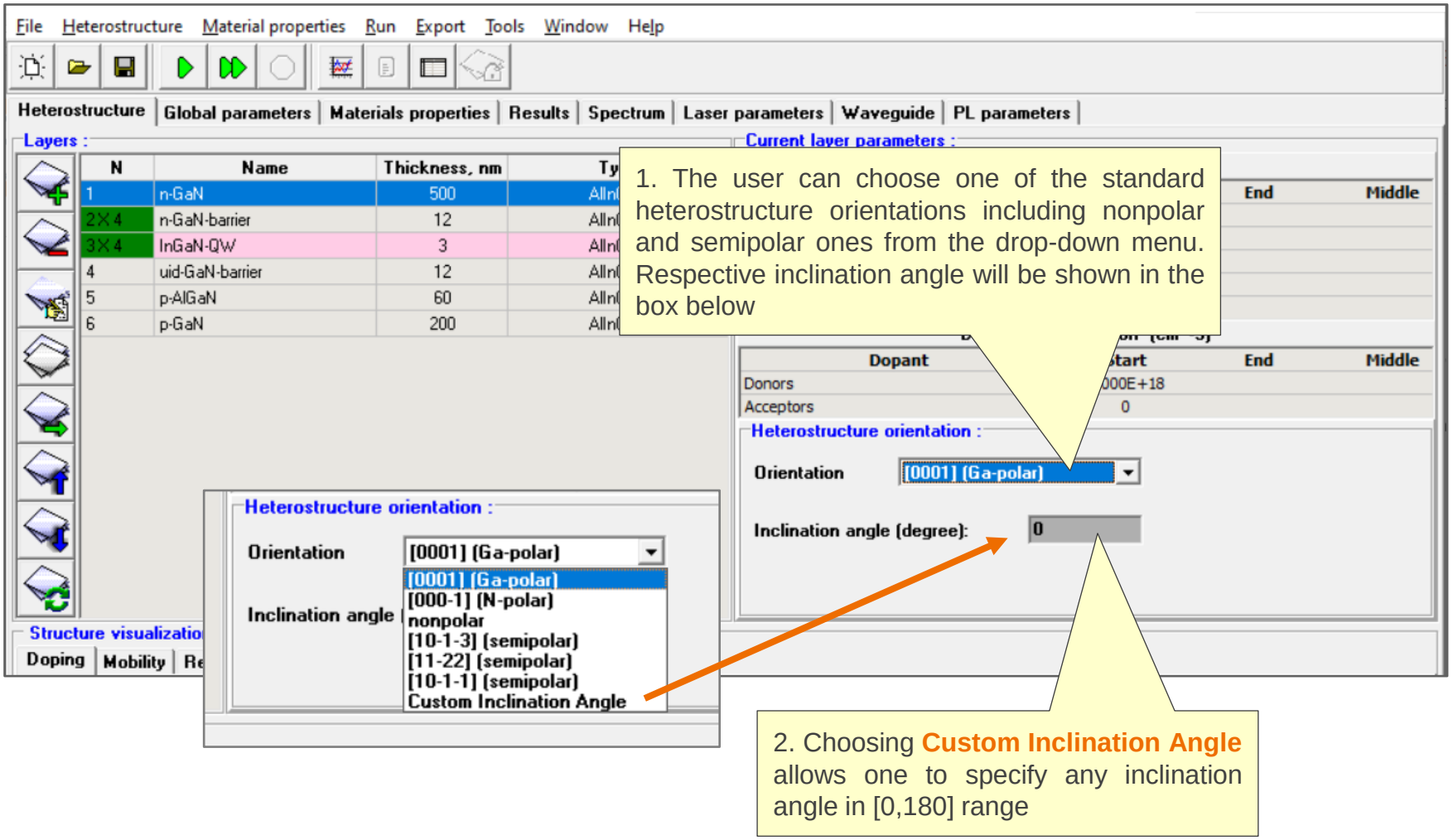
3. A modal window appears where the user is prompted to input the number of periods. Input **3** and press **OK.** To delete a periodic structure, one should input 0 or 1 period

4. The new periodic structure will be marked by green color. You can specify several non-overlapping periodic structures. In this case, they will be marked by alternating green and blue colors

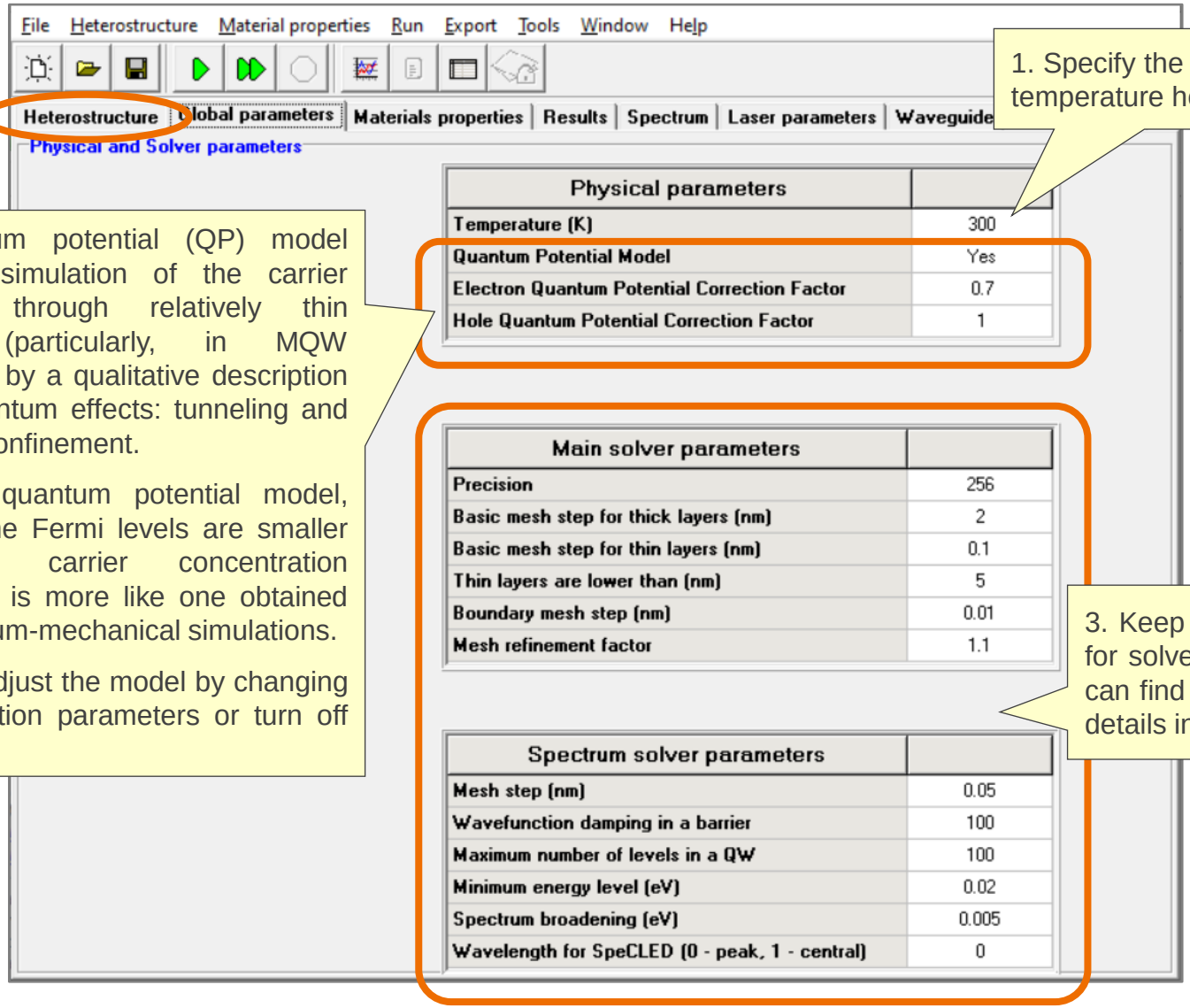
Step 2 (Continued): Finalizing the structure



Step 3: Specification of polarity



Step 3 (Continued): Temperature and solver options



1. Specify the p-n junction temperature here

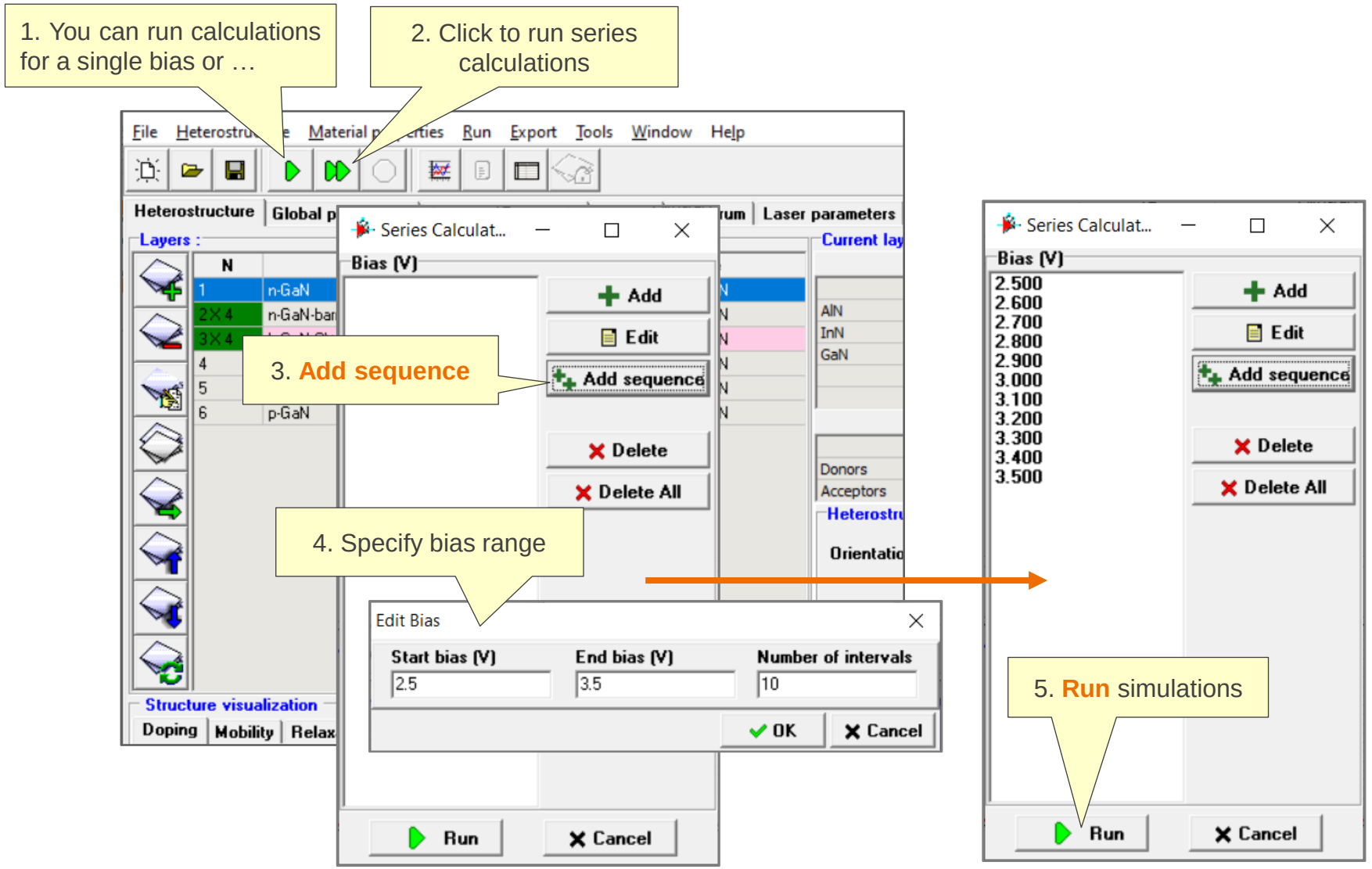
2. Quantum potential (QP) model improves simulation of the carrier transport through relatively thin barriers (particularly, in MQW structures) by a qualitative description of the quantum effects: tunneling and quantum confinement.

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

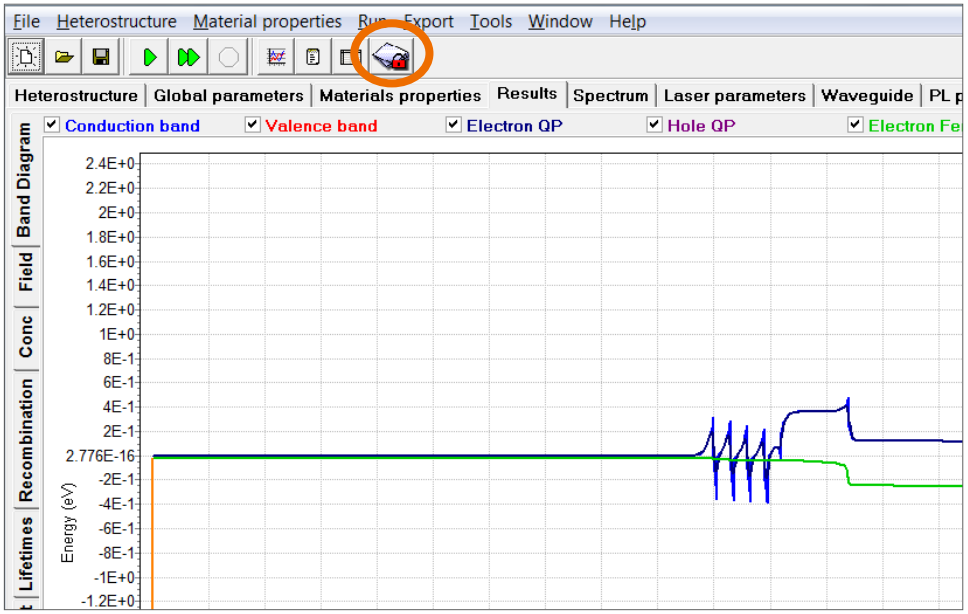
One can adjust the model by changing two correction parameters or turn off the model

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

Step 4: Running the simulation of the band diagram



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”** once at least one result is computed.

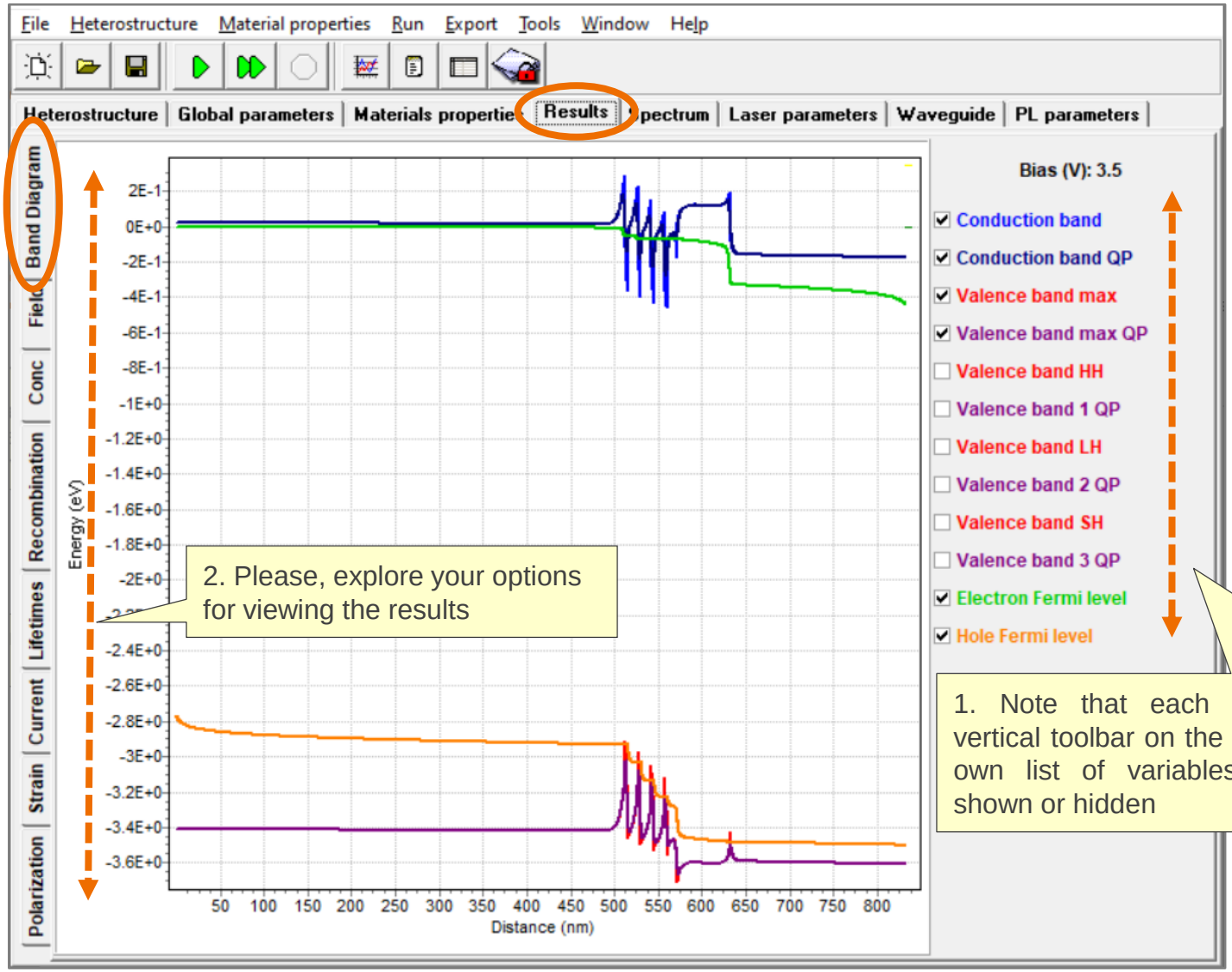
For “locked” project, most of the options for editing heterostructure are disabled. Edit Layer button is enabled, while most of the layer properties appear in read-only mode, that is shown by the grey color of the text fields.

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)

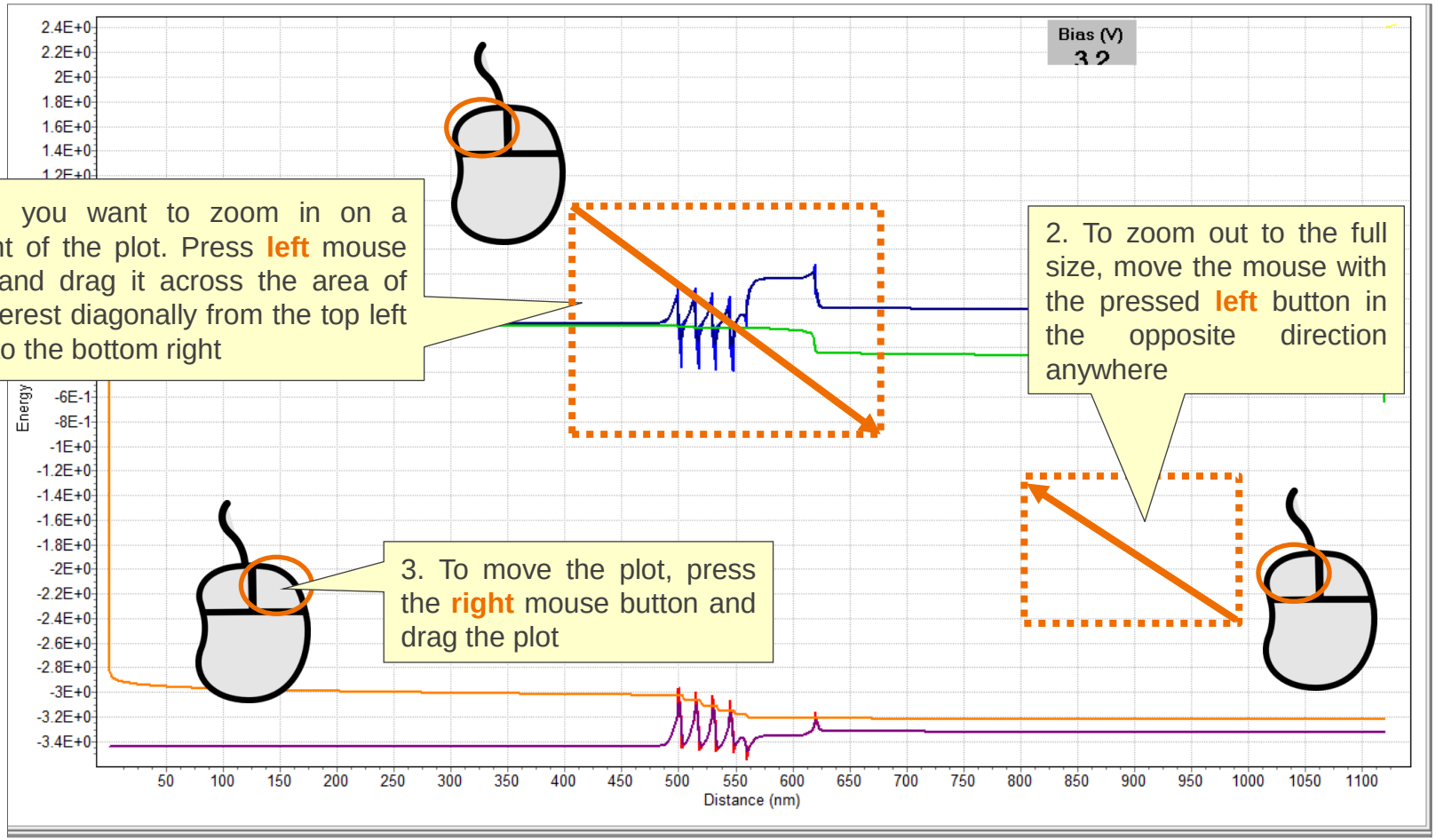
To be able to edit the input data, one needs to clear all the results by **clicking the lock button** and thus unlock the editing.

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.

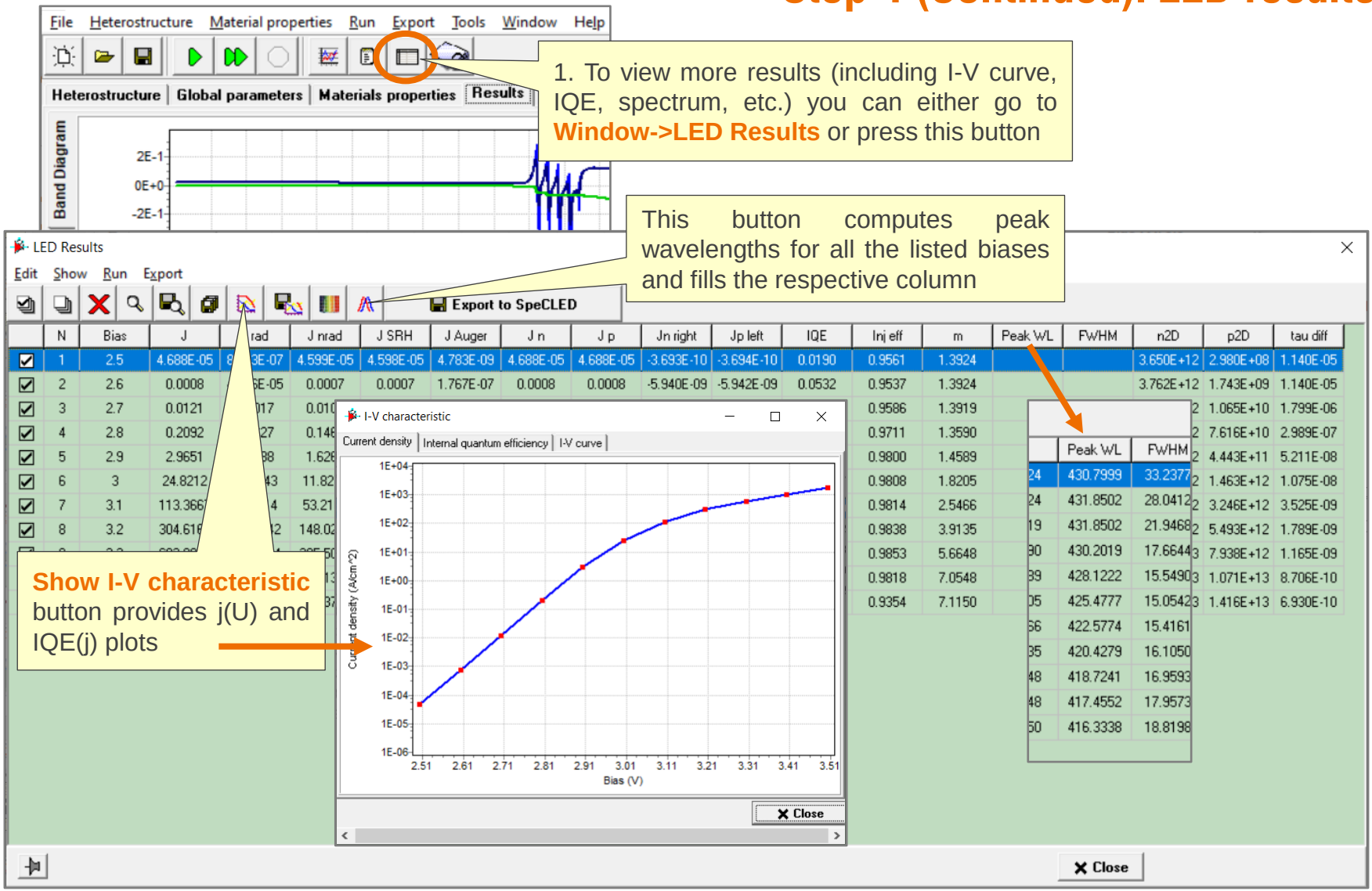
Step 4 (Continued): Results tab



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



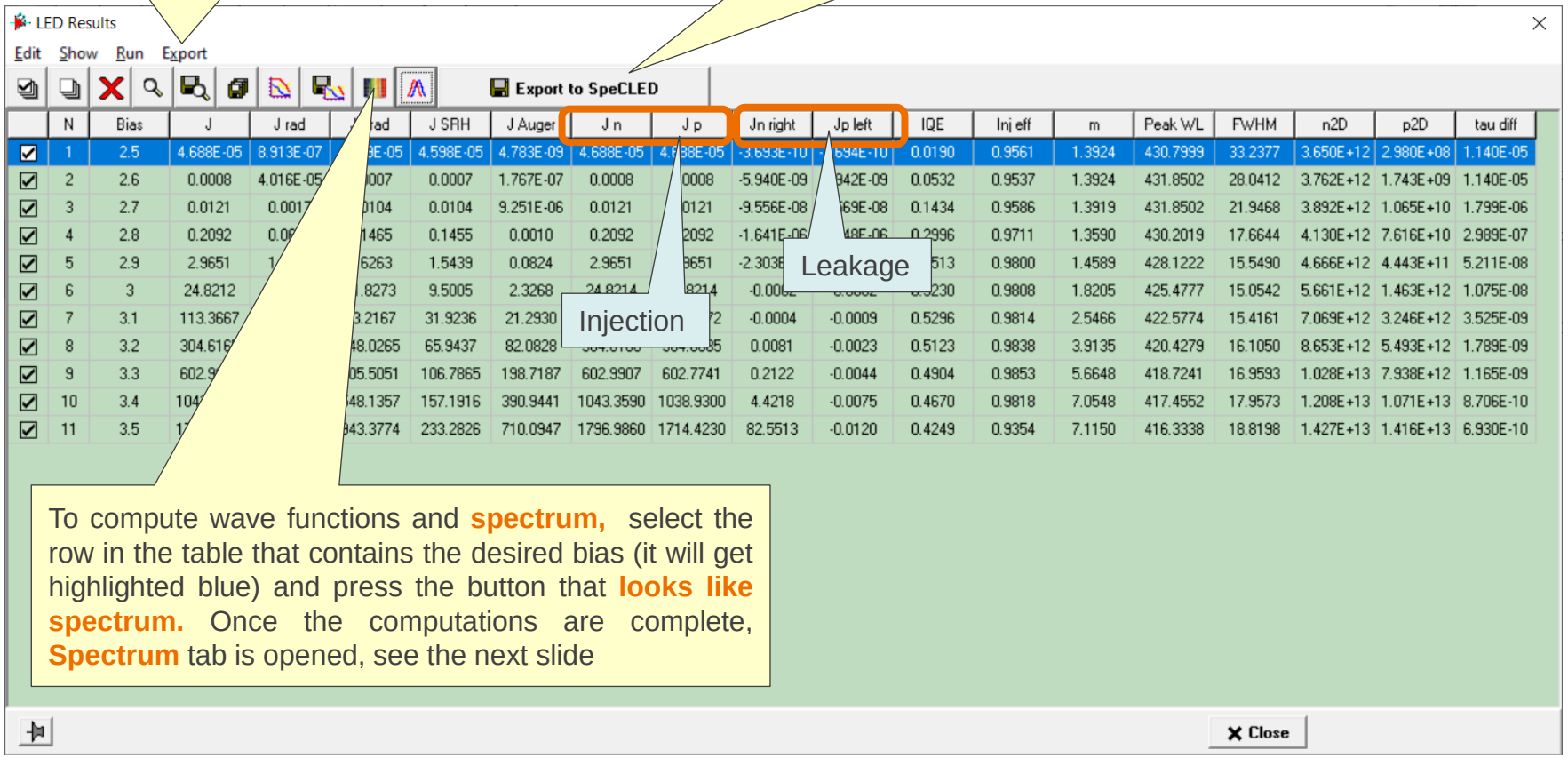
Step 4 (Continued): LED results



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

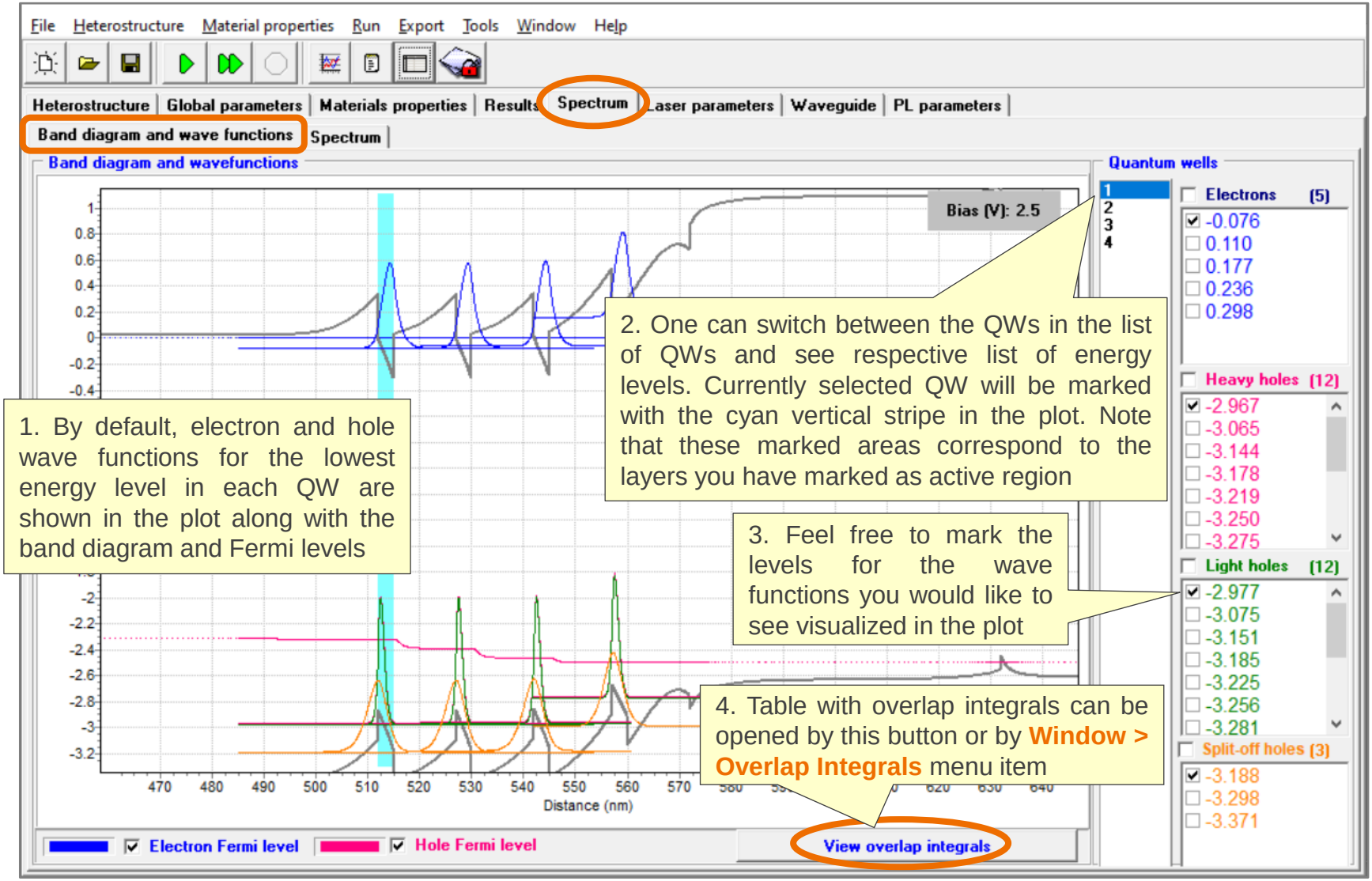
While **Export to SpeCLED** button can be used to export of the results for its further use in SpeCLED, we recommend a newer alternative option (see step 6)



	N	Bias	J	J rad	J SRH	J Auger	J n	J p	Jn right	Jp left	IQE	Inj eff	m	Peak WL	FWHM	n2D	p2D	tau diff
☑	1	2.5	4.688E-05	8.913E-07	4.598E-05	4.783E-09	4.688E-05	4.688E-05	-3.693E-10	-6.94E-10	0.0190	0.9561	1.3924	430.7999	33.2377	3.650E+12	2.980E+08	1.140E-05
☑	2	2.6	0.0008	4.016E-05	0.0007	1.767E-07	0.0008	0008	-5.940E-09	942E-09	0.0532	0.9537	1.3924	431.8502	28.0412	3.762E+12	1.743E+09	1.140E-05
☑	3	2.7	0.0121	0.0017	0104	9.251E-06	0.0121	0121	-9.556E-08	69E-08	0.1434	0.9586	1.3919	431.8502	21.9468	3.892E+12	1.065E+10	1.799E-06
☑	4	2.8	0.2092	0.0	1465	0.0010	0.2092	2092	-1.641E-06	48E-06	0.2396	0.9711	1.3590	430.2019	17.6644	4.130E+12	7.616E+10	2.989E-07
☑	5	2.9	2.9651	1	6263	0.0824	2.9651	9651	-2.303E		513	0.9800	1.4589	428.1222	15.5490	4.666E+12	4.443E+11	5.211E-08
☑	6	3	24.8212		.8273	2.3268	24.8214	8214	-0.000		230	0.9808	1.8205	425.4777	15.0542	5.661E+12	1.463E+12	1.075E-08
☑	7	3.1	113.3667		3.2167	21.2930	72	72	-0.0004	-0.0009	0.5296	0.9814	2.5466	422.5774	15.4161	7.069E+12	3.246E+12	3.525E-09
☑	8	3.2	304.616		48.0265	82.0828			0.0081	-0.0023	0.5123	0.9838	3.9135	420.4279	16.1050	8.653E+12	5.493E+12	1.789E-09
☑	9	3.3	602.9		05.5051	198.7187	602.9907	602.7741	0.2122	-0.0044	0.4904	0.9853	5.6648	418.7241	16.9593	1.028E+13	7.938E+12	1.165E-09
☑	10	3.4	104		48.1357	390.9441	1043.3590	1038.9300	4.4218	-0.0075	0.4670	0.9818	7.0548	417.4552	17.9573	1.208E+13	1.071E+13	8.706E-10
☑	11	3.5	17		943.3774	710.0947	1796.9860	1714.4230	82.5513	-0.0120	0.4249	0.9354	7.1150	416.3338	18.8198	1.427E+13	1.416E+13	6.930E-10

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



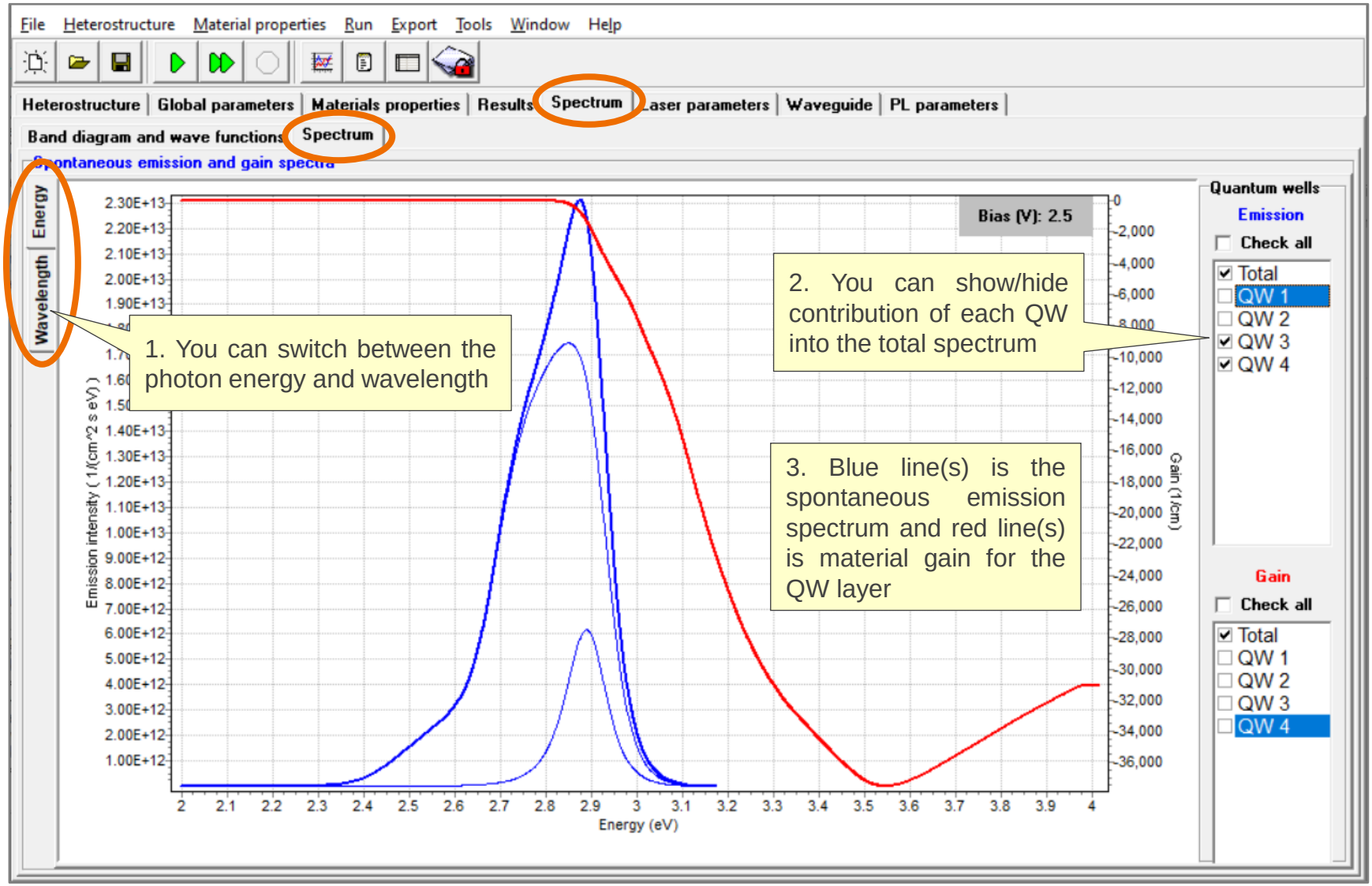
1. By default, electron and hole wave functions for the lowest energy level in each QW are shown in the plot along with the band diagram and Fermi levels

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

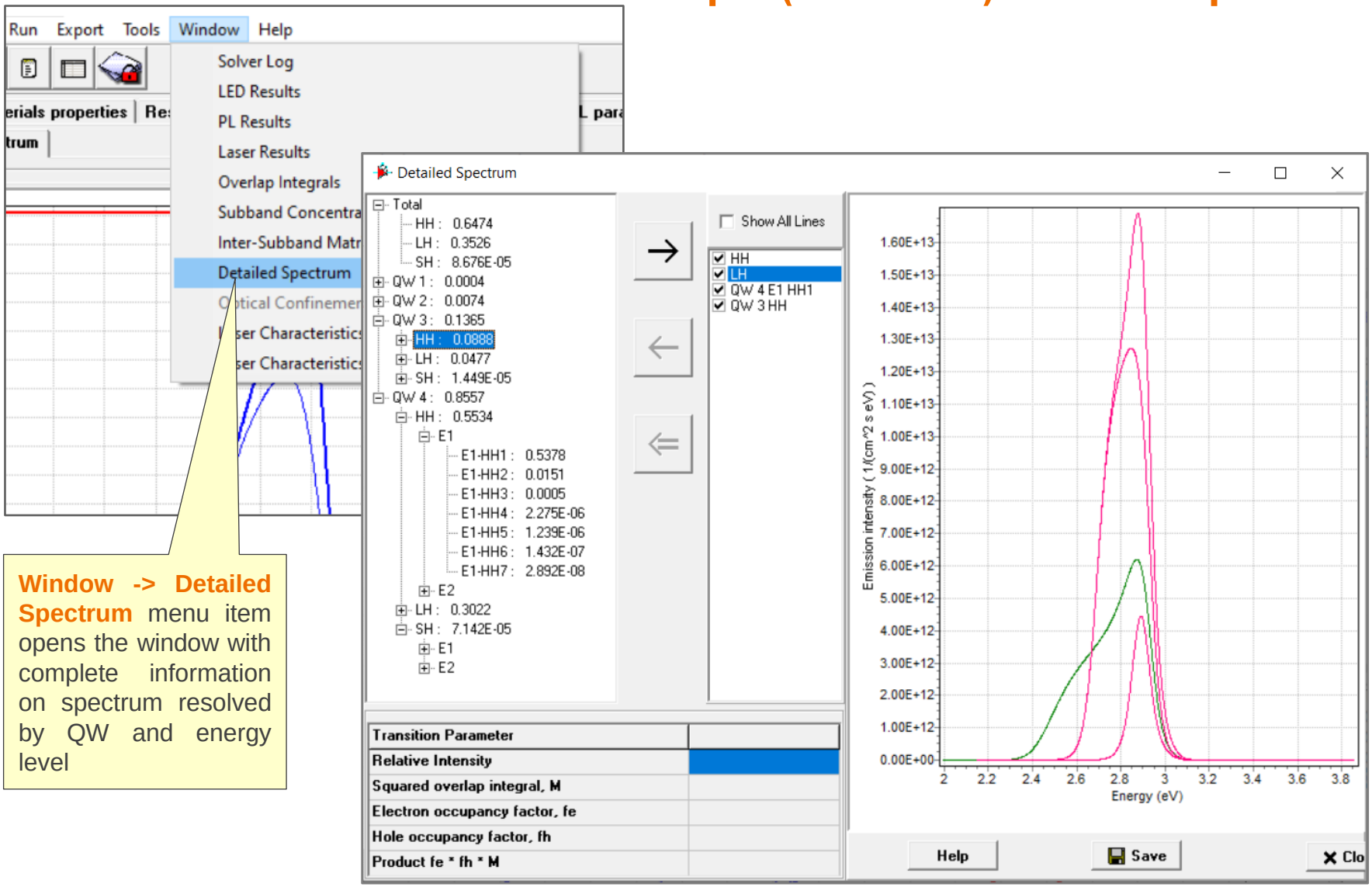
3. Feel free to mark the levels for the wave functions you would like to see visualized in the plot

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

Step 5 (Continued): Emission and gain spectrum

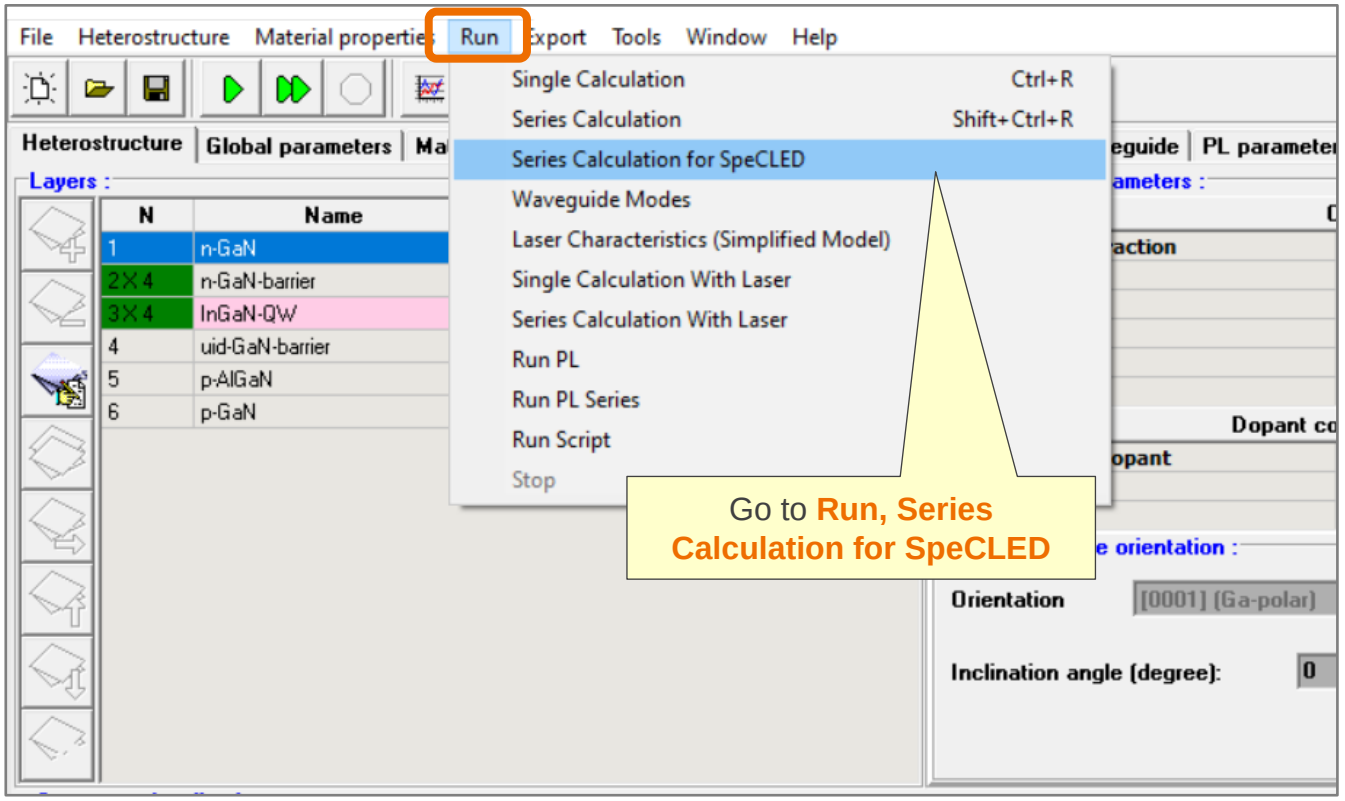


Step 5 (Continued): Detailed spectrum



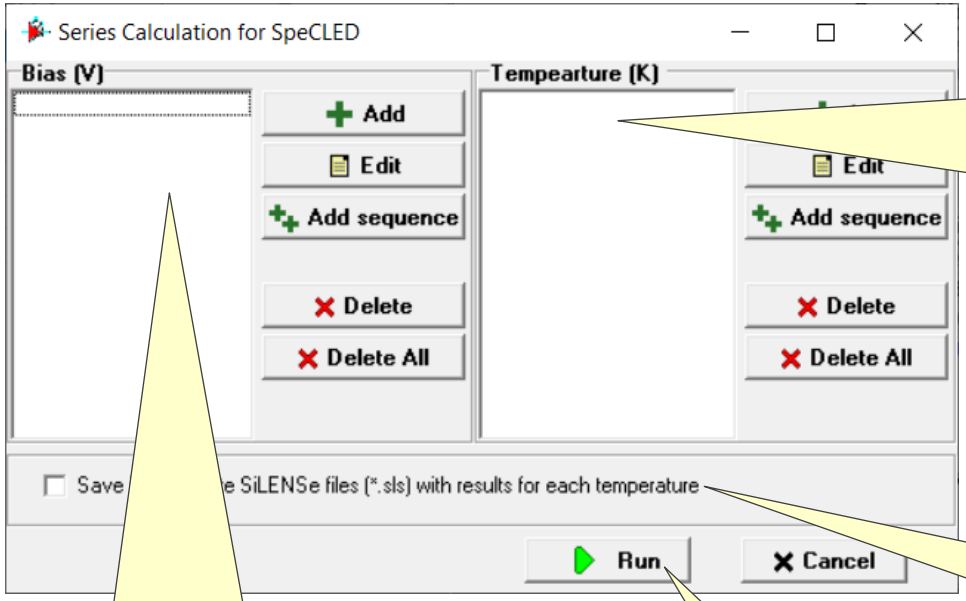
Window -> Detailed Spectrum menu item opens the window with complete information on spectrum resolved by QW and energy level

Step 6: Preparing input data for SpeCLED



Automatic generation of data file according to the user specified variation of both p-n junction bias and temperature is supported. The output data for SpeCLED are organized as a single *.txt file with the same filename as the project file. New approach allows running SpeCLED computations with account of lateral carrier diffusion in the active region and surface recombination.

Step 6: Preparing input data for SpeCLED (2)



2. To run **SpeCLED** simulations with account for self-heating effects, you would need to have data for a range of temperatures that you anticipate in the device. We recommend using the step of 5-20K (for instance, T = 300, 320, 340, 360, 380, 400, 420, 440, 460, 480, 500 K)

3. Check this checkbox if you want the results for each temperatures to be saved as a separated project files.

1. Series computations should cover your typical range of the p-n junction bias variation. At the biases providing current density of interest, the recommended bias step is 10-50 mV.

Note that with increase of temperature the p-n junction bias corresponding to a certain current density becomes lower.

4. **Run** button starts calculations followed by the data export into the *.txt file.

End of Tutorial 1

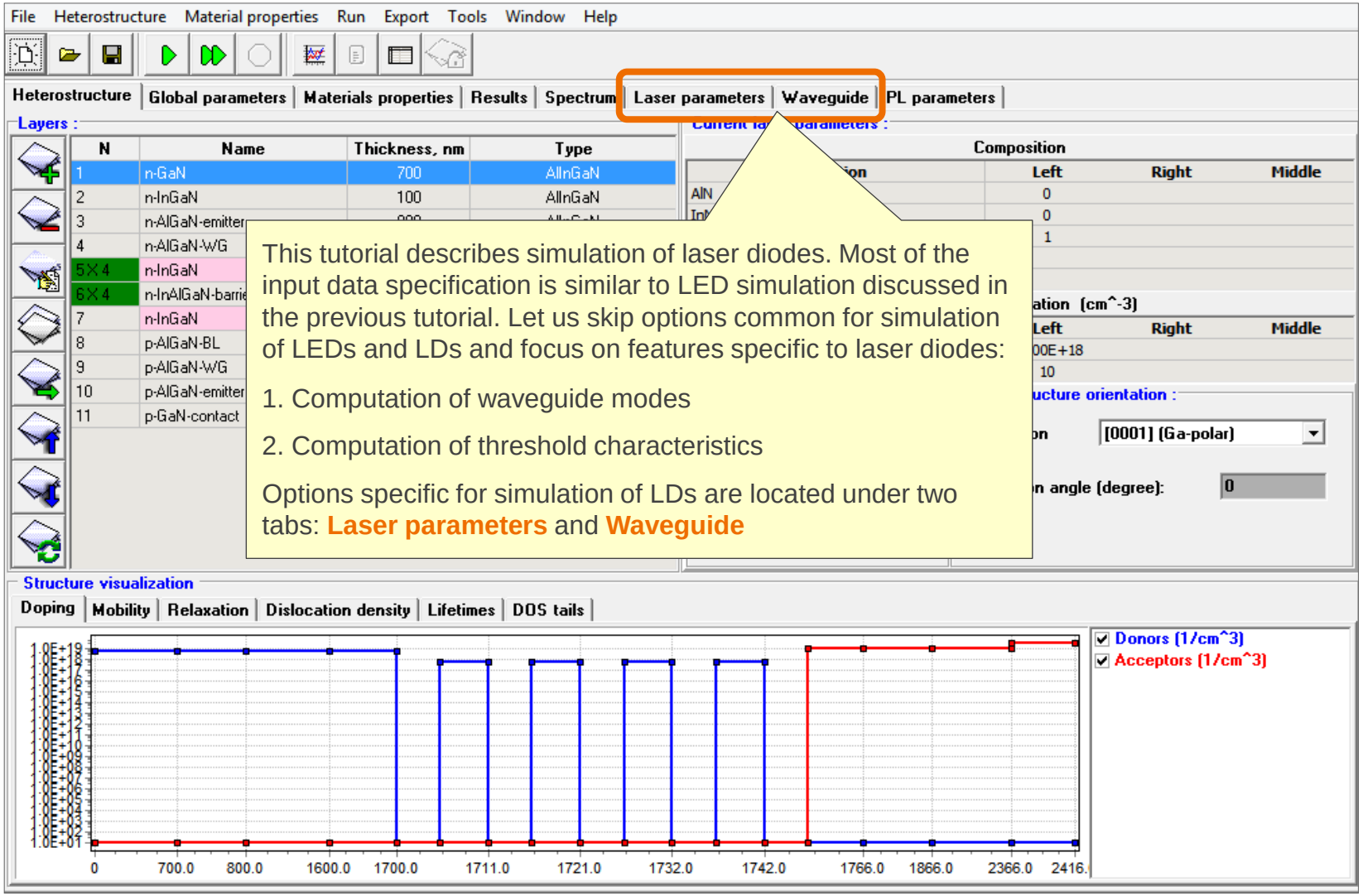
Tutorial 2

SiLENSe Laser Edition 5.12

Using SiLENSe for Modeling of Lasers:

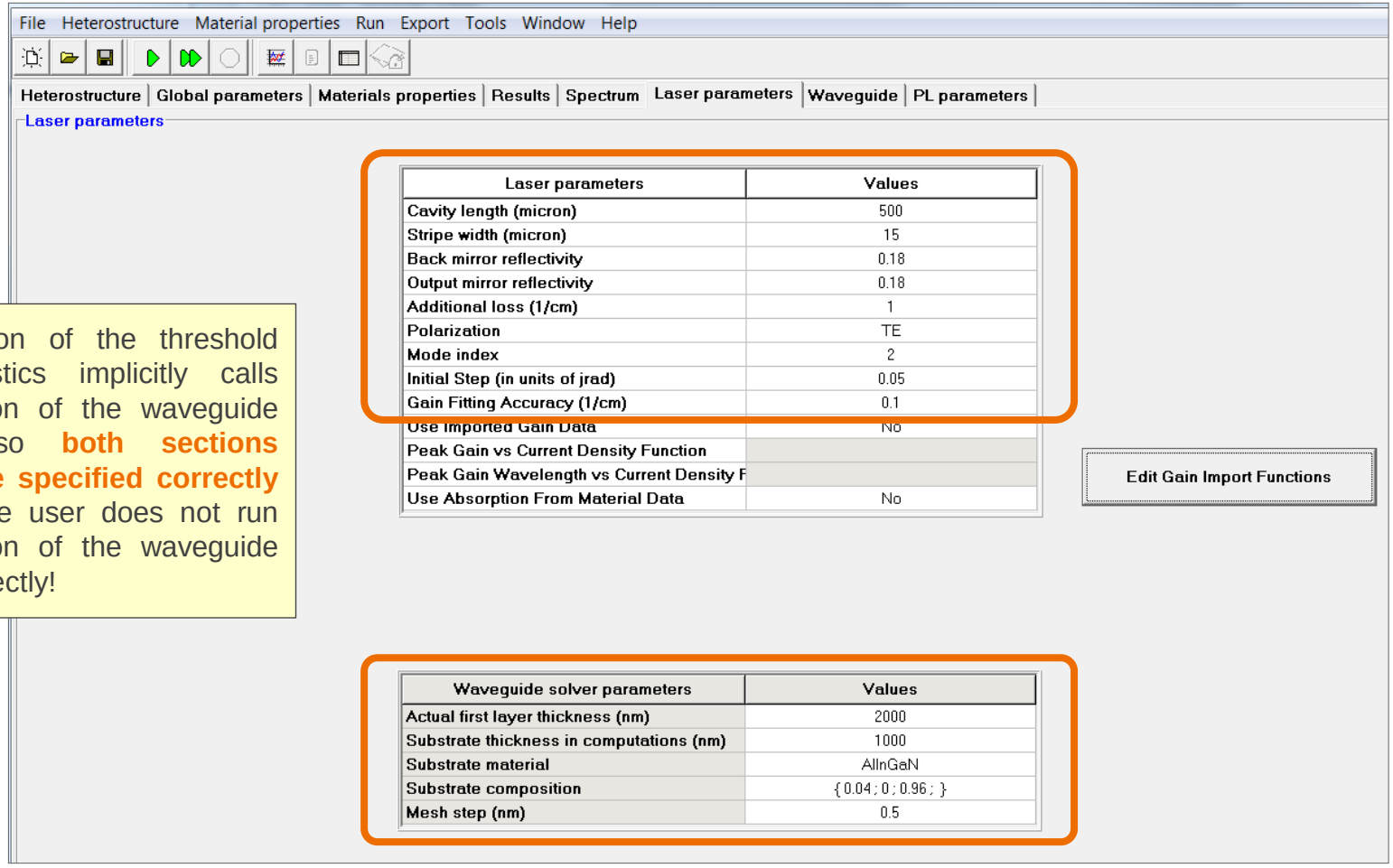
Simulation of InGaN MQW UV laser diode

Features specific to laser diodes



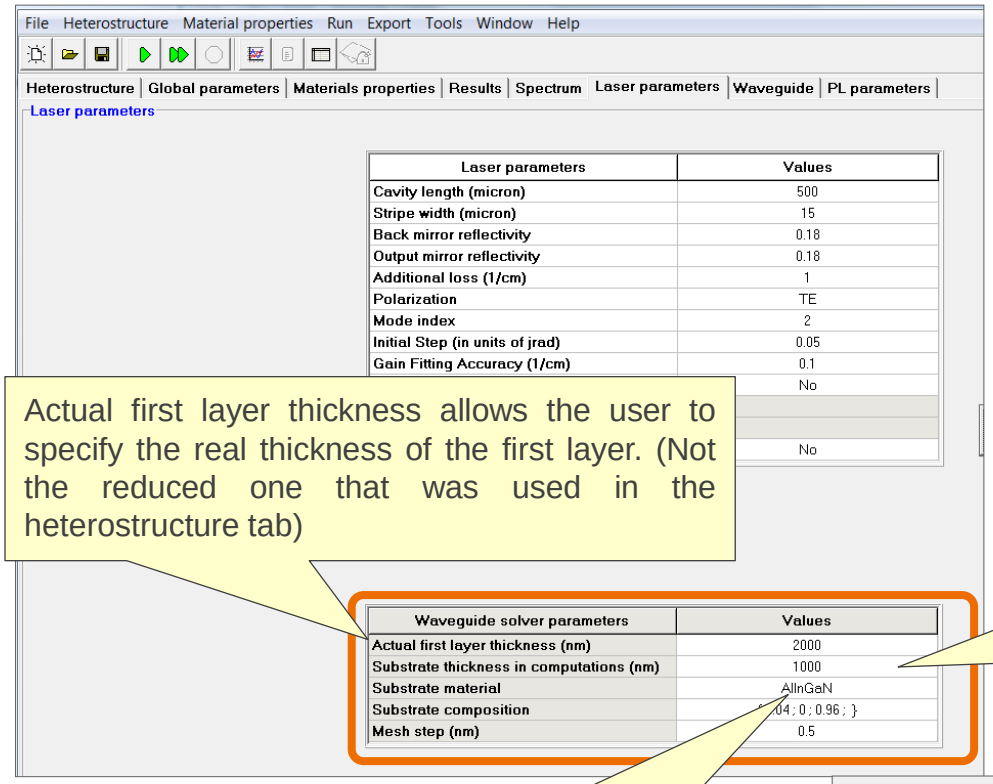
Specifying options specific for LDs

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.



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

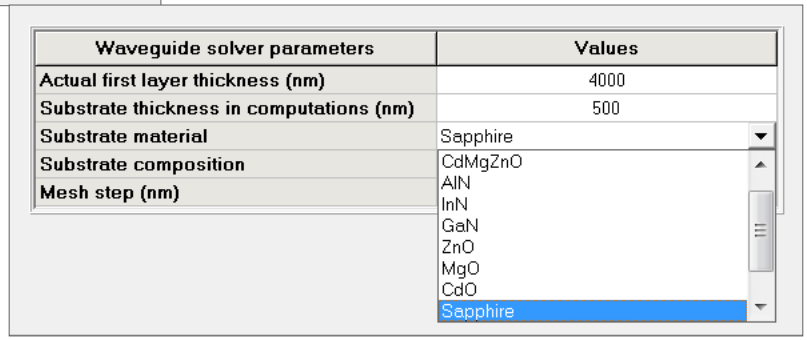


Actual first layer thickness allows the user to specify the real thickness of the first layer. (Not the reduced one that was used in the heterostructure tab)

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**

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

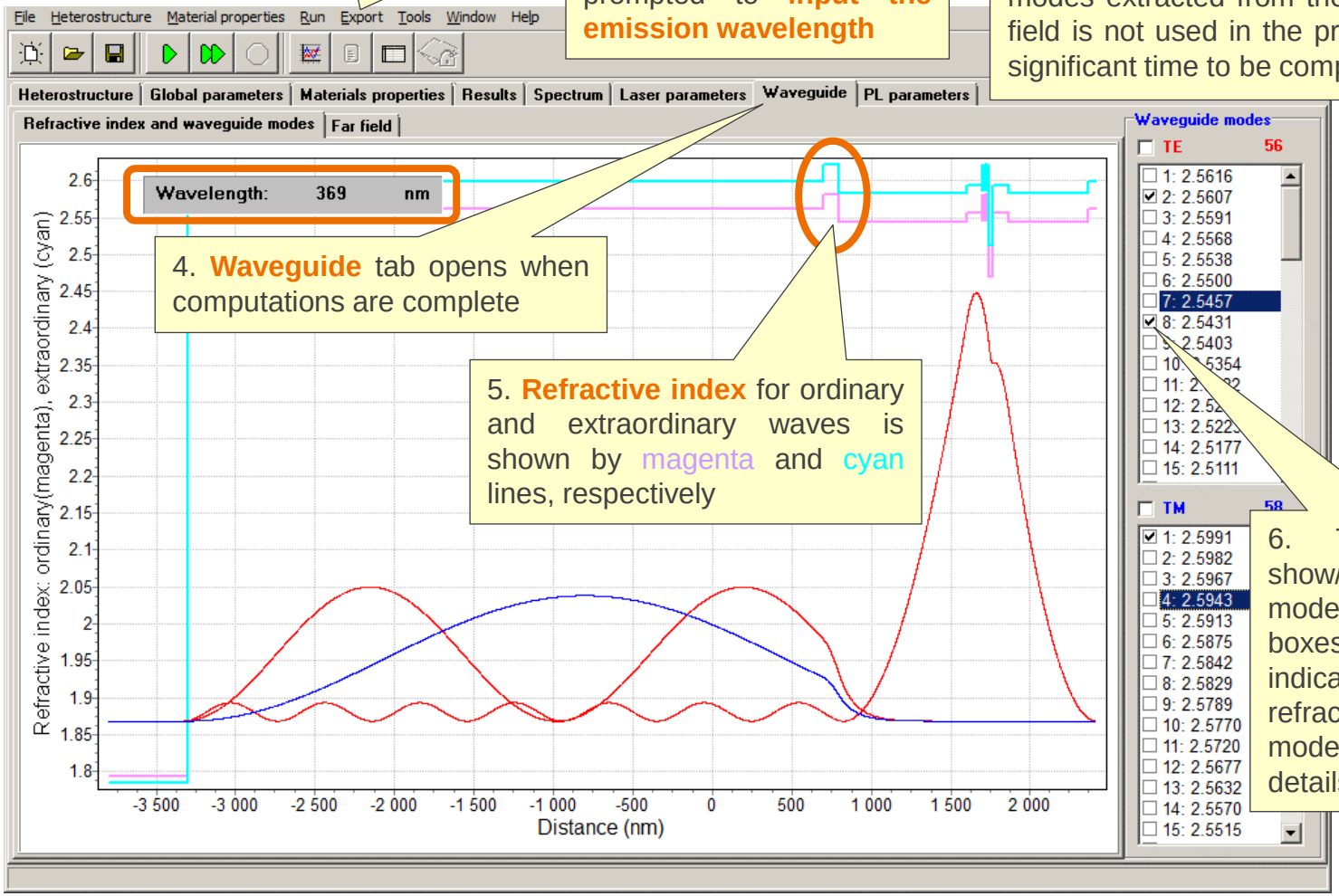


Computation of waveguide modes

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)

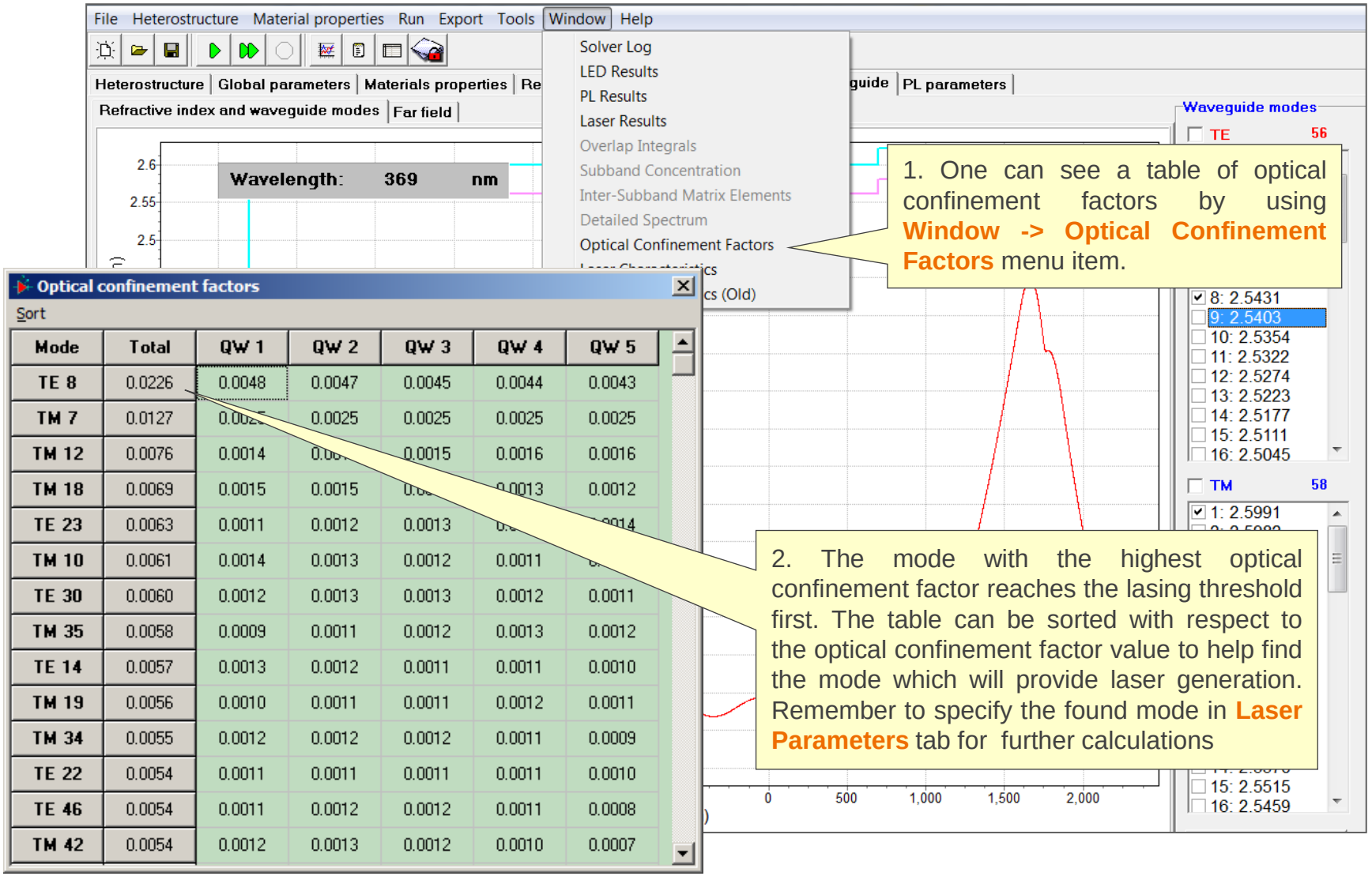


4. **Waveguide** tab opens when computations are complete

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

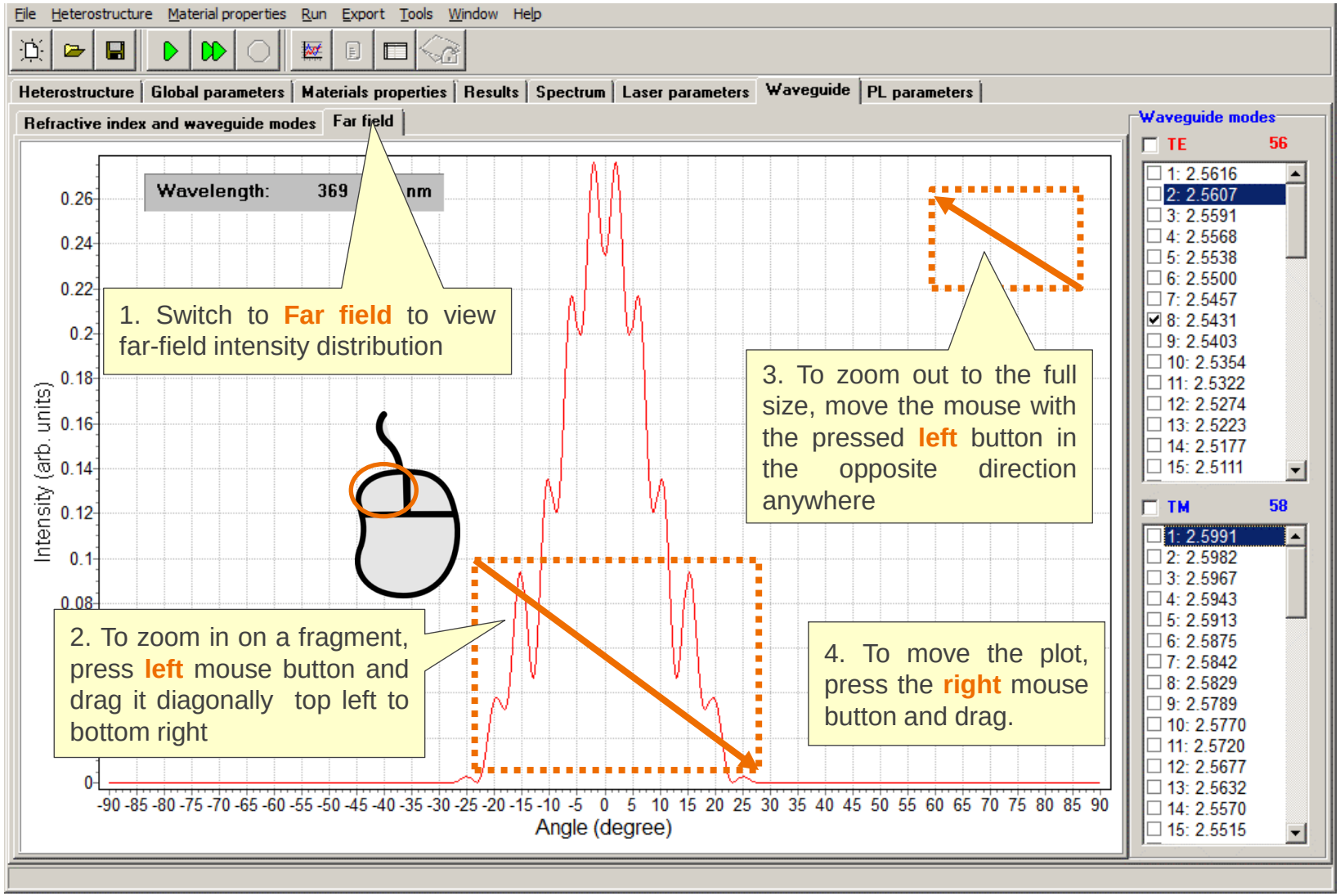


Optical confinement factors

Sort

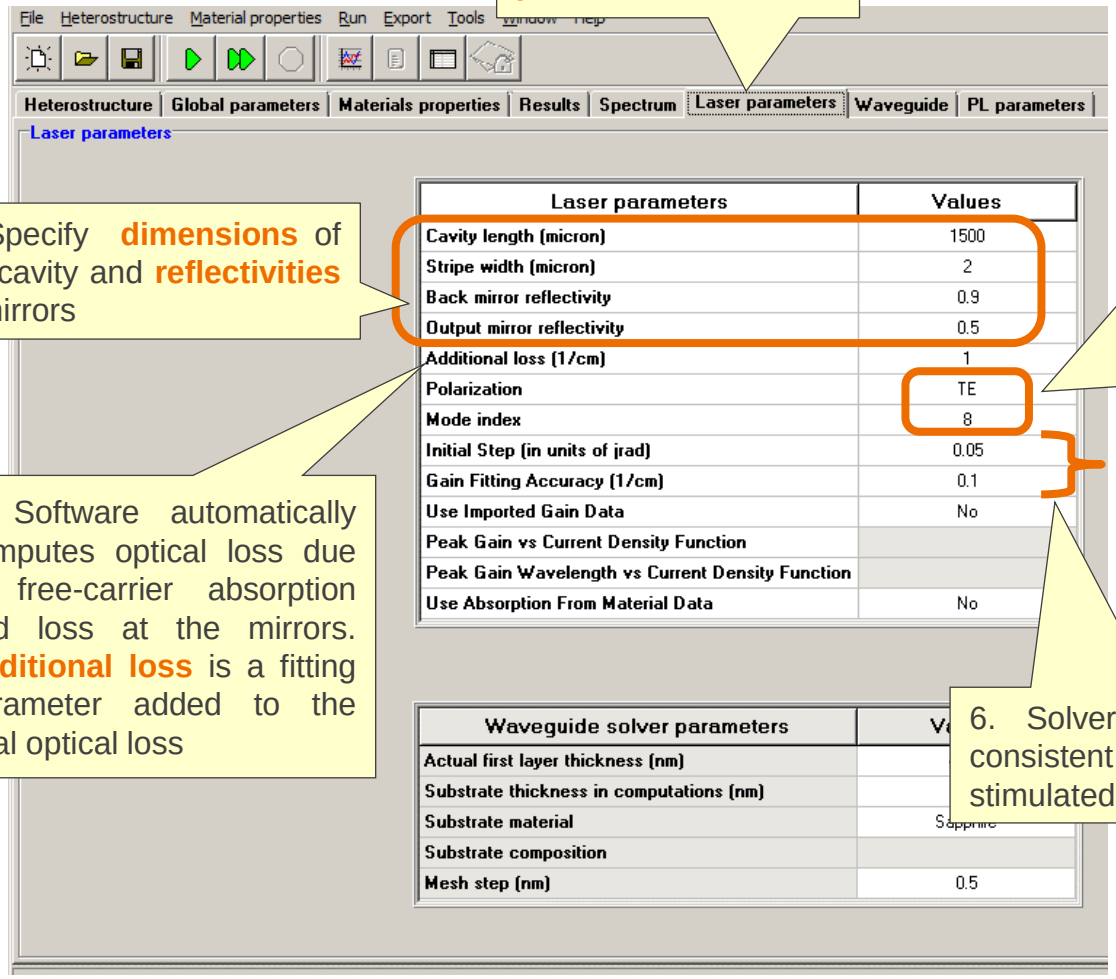
Mode	Total	QW 1	QW 2	QW 3	QW 4	QW 5
TE 8	0.0226	0.0048	0.0047	0.0045	0.0044	0.0043
TM 7	0.0127	0.0025	0.0025	0.0025	0.0025	0.0025
TM 12	0.0076	0.0014	0.0015	0.0016	0.0016	
TM 18	0.0069	0.0015	0.0015	0.0013	0.0012	
TE 23	0.0063	0.0011	0.0012	0.0013		
TM 10	0.0061	0.0014	0.0013	0.0012	0.0011	
TE 30	0.0060	0.0012	0.0013	0.0013	0.0012	0.0011
TM 35	0.0058	0.0009	0.0011	0.0012	0.0013	0.0012
TE 14	0.0057	0.0013	0.0012	0.0011	0.0011	0.0010
TM 19	0.0056	0.0010	0.0011	0.0011	0.0012	0.0011
TM 34	0.0055	0.0012	0.0012	0.0012	0.0011	0.0009
TE 22	0.0054	0.0011	0.0011	0.0011	0.0011	0.0010
TE 46	0.0054	0.0011	0.0012	0.0012	0.0011	0.0008
TM 42	0.0054	0.0012	0.0013	0.0012	0.0010	0.0007

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



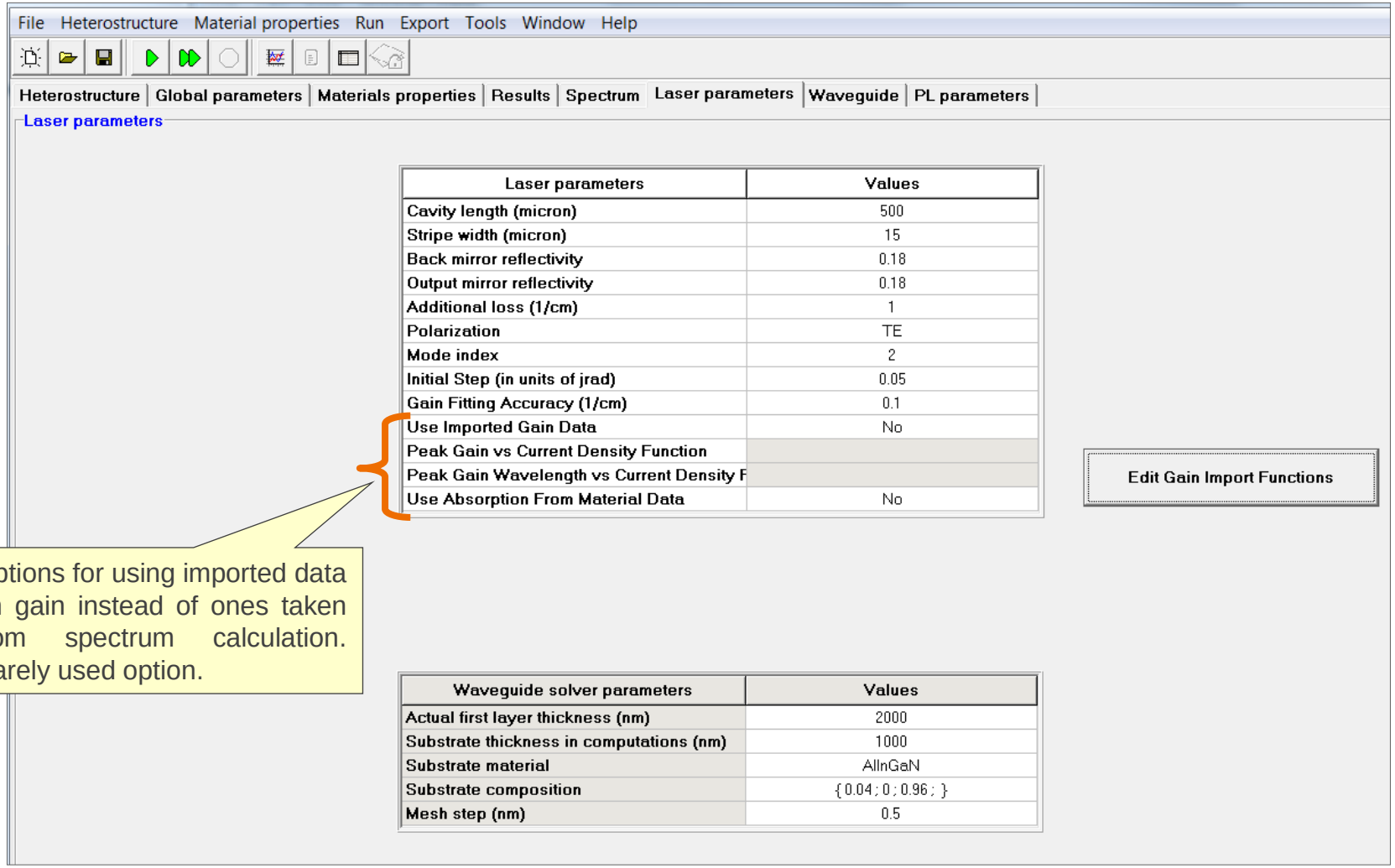
2. Specify **dimensions** of the cavity and **reflectivities** of mirrors

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

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 the section on viewing the confinement factors)

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

Parameters for computation of threshold characteristics and laser output power beyond the threshold. Additional options



Laser parameters	Values
Cavity length (micron)	500
Stripe width (micron)	15
Back mirror reflectivity	0.18
Output mirror reflectivity	0.18
Additional loss (1/cm)	1
Polarization	TE
Mode index	2
Initial Step (in units of jrad)	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 F	
Use Absorption From Material Data	No

Waveguide solver parameters	Values
Actual first layer thickness (nm)	2000
Substrate thickness in computations (nm)	1000
Substrate material	AlInGaN
Substrate composition	{ 0.04 ; 0 ; 0.96 ; }
Mesh step (nm)	0.5

Computation flow in self-consistent laser model (1)

Modal gain is computed as a sum of the gain values (at given wavelength) with account of confinement factors of each QW

Optical losses include:

• Losses on back and output mirrors;

• Free-carrier losses;

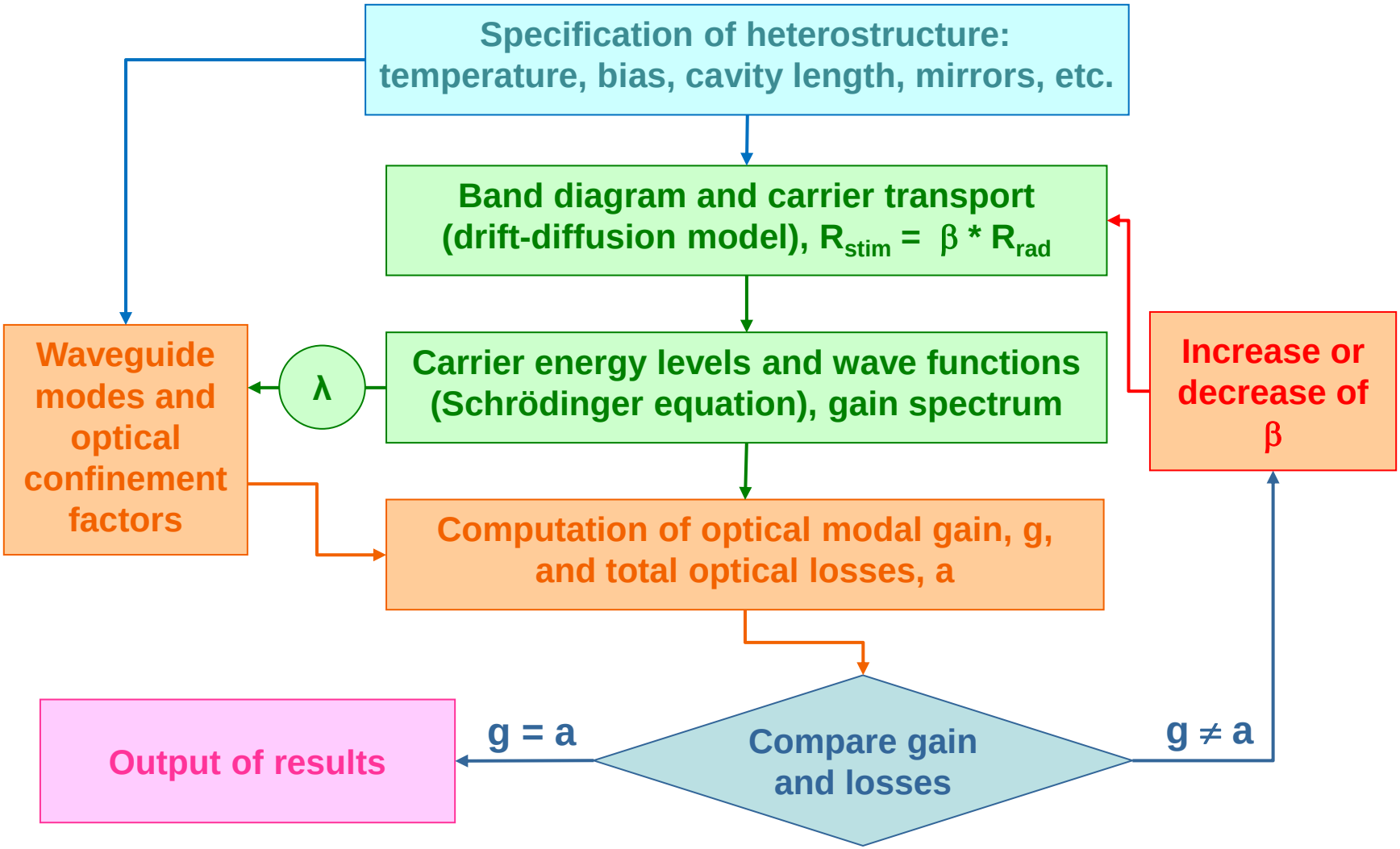
• Additional optical losses in waveguide (can be used as fitting parameter)

Threshold is determined by comparing modal gain and total modal losses. Specification of global parameters (like temperature). Above the threshold, the stimulated recombination is included self-consistently into the drift-diffusion model as following. In the quantum wells, stimulated recombination rate is assumed to be proportional to the spontaneous radiative recombination rate, $R_{stim} = \beta R_{rad}$. Coefficient β is adjusted in order to fit the steady-state condition that modal gain is equal to total optical losses. Increase of β leads to lowering of the carrier concentration in QWs and lowering of the gain.

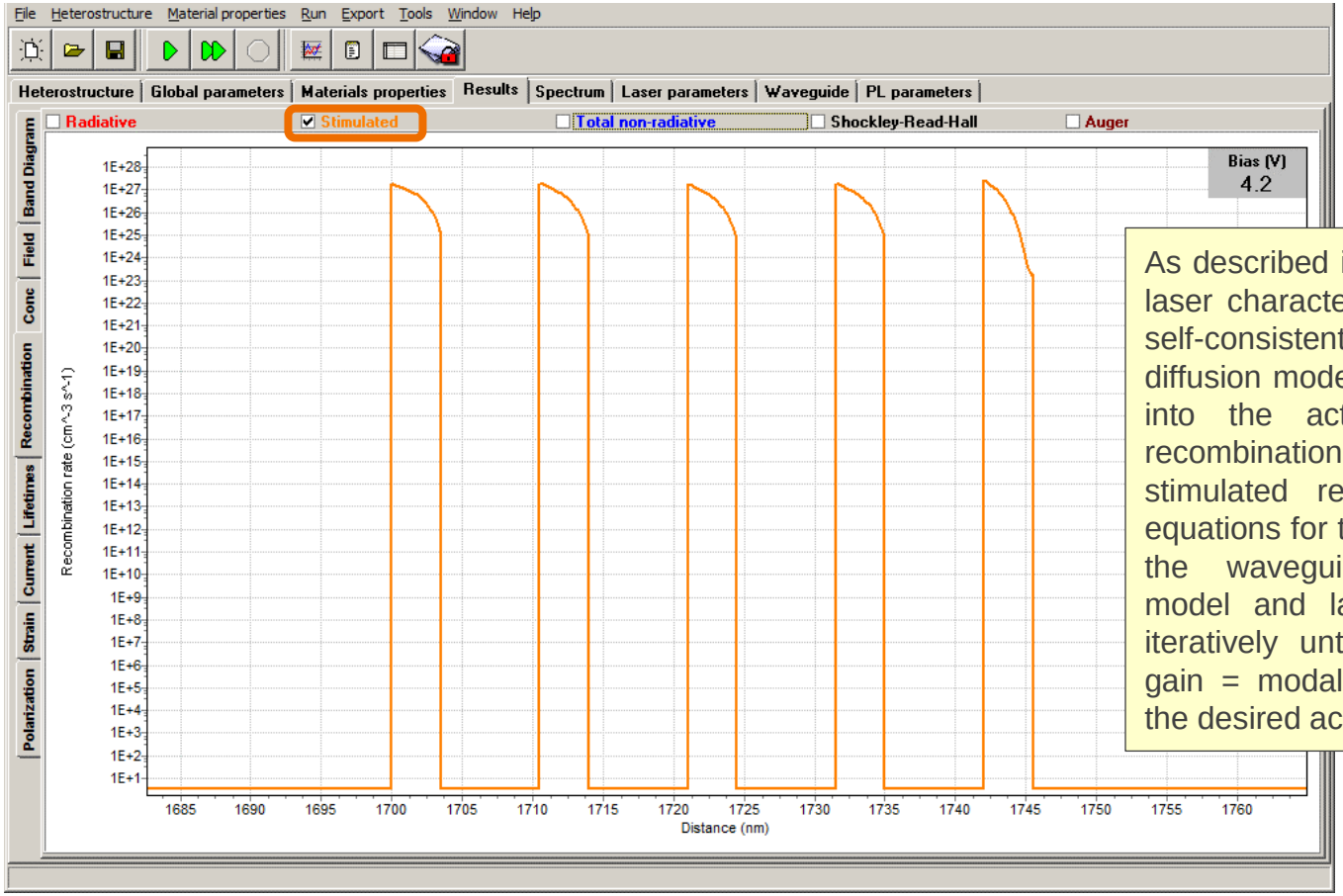
Output laser power equals to the integrated stimulated recombination rate multiplied by the factor describing losses.

See the next slide for a schematic view

Computation flow in self-consistent laser model (2)



Computation of laser characteristics

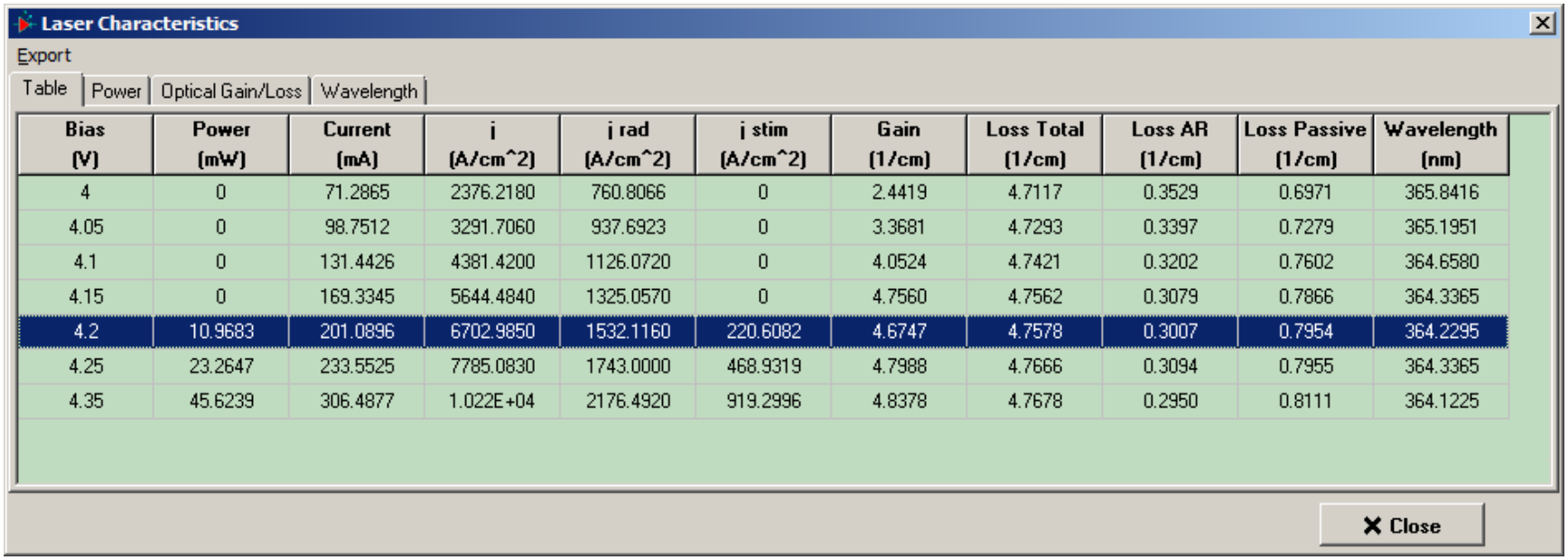


As described in the previous slide, the laser characteristics are computed by self-consistent solution of the drift-diffusion model for the carrier injection into the active region and their recombination there (including stimulated recombination) and rate equations for the number of photons in the waveguide. 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 -> Series 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



Bias (V)	Power (mW)	Current (mA)	j (A/cm^2)	j rad (A/cm^2)	j stim (A/cm^2)	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

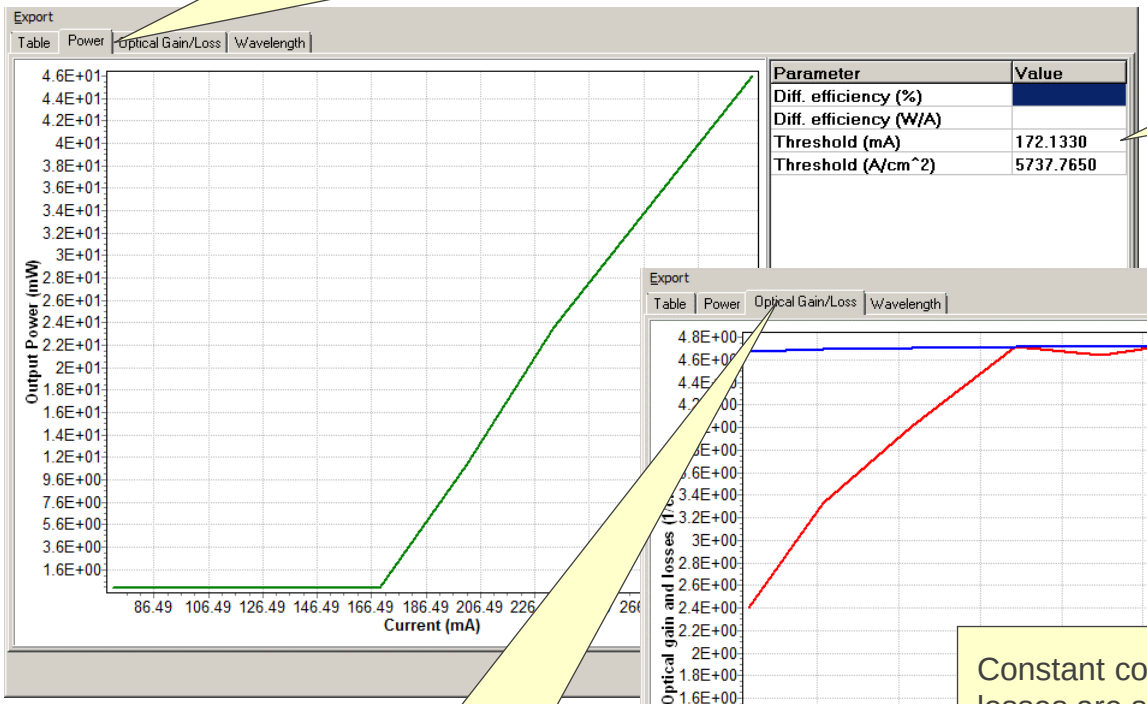
(later one can open it by using **Window -> Laser Characteristics** menu item)

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.

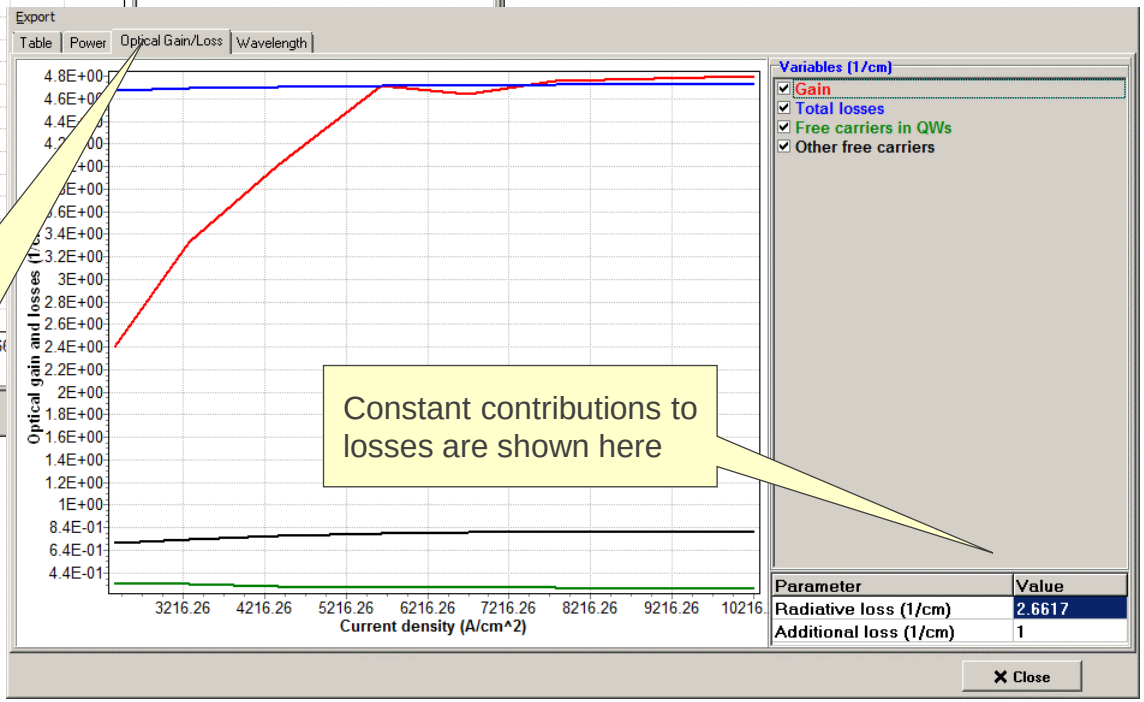
Similarly to LED results, the band diagram, carrier concentrations, etc. are stored in the project file. One can see them by using **Laser Results** window (**Window -> Laser Results** menu item). It works very similar to **LED Results** window described in the previous tutorial, see the next page.

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)



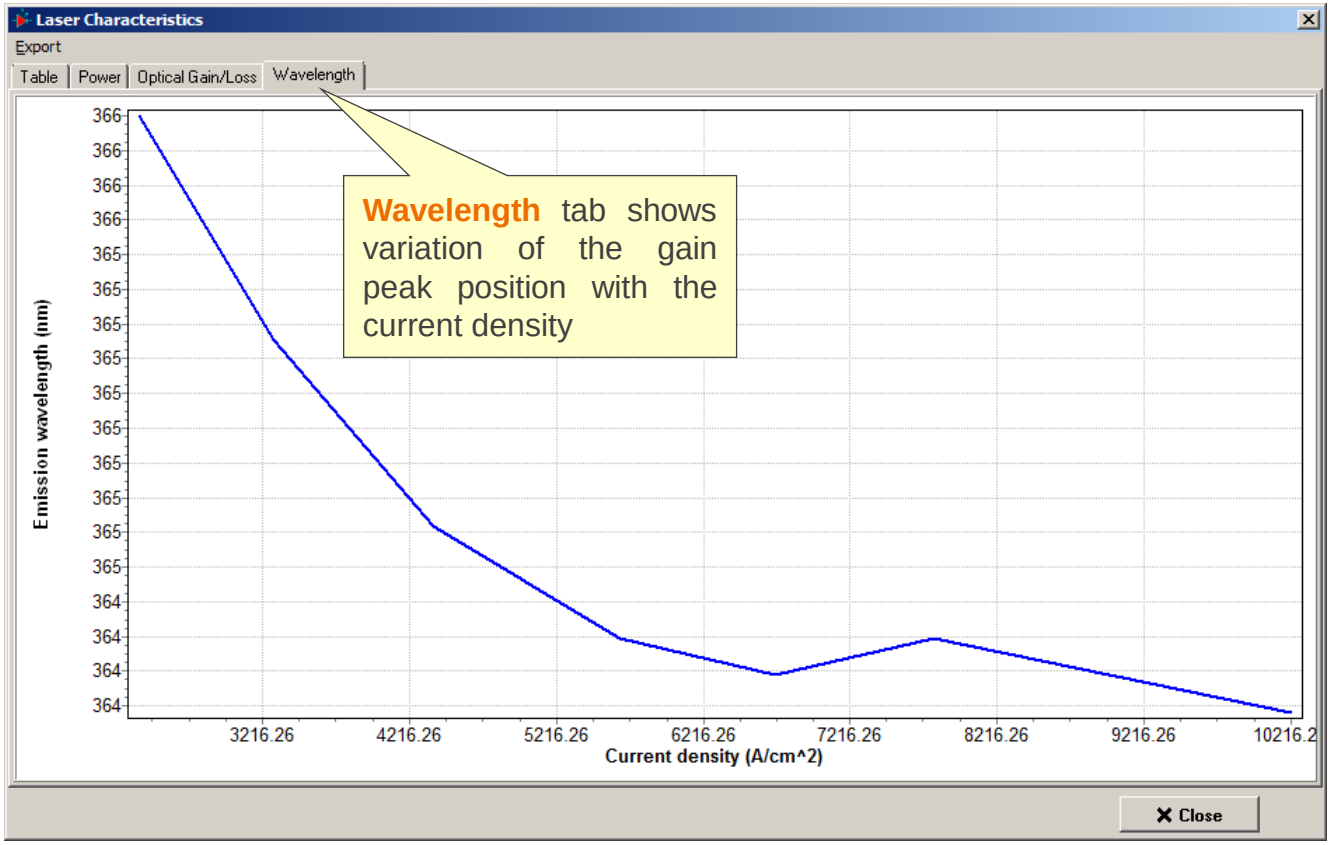
Threshold current and the respective current density are shown here



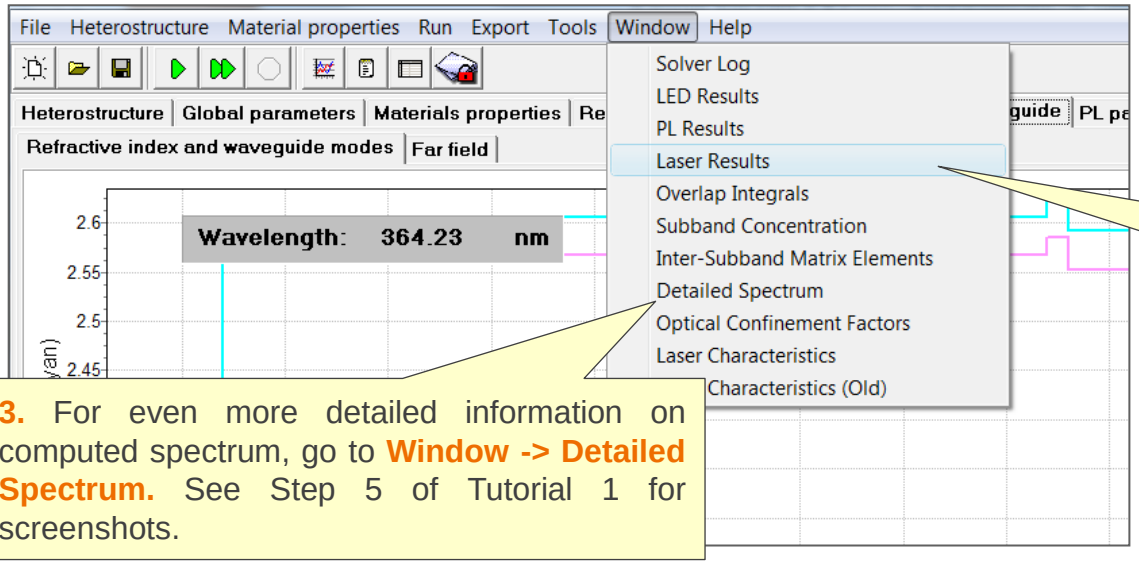
Optical Gain/Loss tab shows variation of the gain and loss as a function of current density

Constant contributions to losses are shown here

Viewing the results (Continued)



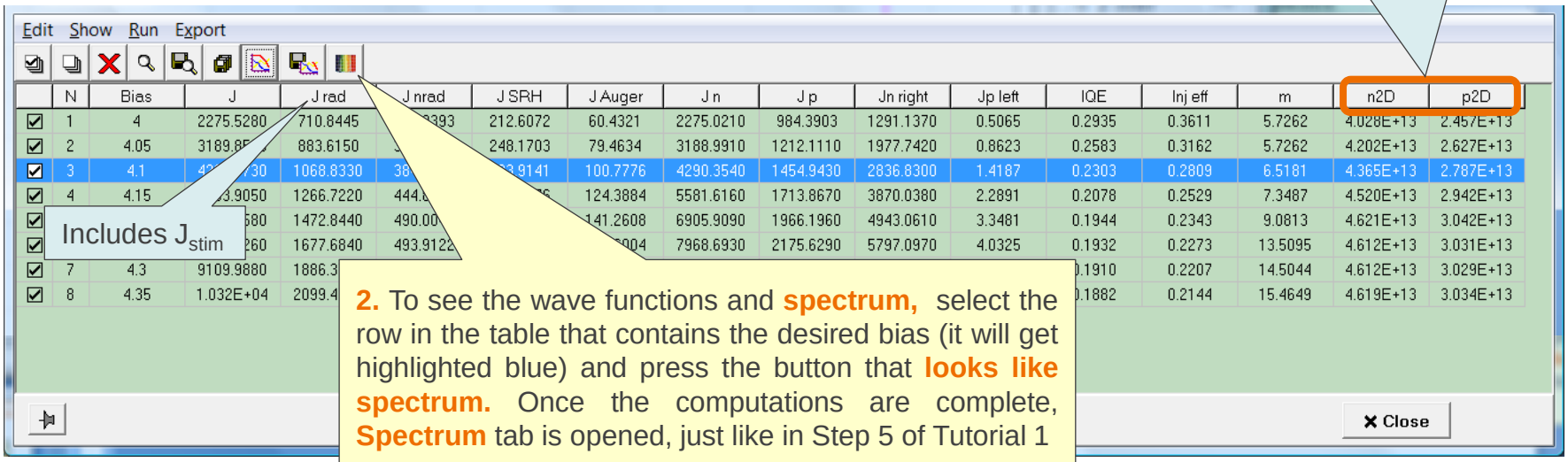
Viewing the results (continued)



1. For more results, go to **Window -> Laser Results** menu item

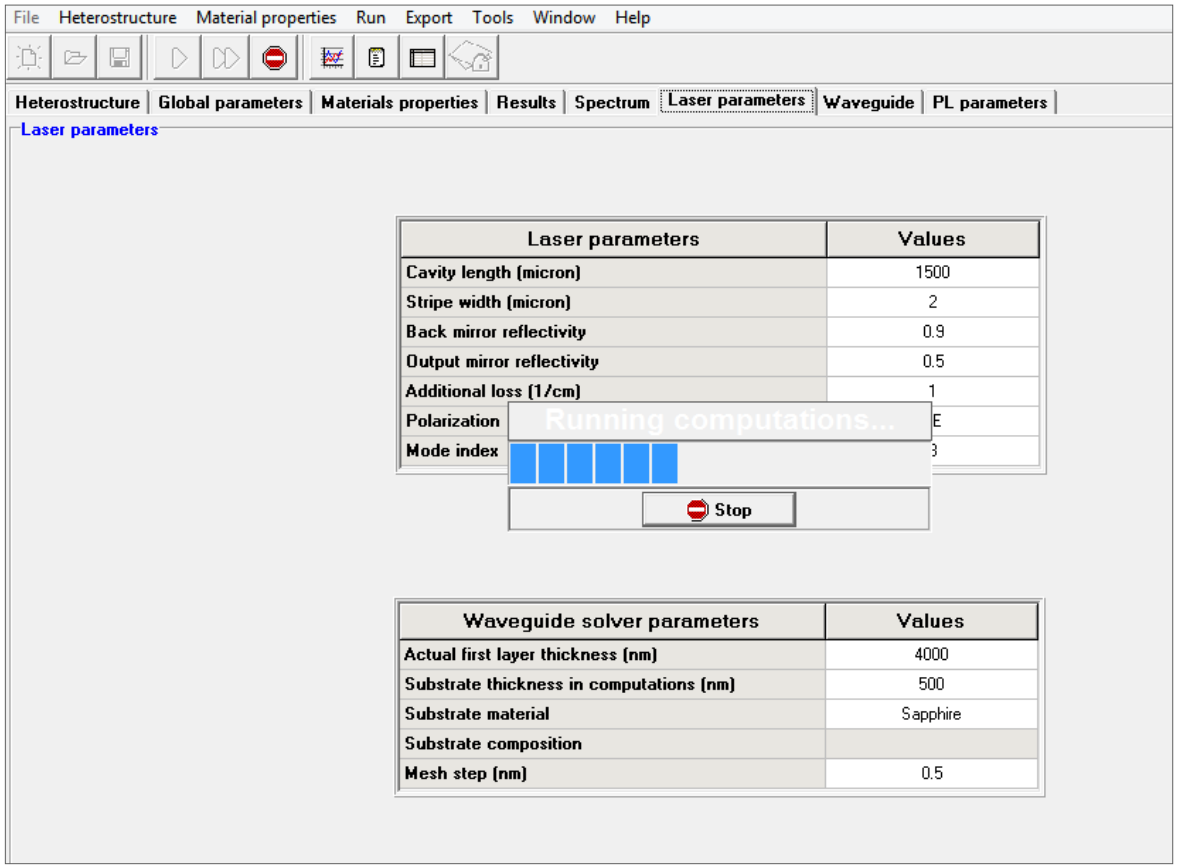
3. For even more detailed information on computed spectrum, go to **Window -> Detailed Spectrum.** See Step 5 of Tutorial 1 for screenshots.

2D carrier concentrations integrated over all the QWs



2. To see the 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, just like in Step 5 of Tutorial 1

Computation of threshold characteristics (old model)



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.

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

End of Tutorial 2

Tutorial 3

SpeCLED 2008

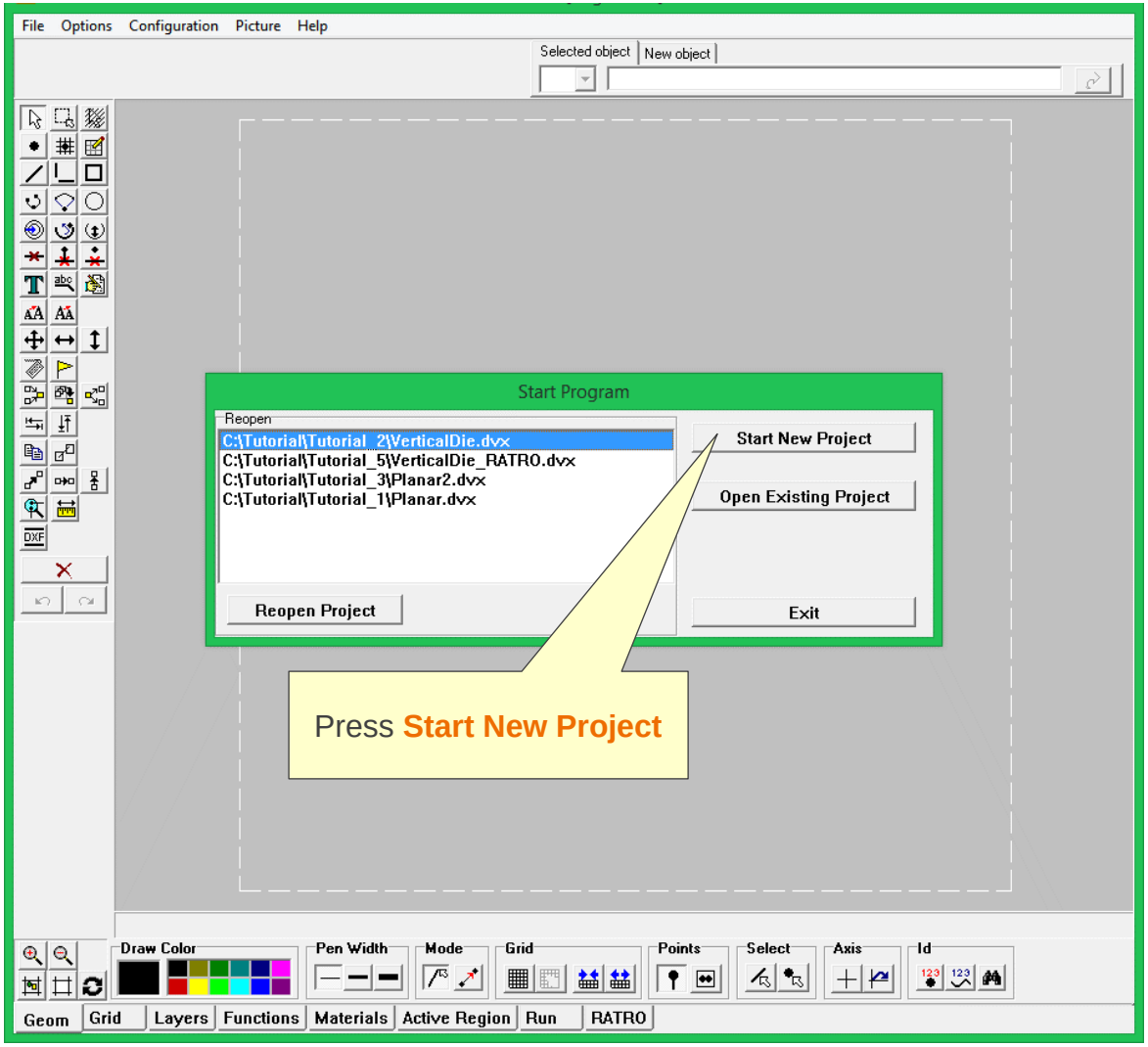
Specifying a New Problem in SpeCLED:

Simulation of a Planar Chip

This tutorial shows how to create new project similar to example “Planar 2” supplied with the software, specify all necessary input data, and start simulations. It includes the following steps:

1. Choosing the die type and specification of the layer thickness
2. Drawing lateral geometry
3. Specification of layers (building 3D geometry from 2D lateral geometry blocks)
4. Generation of the computational grid
5. Specification of the material properties
6. Specification of the active region properties
7. Specification of the heat transfer problem and other global parameters
8. Running the computations

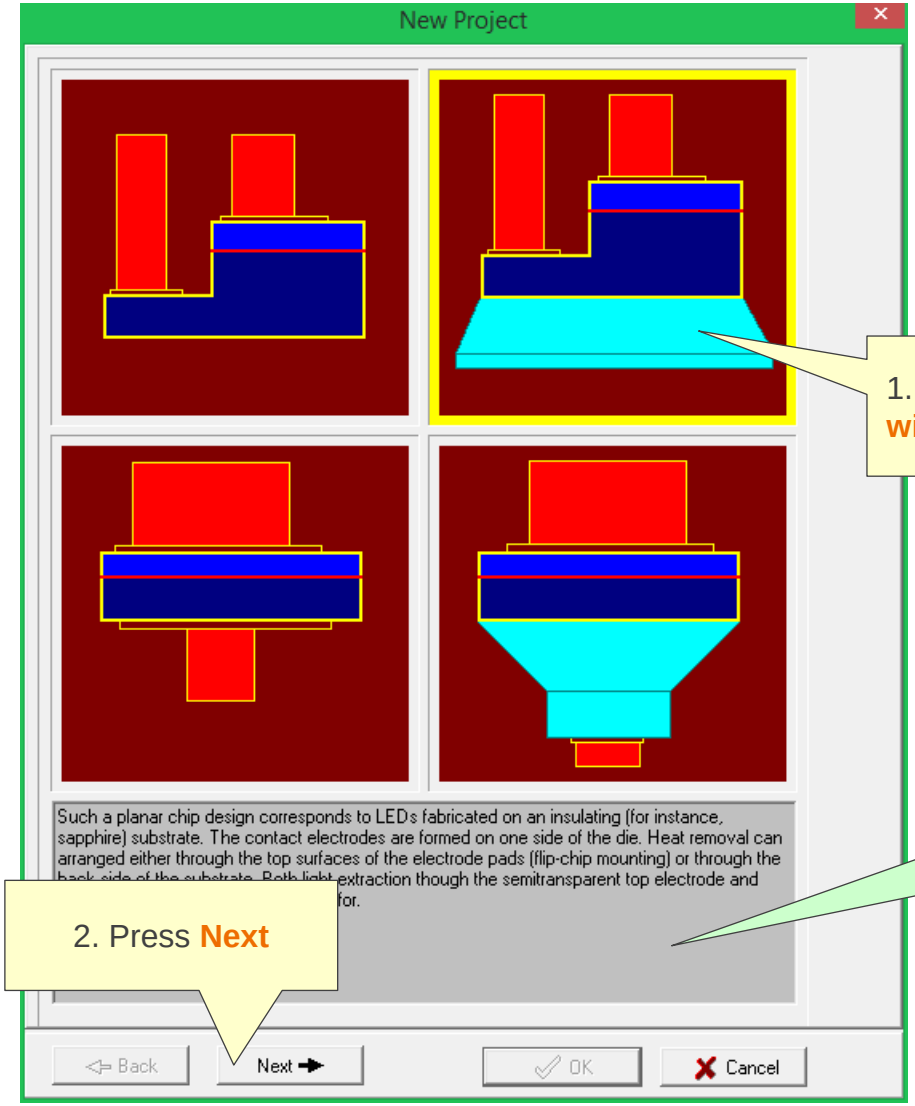
Step 1: Opening a new project



Select **Start -> All Programs -> SpeCLED 2008 -> SpeCLED 2008** or click start SpeCLED GUI. You can also use the respective desktop icon or just clock on the SpeCLED_RATRO.exe

After SpeCLED GUI is started, **Start Program dialog window** appears. It allows the user to either start a new project or open an existing one. A list of recent projects is available.

Step 1 (Continud): Choosing the die type



Project Configuration window is opened

At the start of a new project, user should first select the type of the chip to be modeled

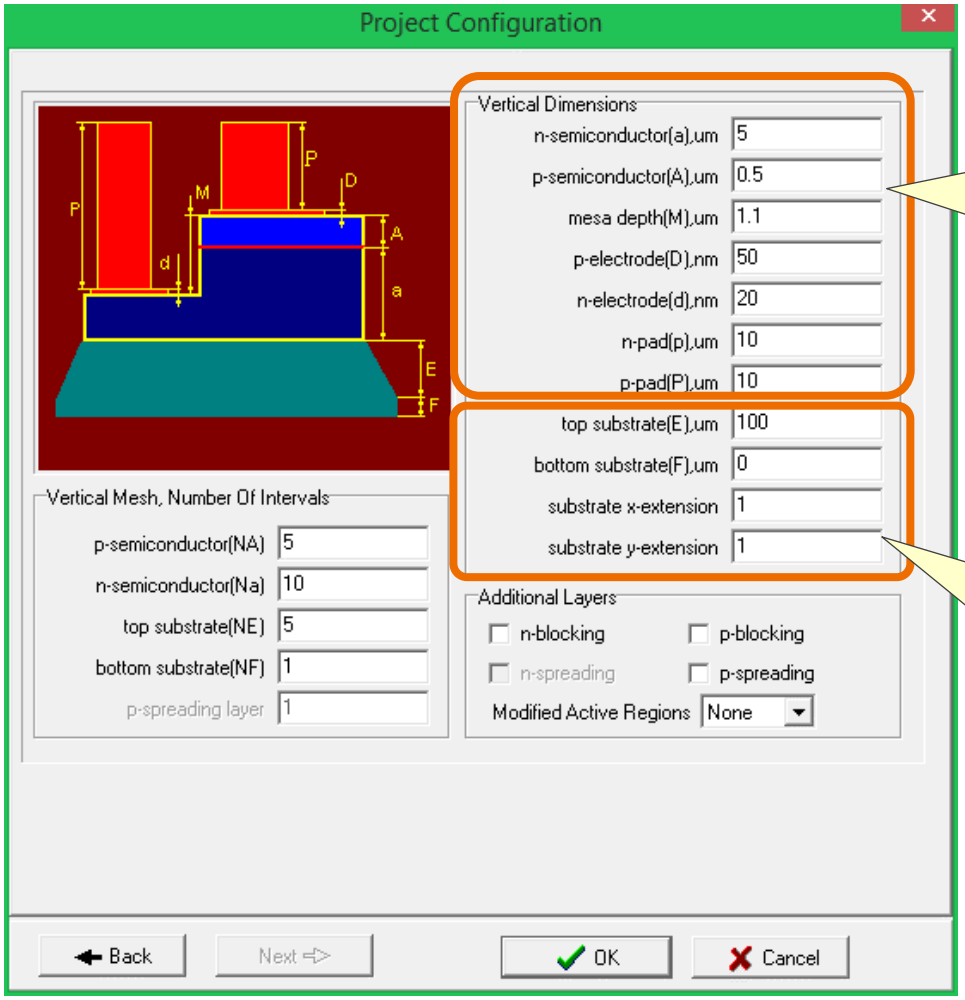
Four options are available: planar and vertical dies with and without a substrate

1. Select **Planar Chip with a Substrate**

You can try choosing different types of the chip. Each time, thorough description of the chosen chip will appear in the window below.

2. Press **Next**

Step 1 (Continued): Specification of the layer thicknesses



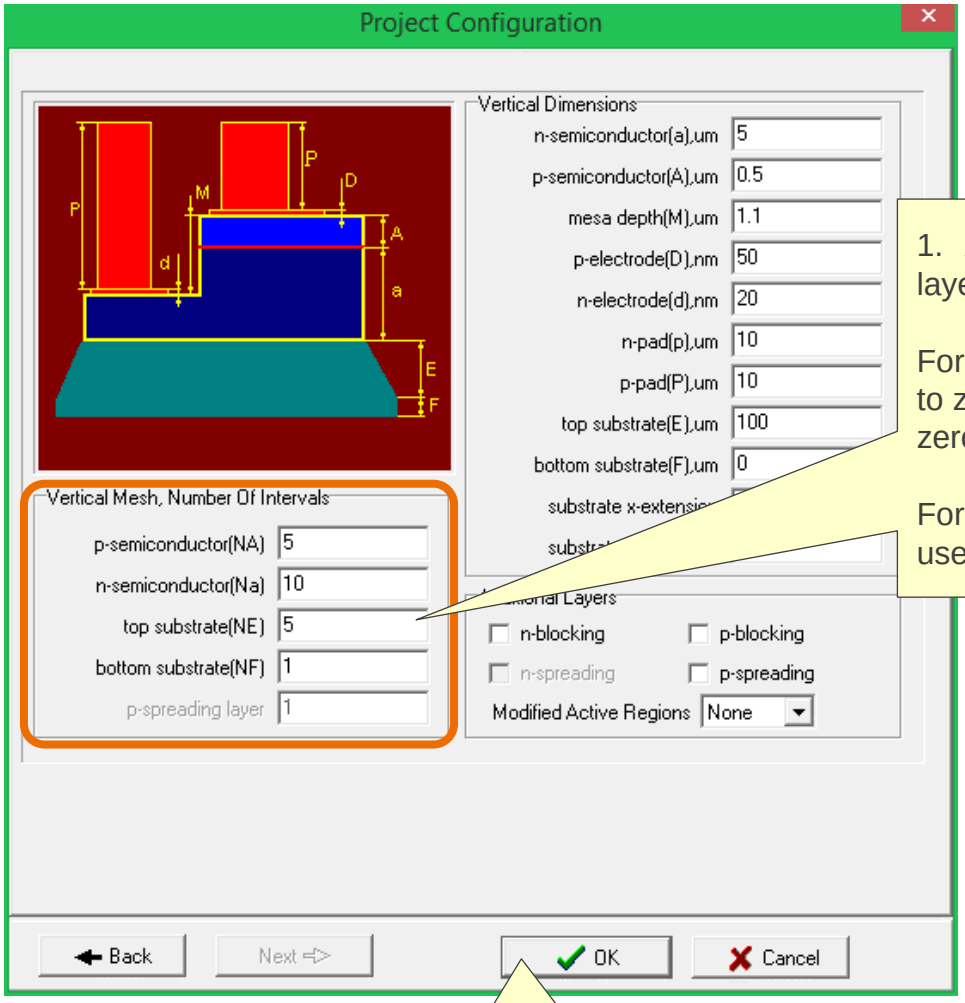
Project Configuration window is opened

1. Assign thickness of the semiconductor layers, electrodes, and pads, and substrate as follows:
n-semiconductor(a) = 5
p-semiconductor(A) = 0.5
mesa depth (M) = 1.1
p-electrode (D) = 50
n-electrode (d) = 20
n-pad(p) = 10
p-pad(P) = 10

2. Assign parameters describing the substrate thickness:
top (part of the) substrate(E) = 100
bottom (part of the) substrate (F) = 0

3. Assign relative width of the bottom part of the substrate (1 for straight vertical, <1 for narrowing, >1 for widening):
substrate x-extension = 1
substrate y-extension = 1

Step 1 (Continued): Specification of the layer thickness



1. Assign vertical mesh for p- and n-layers, electrodes and pads.

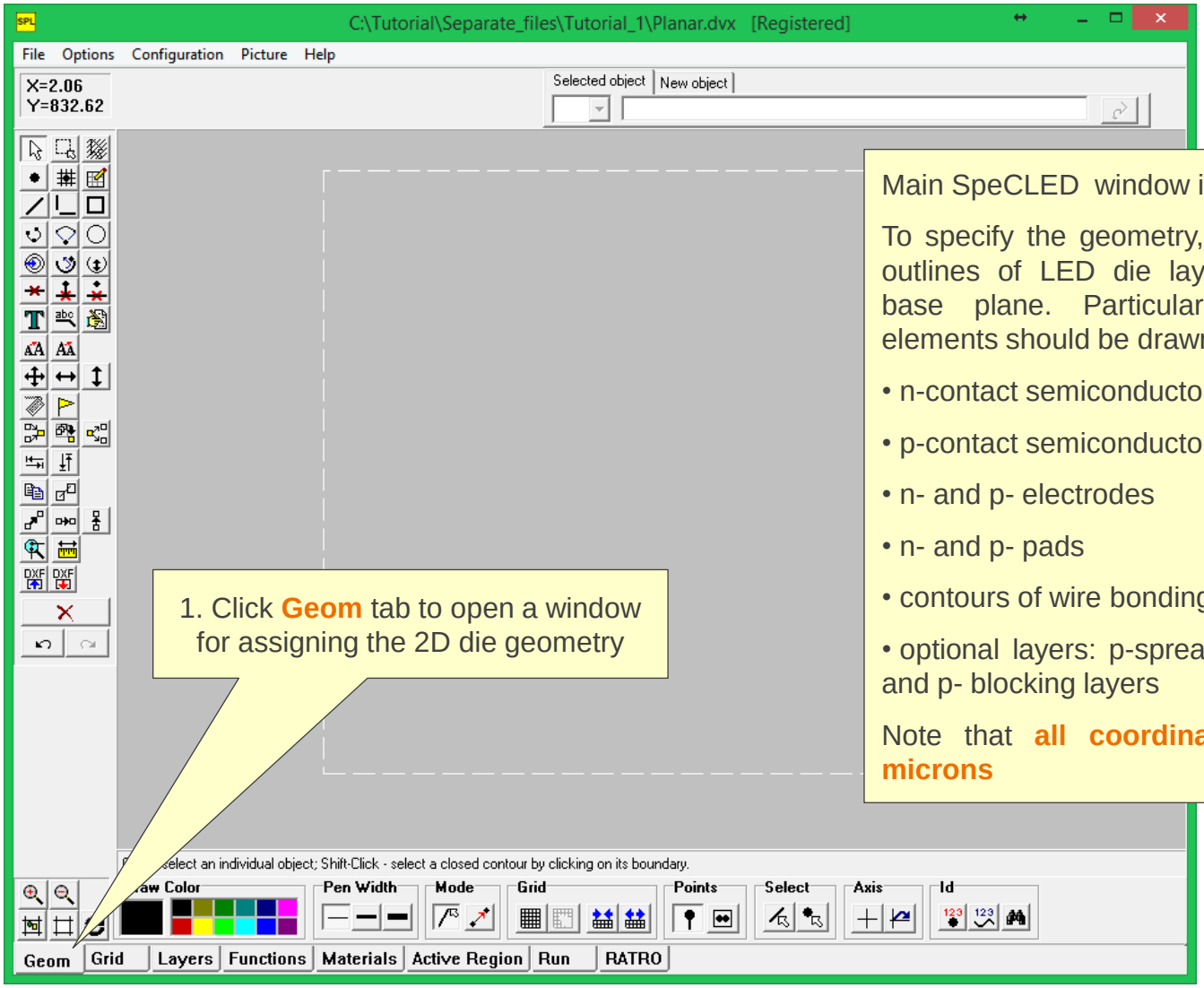
For a vertical substrate with size F equal to zero, NF can be set to an arbitrary non-zero value, for instance, to 1.

For p-spreading layer, we recommend use only 1 step.

2. Press **OK**

Note that the user can also access and edit the parameters described in this window later at any time by using **Configuration** menu item

Step 2: Drawing the outlines of the layers



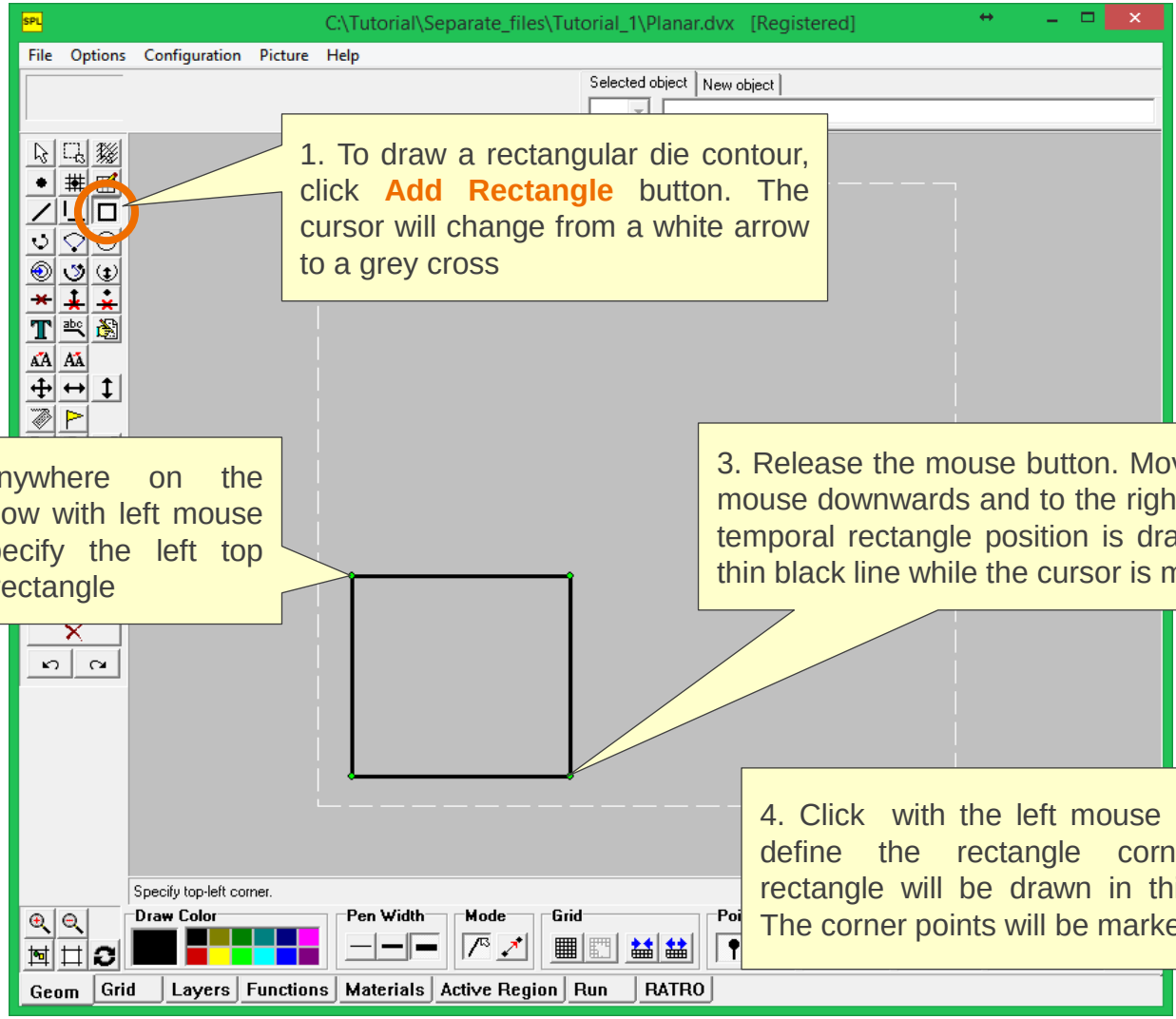
Main SpeCLED window is opened

To specify the geometry, one needs to draw an outlines of LED die layers projected onto the base plane. Particularly, the following die elements should be drawn:

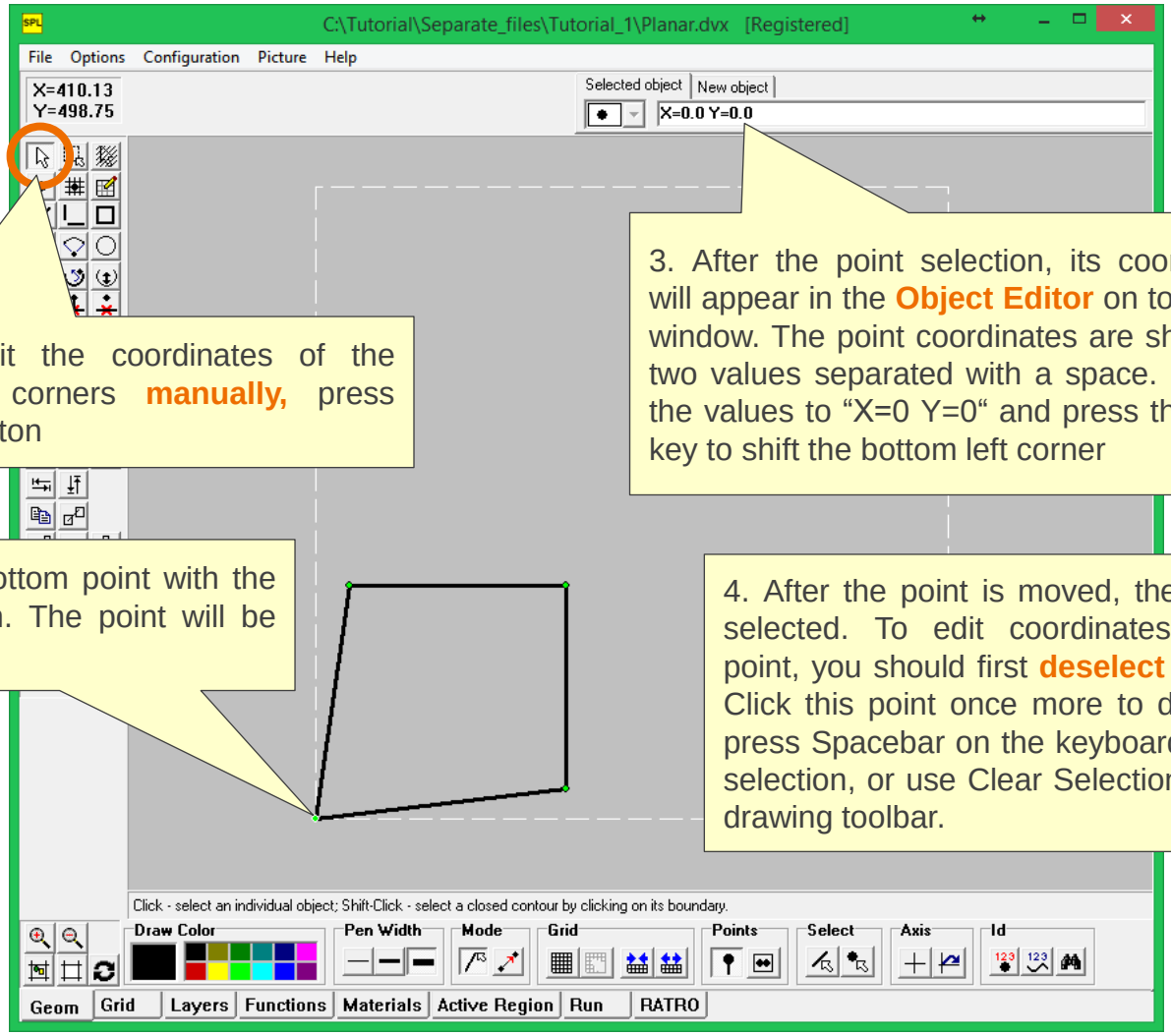
- n-contact semiconductor layer
- p-contact semiconductor layer
- n- and p- electrodes
- n- and p- pads
- contours of wire bonding
- optional layers: p-spreading (ITO) layer and n- and p- blocking layers

Note that **all coordinates are specified in microns**

Step 2 (Continued): Drawing a rectangle



Step 2 (Continued): Editing the coordinates manually



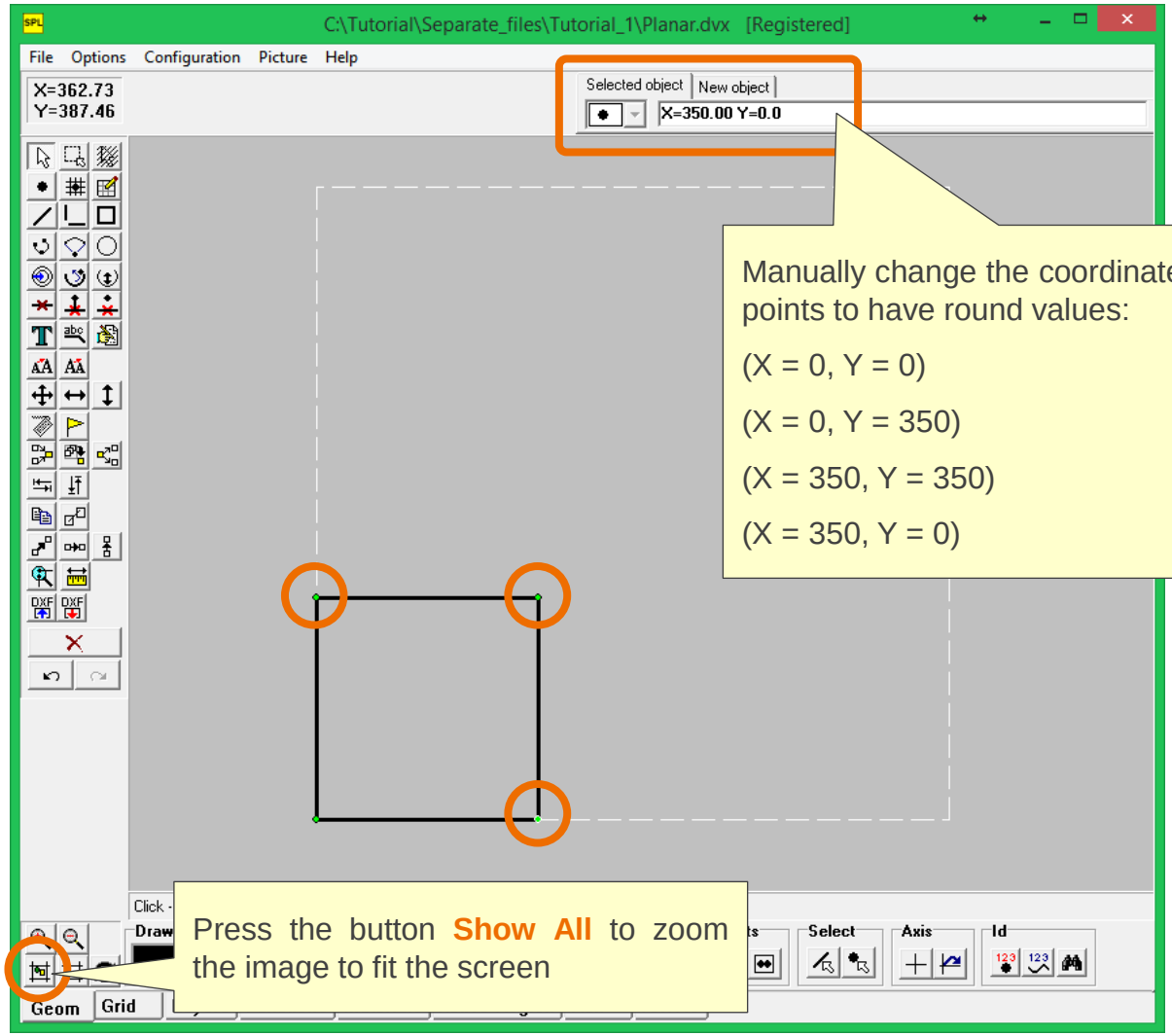
1. To edit the coordinates of the rectangle corners **manually,** press **Select** button

2. Pick the left bottom point with the left mouse button. The point will be marked in white.

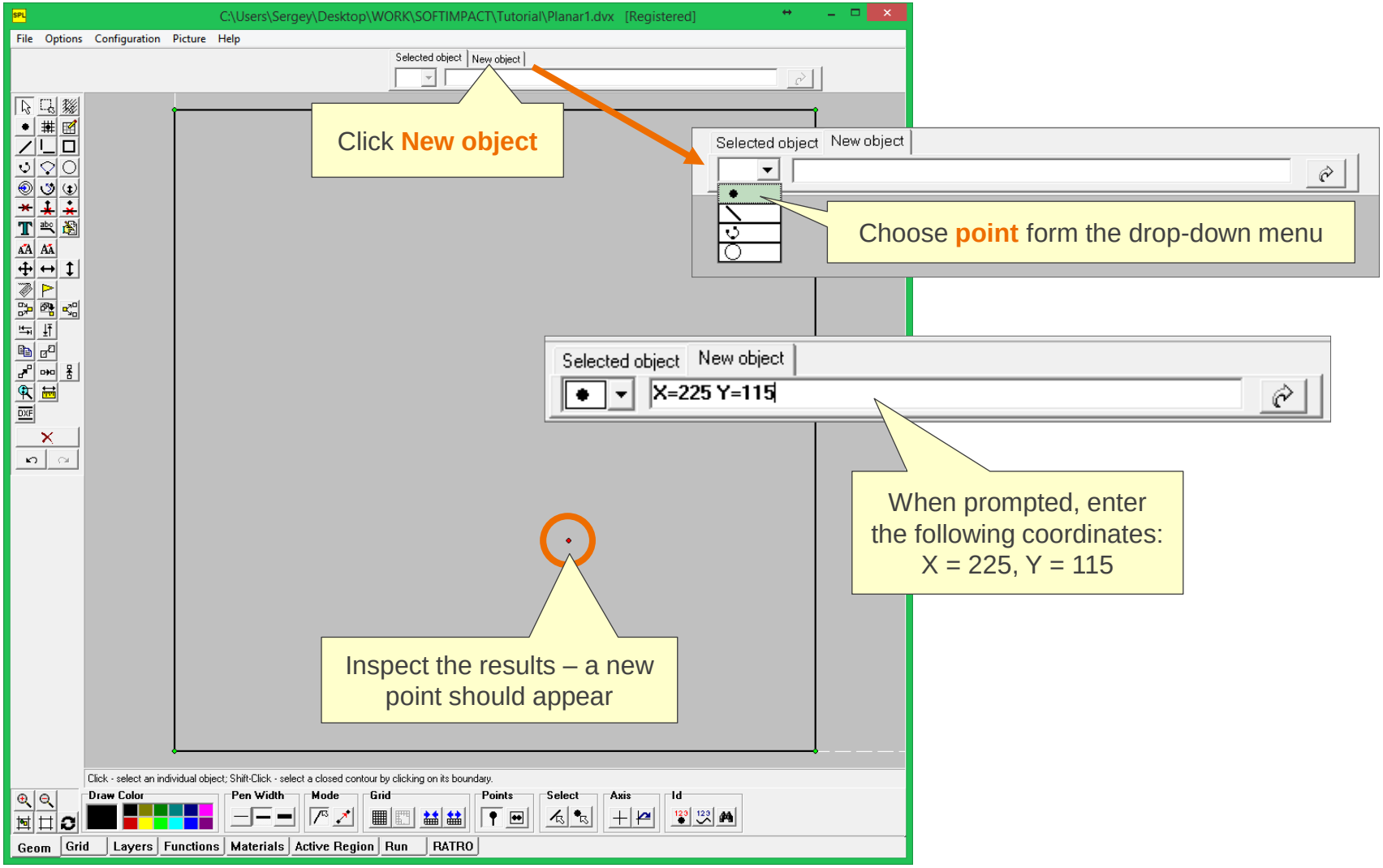
3. After the point selection, its coordinates will appear in the **Object Editor** on top of the window. The point coordinates are shown as two values separated with a space. Change the values to “X=0 Y=0“ and press the Enter key to shift the bottom left corner

4. After the point is moved, the point is still selected. To edit coordinates of another point, you should first **deselect** the first one. Click this point once more to deselect it, or press Spacebar on the keyboard to clear the selection, or use Clear Selection button from drawing toolbar.

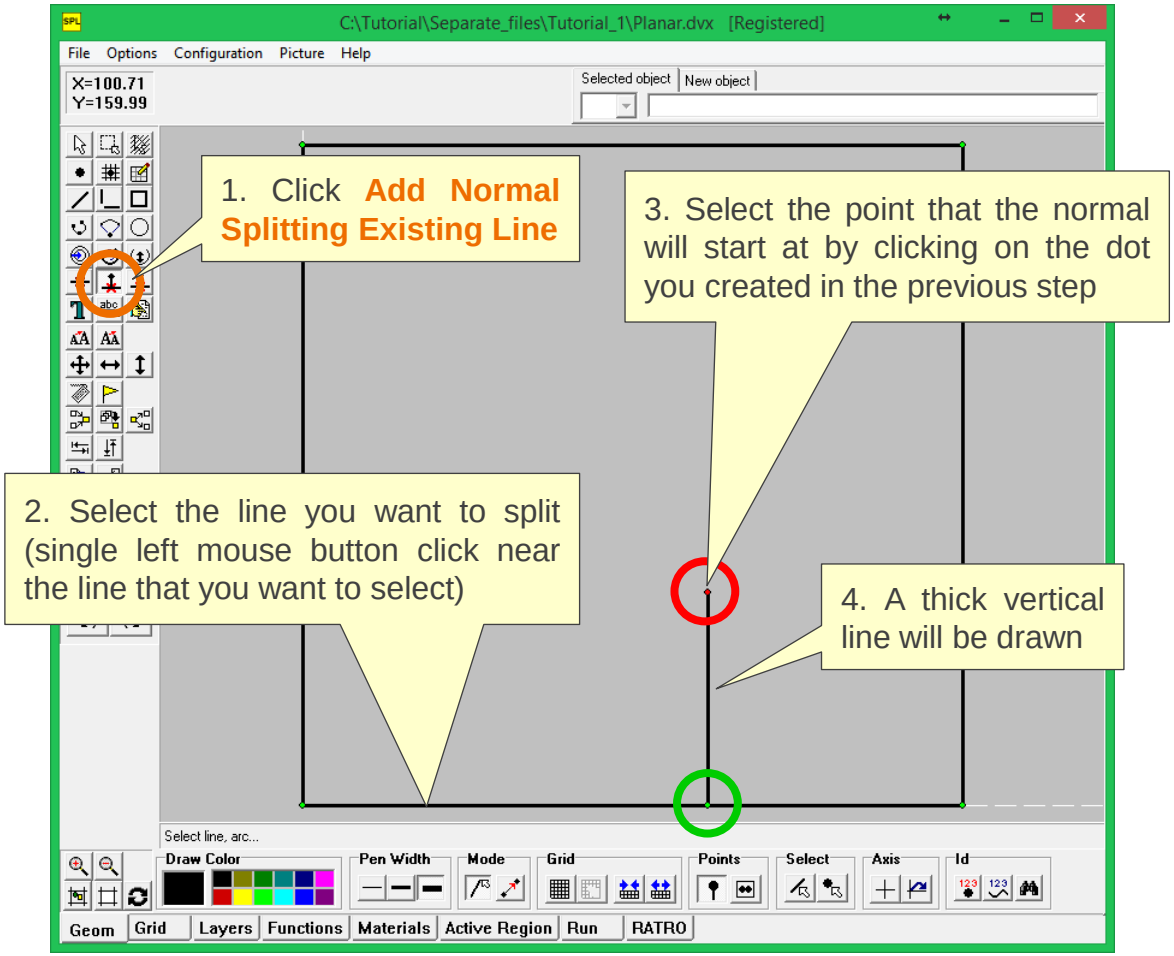
Step 2 (Continued): Editing the coordinates manually



Step 2 (Continued): Adding an object



Step 2 (Continued): Normal splitting



To draw a vertical boundary of the mesa, use one of the tools dropping a normal to the line from a selected point.

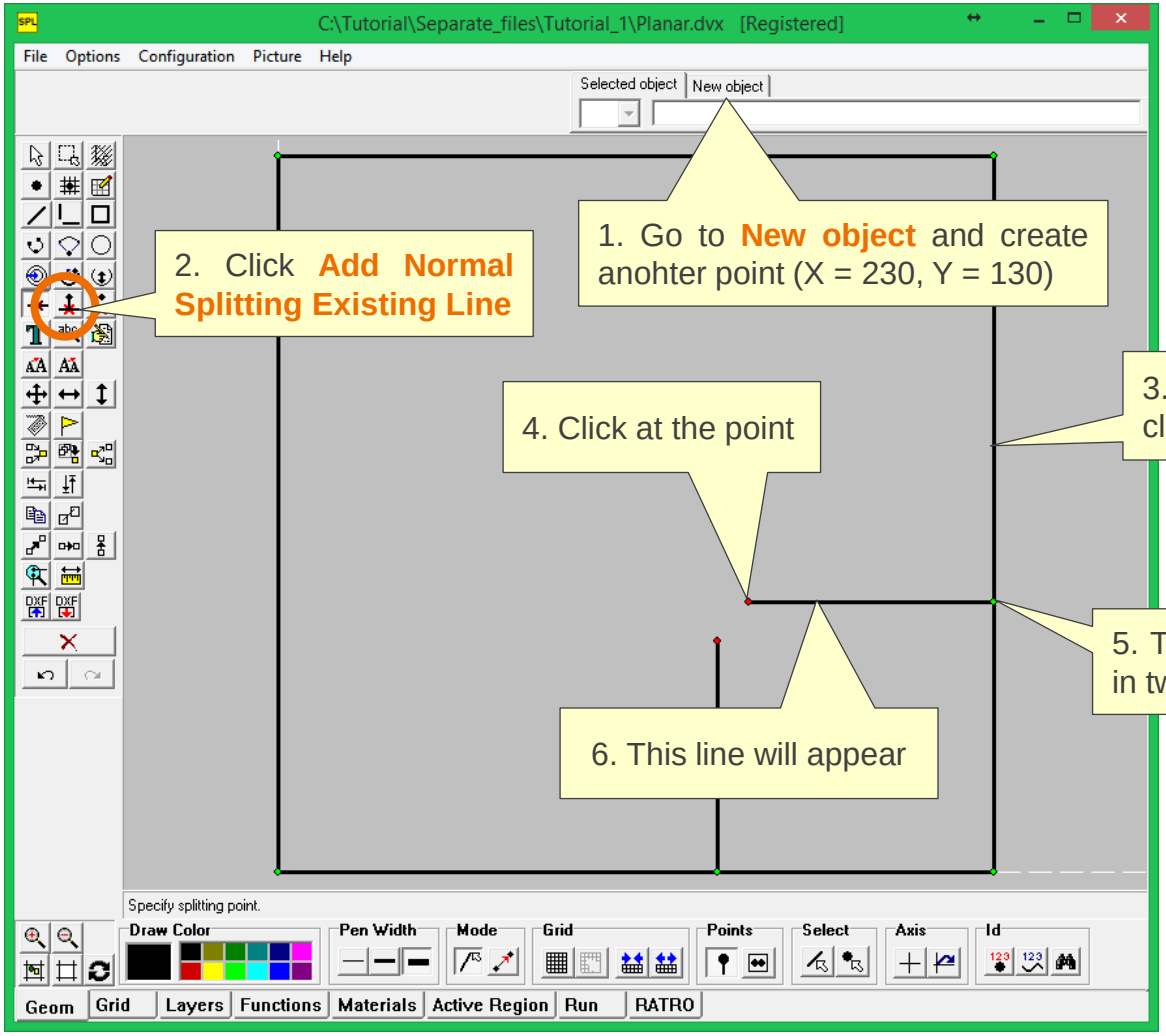
As a result, the original bottom line will split in two parts and the vertical line connecting a point and the bottom line will be added.

Note that the bottom ending point will be marked green – the point is shared by several lines. At the same time, the point in the middle will stay red as dangling.

Note that **Red** color of an ending point marks a dangling line

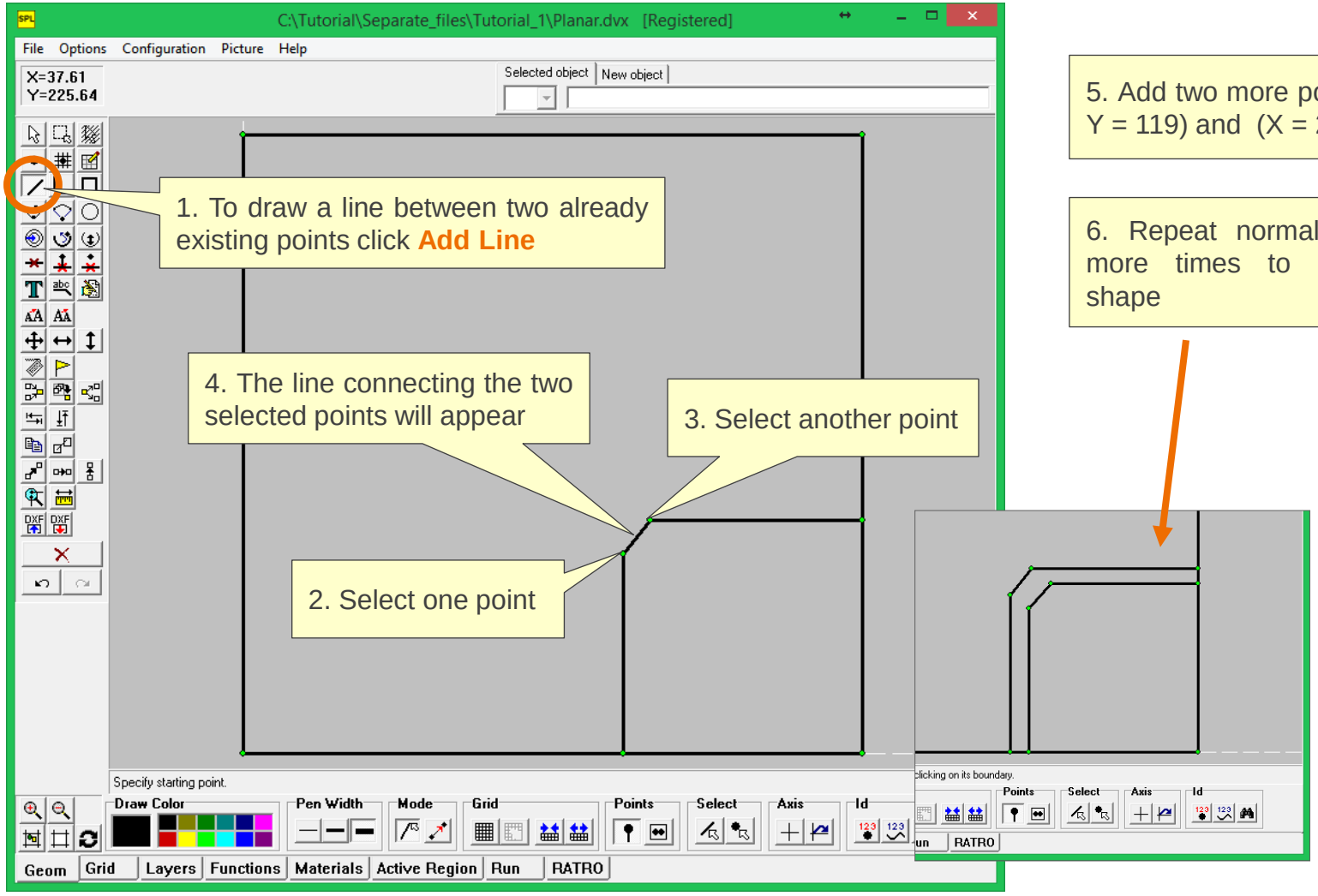
Green color marks an internal point of a contour, in other words, point connecting two or more lines

Step 2 (Continued): Adding another side



To add one more side to the mesa, repeat two previous steps.

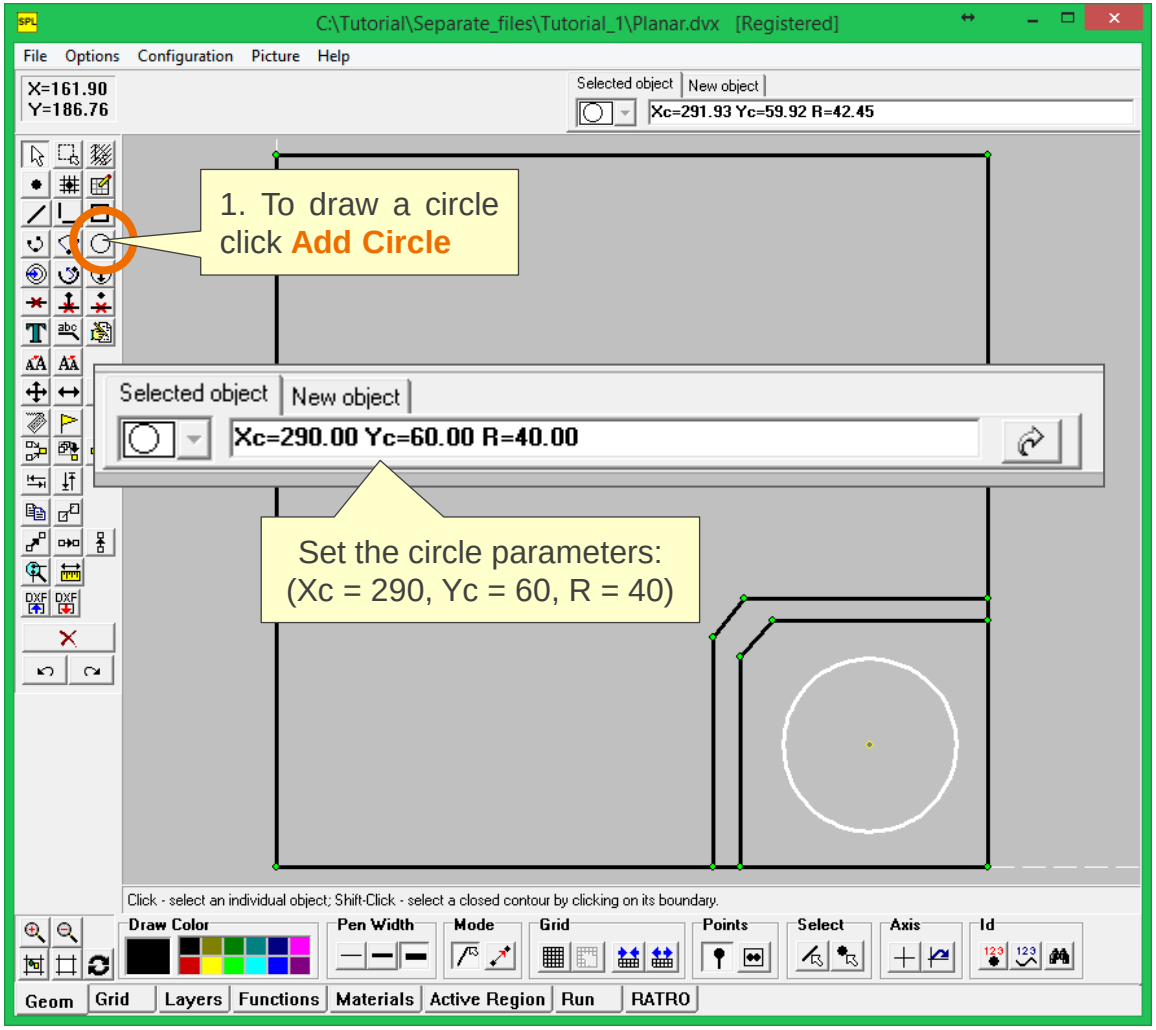
Step 2 (Continued): Linking the points



5. Add two more points (X = 244, Y = 119) and (X = 228, Y = 103)

6. Repeat normal splitting two more times to complete the shape

Step 2 (Continued): Adding a circle to draw n-pad



2. Define the circle center (click and release the left mouse button)

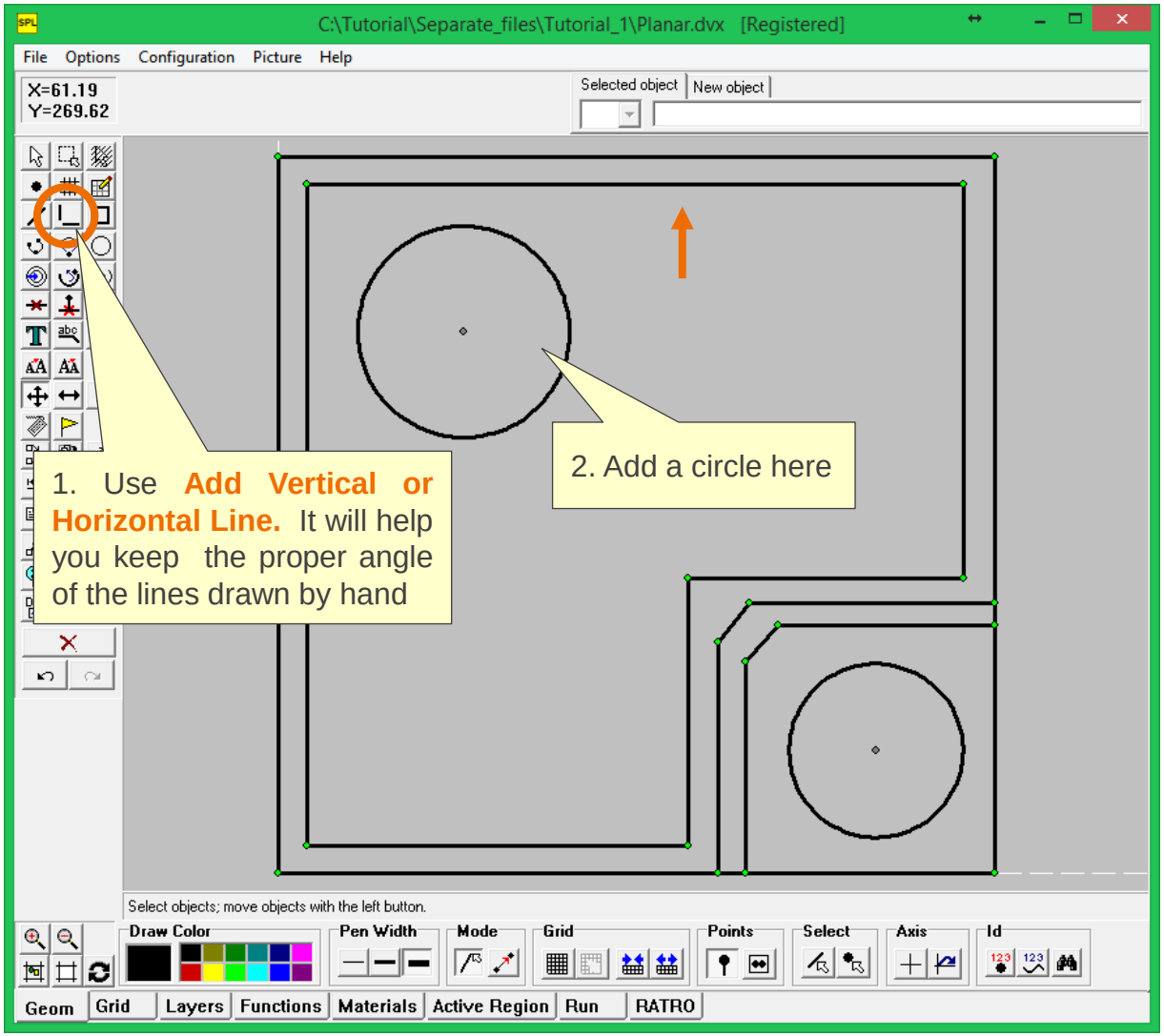
3. Move the cursor from the circle center. Press the button again and move the mouse keeping the button pressed. The current circle position defined by the current cursor position will be shown in a thin gray line

4. Release the button to assign the circle position.

5. Position of the selected circle can be edited in the **Object Editor** like the position of a line. You can edit three values: center coordinates Xc and Yc and the radius R

6. Alternatively, you could have used **New object** tab to add a circle and manually edit its parameters

Step 2 (Continued): Adding vertical or horizontal lines



To draw the p-electrode and p-pad we need to add several vertical and horizontal lines

Draw the contours of the p-electrode using **Add Vertical or Horizontal Line** tool with the following coordinates:

(X = 14, Y = 336)

(X = 14, Y = 14)

(X = 200, Y = 14)

(X = 200, Y = 144)

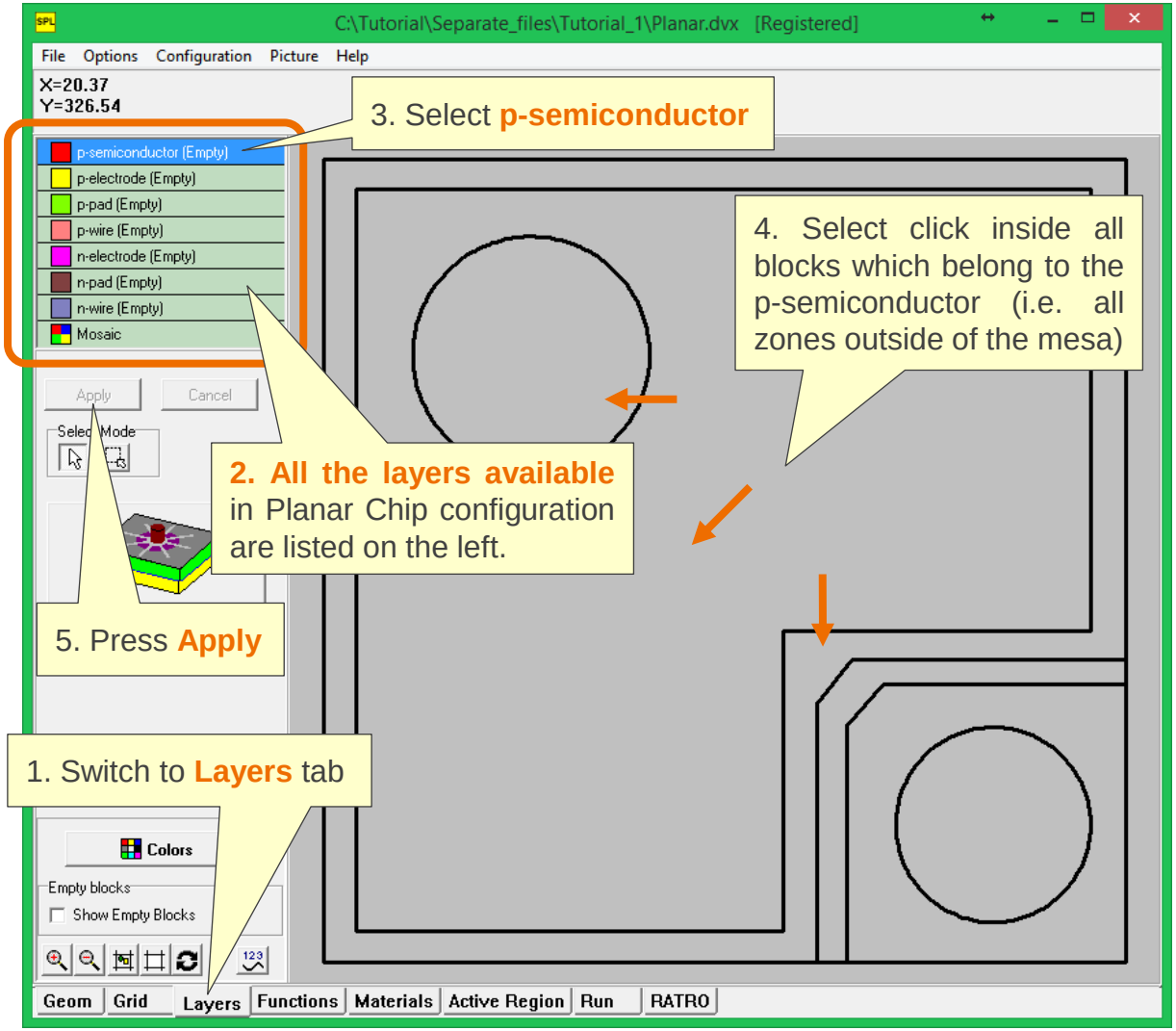
(X = 336, Y = 144)

(X = 336, Y = 336)

Draw the contour of p-pad using **Add Circle** with the following coordinates:

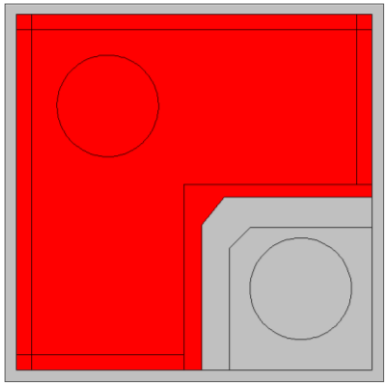
(Xc = 90, Yc = 265, R = 50)

Step 3: Specification of layers



Now the contours are drawn and one needs to convert them into a 3D geometry. You have assigned the thickness of the layer right after the selection of the chip type, but the layers there are listed “by name” (mesa depth, p-electrode, n-pad, etc.) and the software does not know “who is who”. Now we will sort it out by establishing connection between outlines and functional elements

As you pick them, they are filled with the **Red** color, see below. To exclude block from selection, click it again.



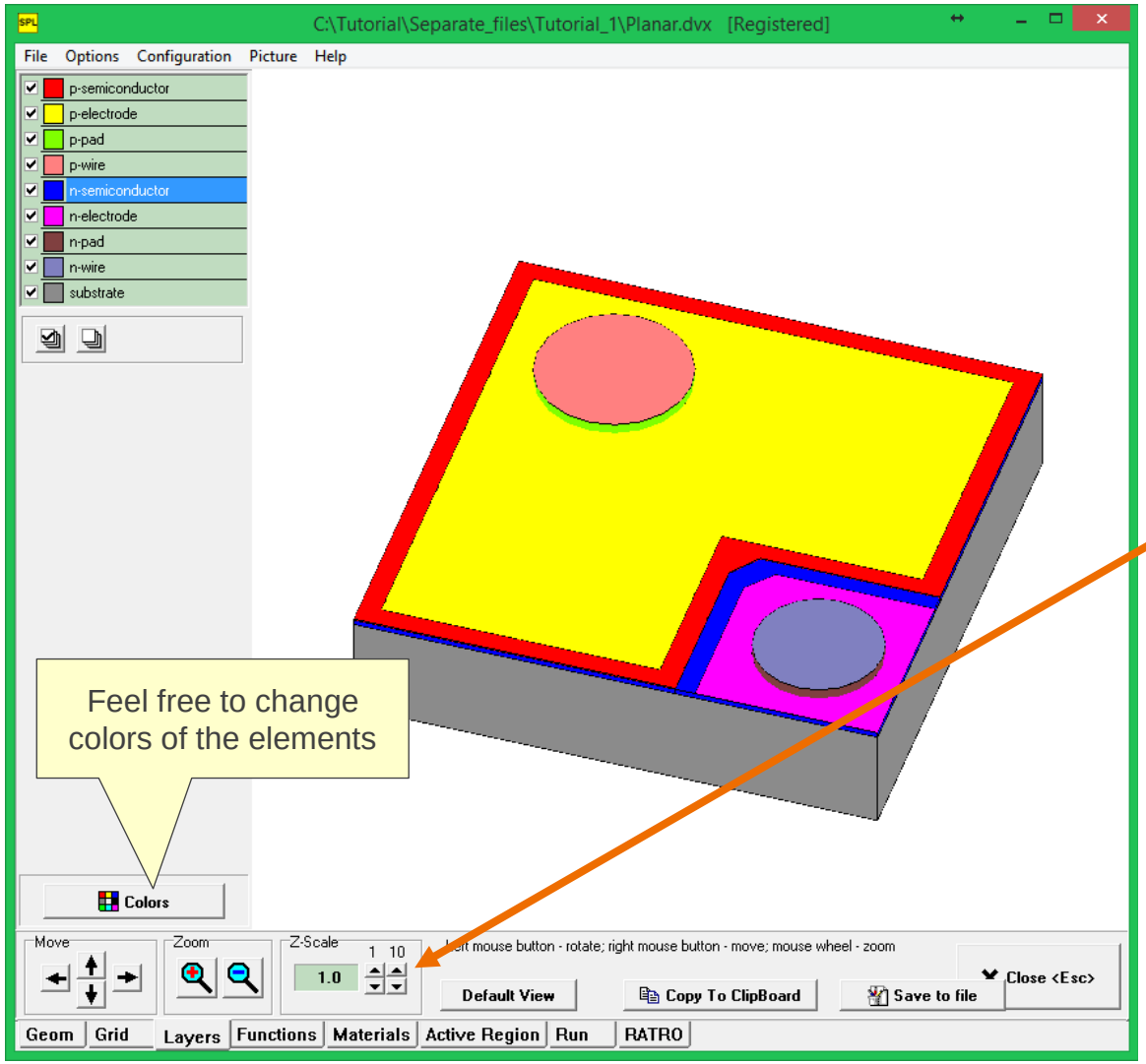
Step 3 (Continued): Specification of layers

All other chip elements to be specified as follows:

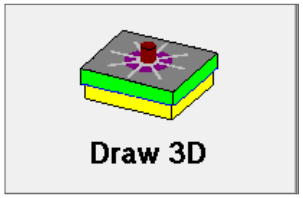
1. p-semiconductor: all area except the etched mesa. The active region area has the same shape as p-semiconductor. For vertical LEDs, p-semiconductor layer is not specified. It is assumed to cover all the die area.
2. Electrodes and pads: metallic layers, where distribution of the electric potential and electric current is computed. It is suggested (but not obligatory) that electrodes are used to represent thin semitransparent metallic layers, while pads represent thick layers. Electrode layer to be specified even if the contact is thick (in this case, the electrode might has the same geometry as the respective pad).
3. Wires: areas of wire bonding. They are used only to set up boundary conditions for the electric potential.

Note the following requirements: p-semiconductor has to include p-electrode, which has to include p-pad, which has to include p-wire. Similarly, mesa has to include n-electrode, which has to include n-pad, which has to include n-wire. If optional p-spreading layer is used, it should be inside p-semiconductor and include p-electrode

Step 3 (Continued): 3D view



Now the die geometry is specified and you can check it in 3D View. Click **Draw 3D** button on the left.



Window **3D View** will be opened

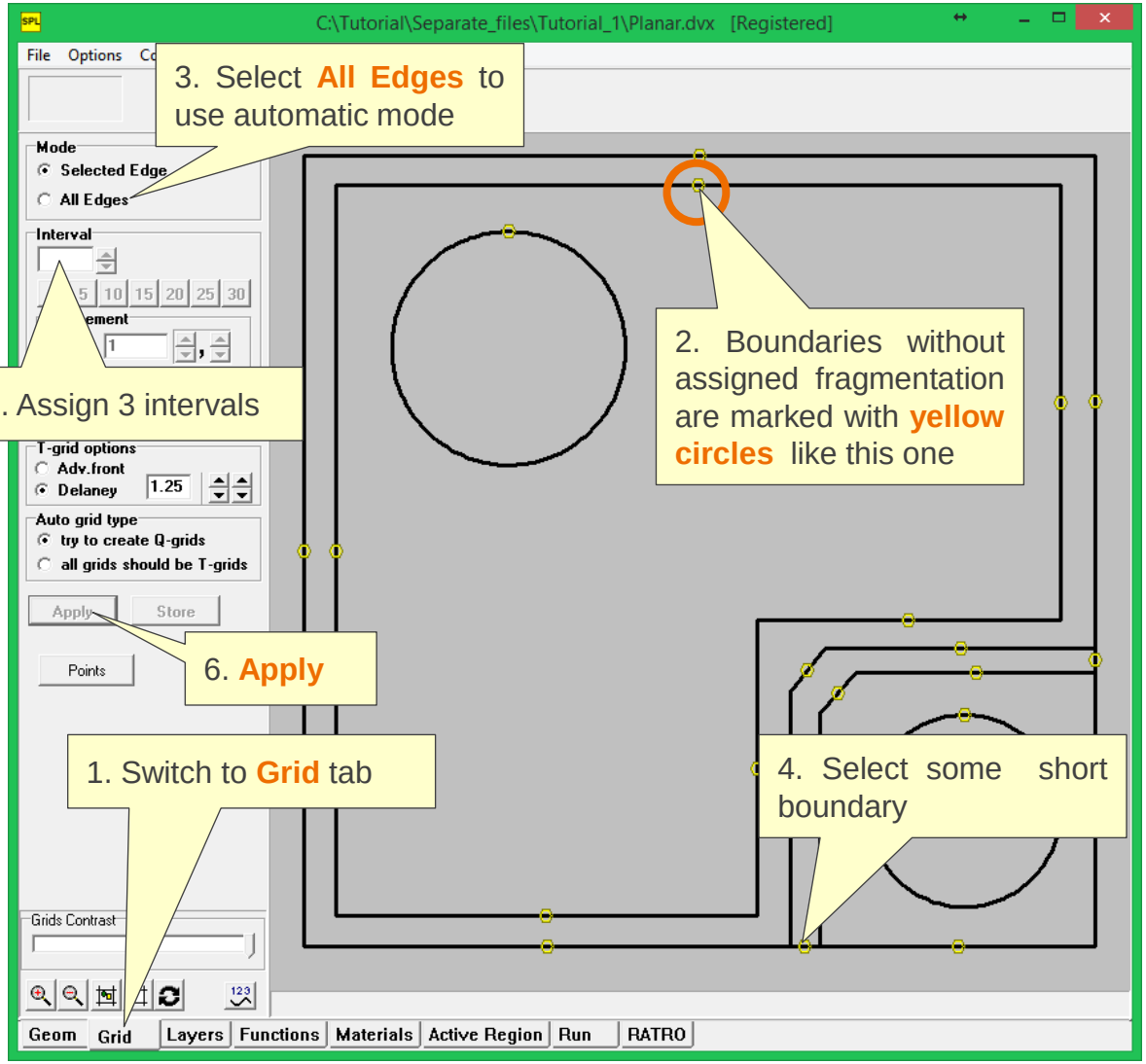
The planar die height is much smaller than its width. One can change z-scale to inspect fine details

The semiconductor layers and pads are shown proportional their actual thickness in microns

The electrode thickness is assumed to be negligible, so they are shown with some fixed small non-zero thickness

One can show or hide die elements by the respective check boxes

Step 4: Generation of the computational grid



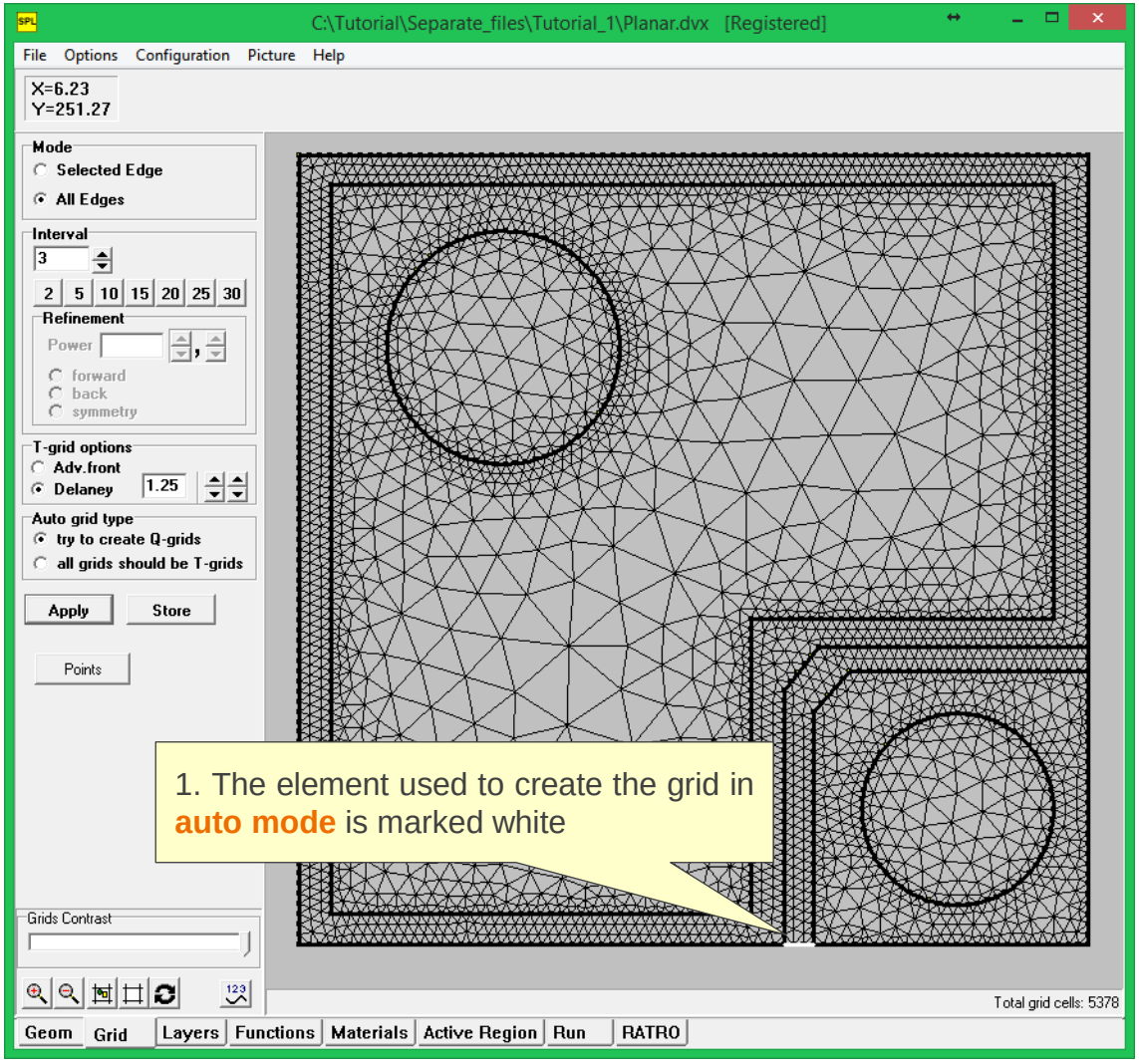
Switch to the tab window **Grid** to generate the computational grid

To generate the grid in a 2D domain, the user should assign the fragmentation of the domain boundaries

In Automatic Mode **(All Edges),** all boundaries are split in grid faces of the same size. It can often serve as an excellent starting point provided that the reasonable step of the boundary fragmentation is chosen.

We recommend choosing a short boundary and splitting it in several fragments. The same fragmentation density will be applied to all the other lines, see the next page.

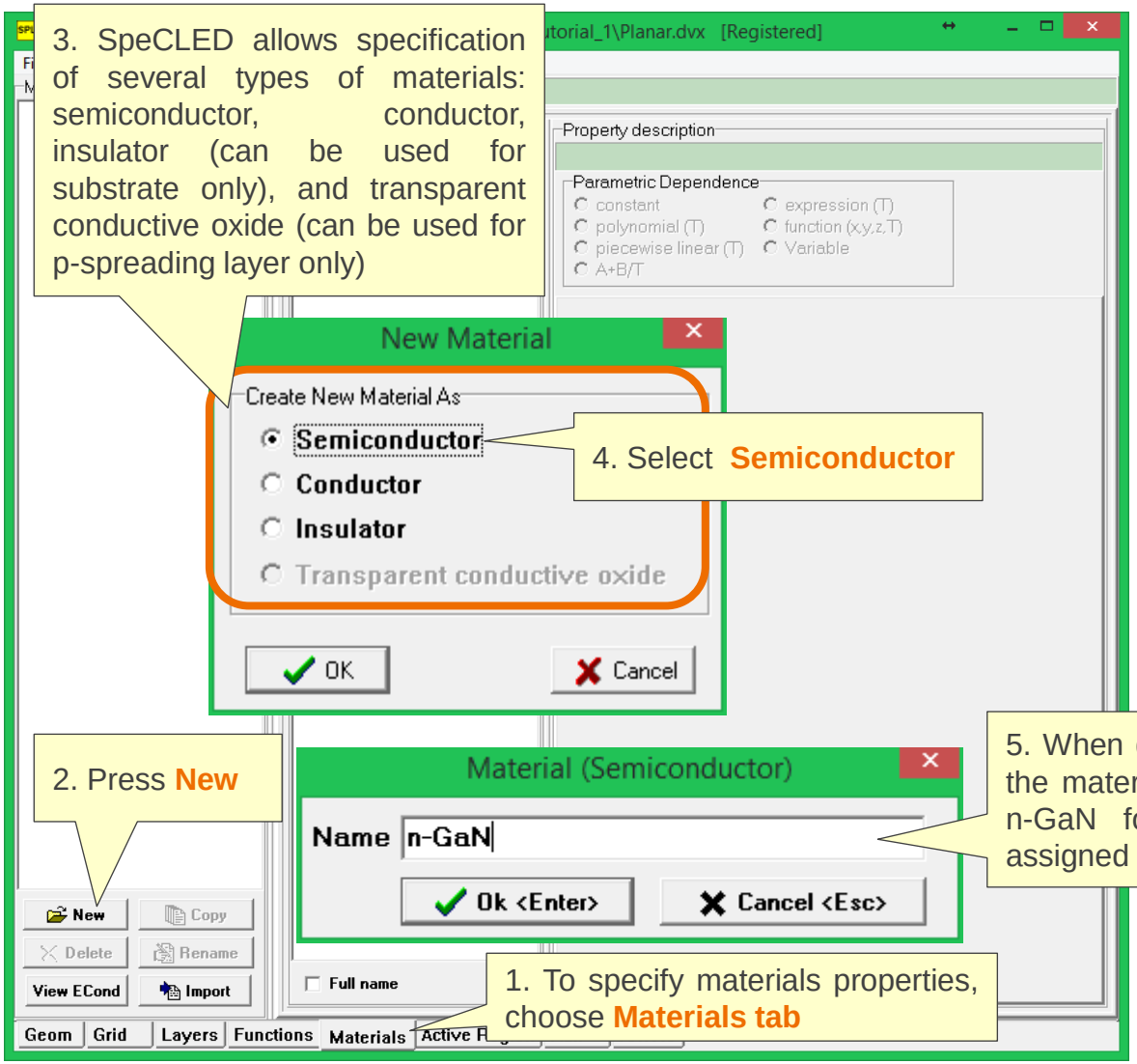
Step 4 (Continued): computational grid in auto mode



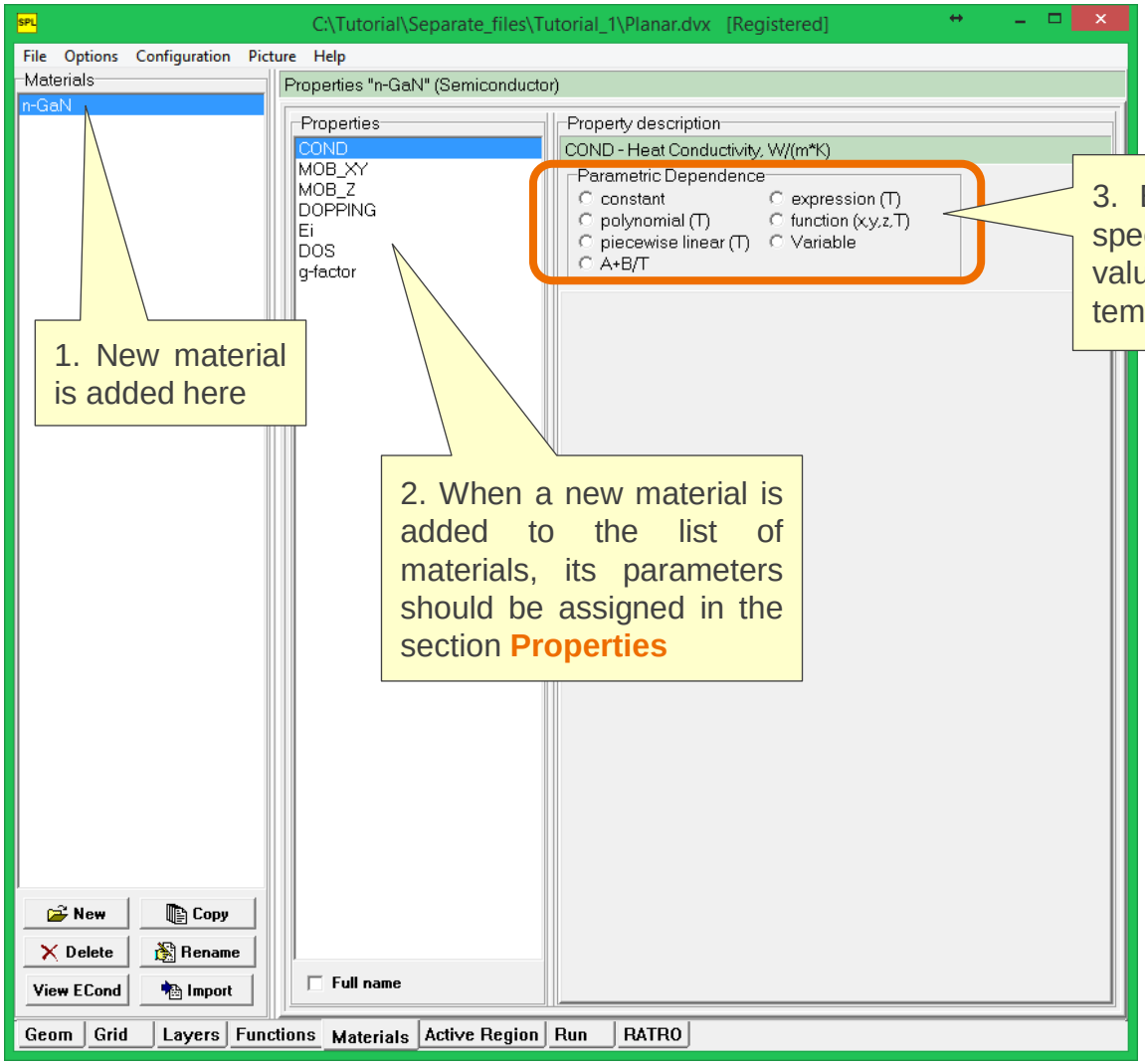
Later, one can manually refine grid by choosing **Selected Edge** mode, and correct fragmentation of several boundaries.

Please, note that the rougher the grid, the faster will be your computations and the lower will be accuracy. We recommend that you start with a rough grid, similar to shown on the left, to get the first solution and inspect it in terms of possible errors of the input. Once you are sure that the input is correct, try refining the grid (for instance, by assigning more intervals to the same short boundary you used at the previous stage) and compare the two solutions. For estimates, it is often sufficient to use a rough grid, while for final results and for studying the effect of minor changes it is important to have a detailed grid. Also, note that the grid should be particularly good at the areas of high currents or high gradients.

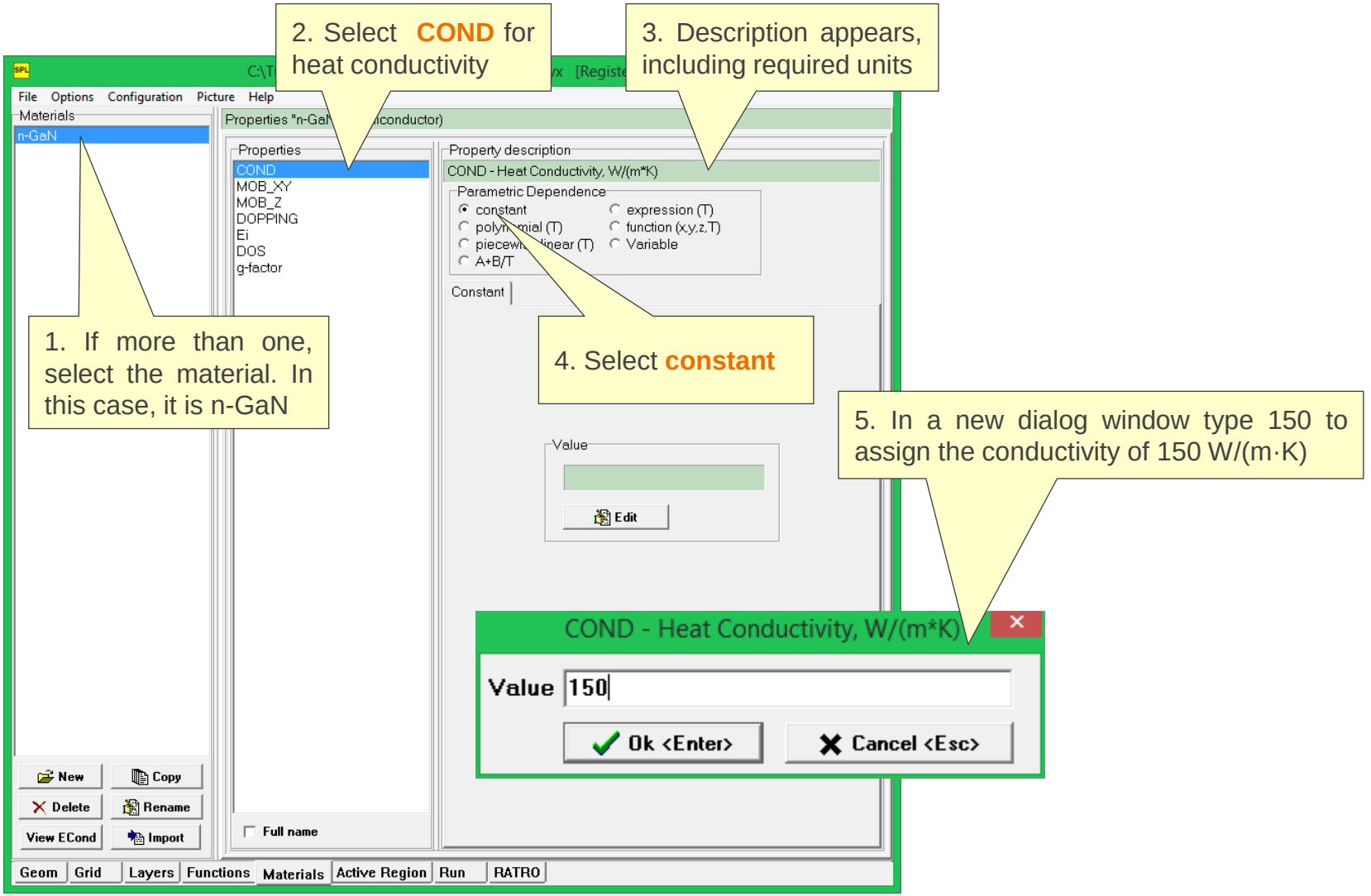
Step 5: Specification of material properties



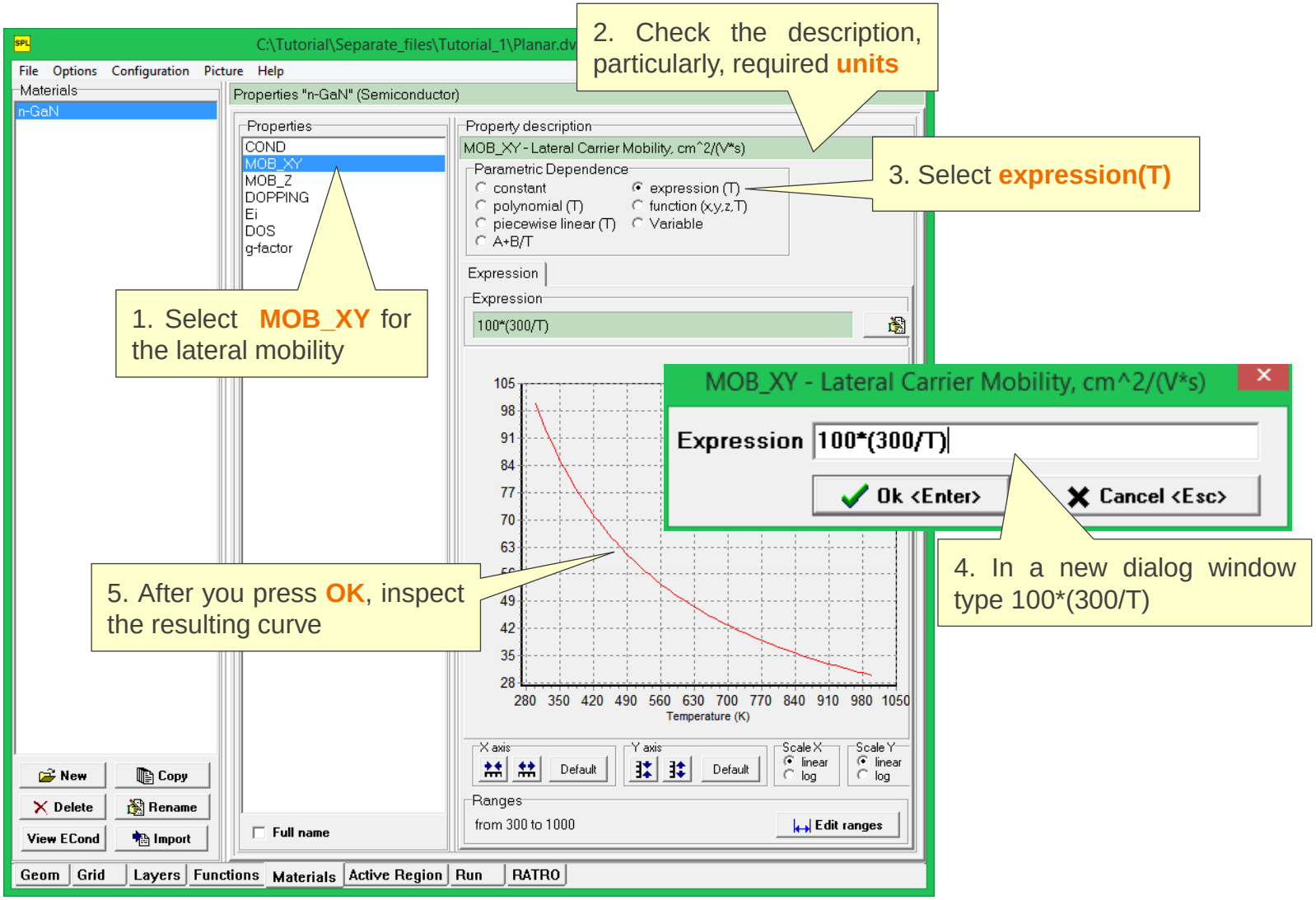
Step 5 (Continued): Specification of material properties



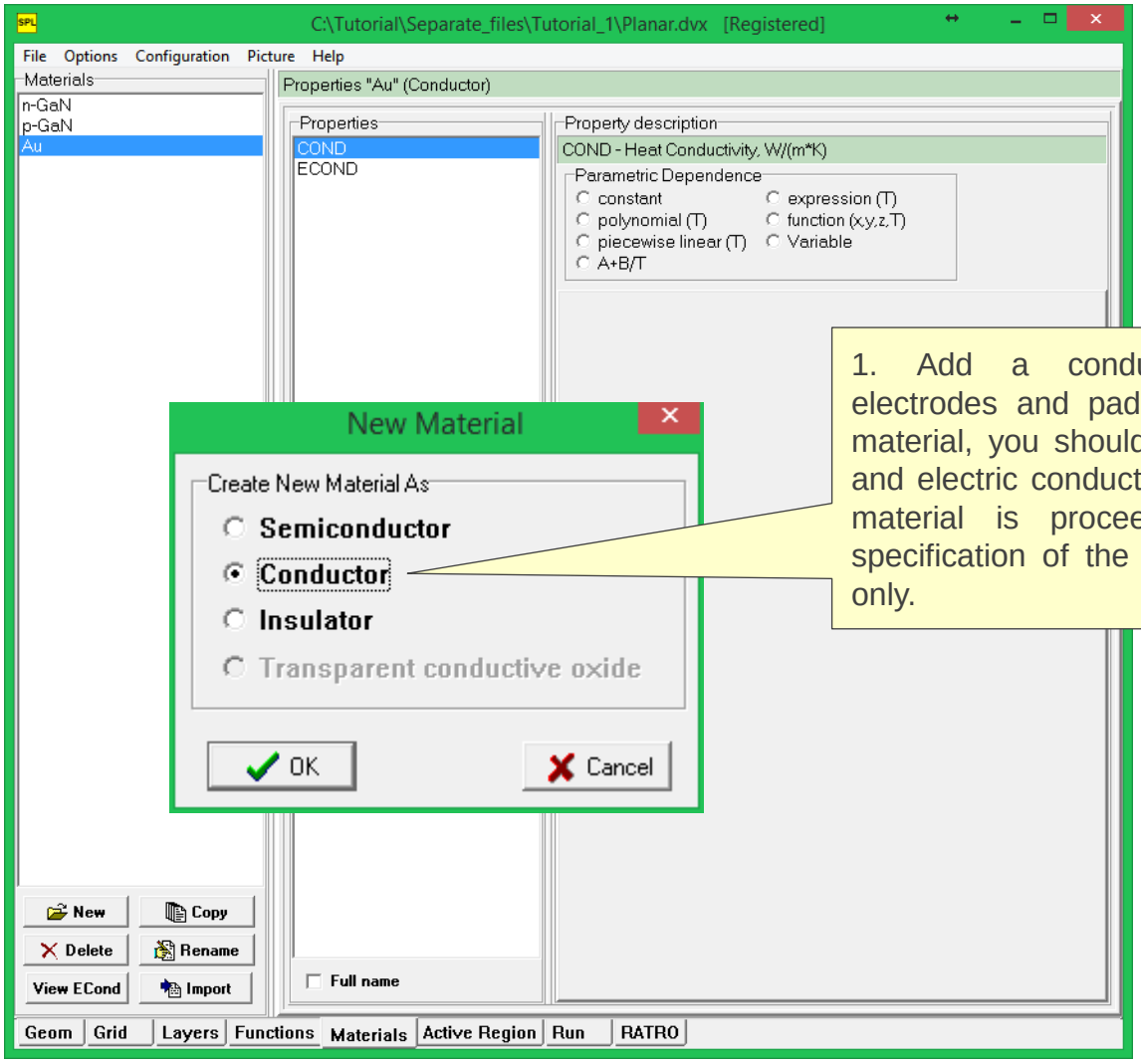
Step 5 (Continued): Using a constant value for properties



Step 5 (Continued): Using functions to specify properties



Step 5 (Continued): Conductors and insulators



1. Add a conductor material for electrodes and pads. For a Conductor material, you should assign the thermal and electric conductivities only. Insulator material is proceeded similarly with specification of the thermal conductivity only.

2. Just like it the previous step, assign the following parameters:

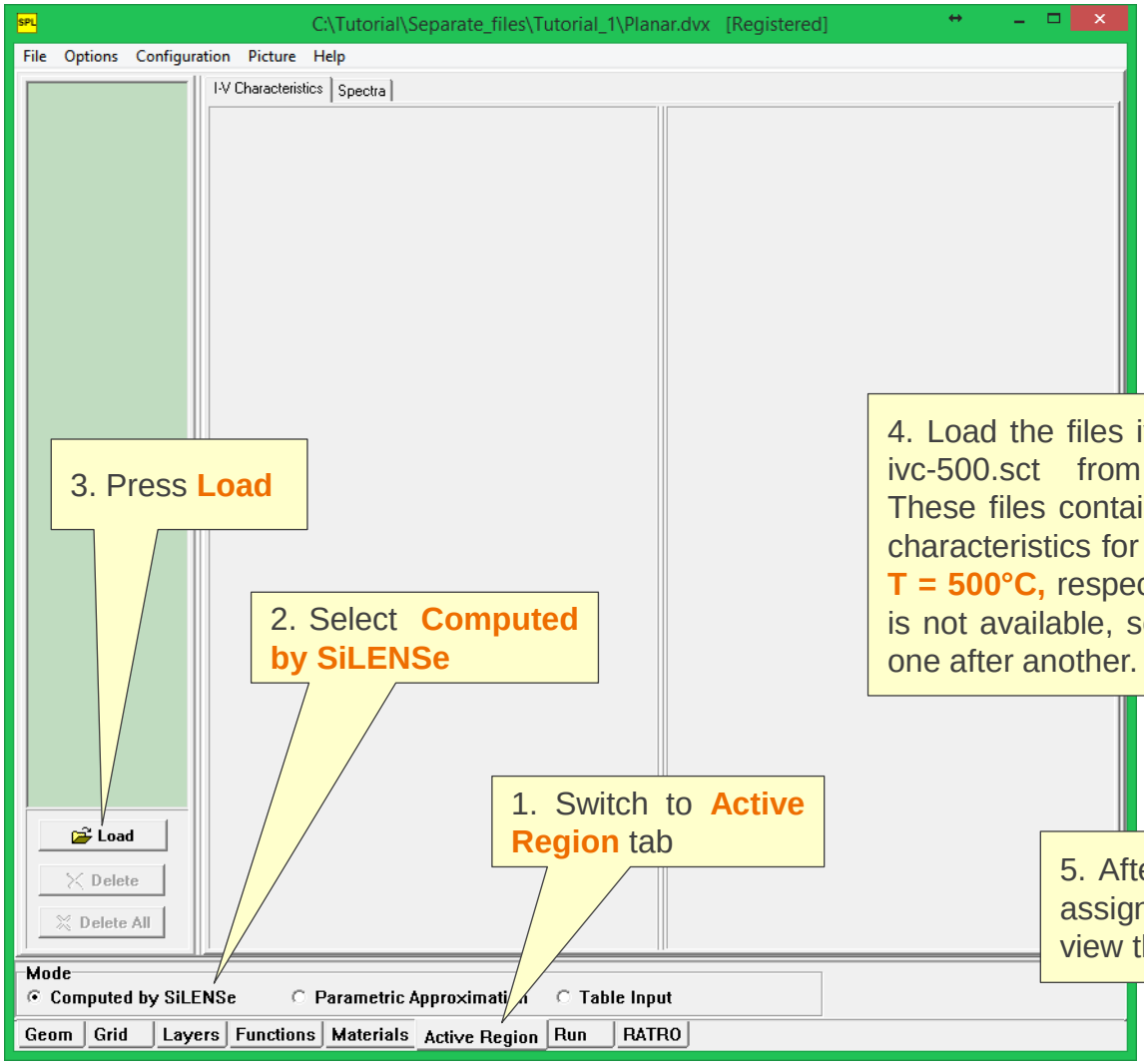
COND (heat conductivity)

315 W/(m·K)

ECOND (electric conductivity)

4.1×105 (Ω·cm)-1

Step 6: Importing active region properties from SiLENSe

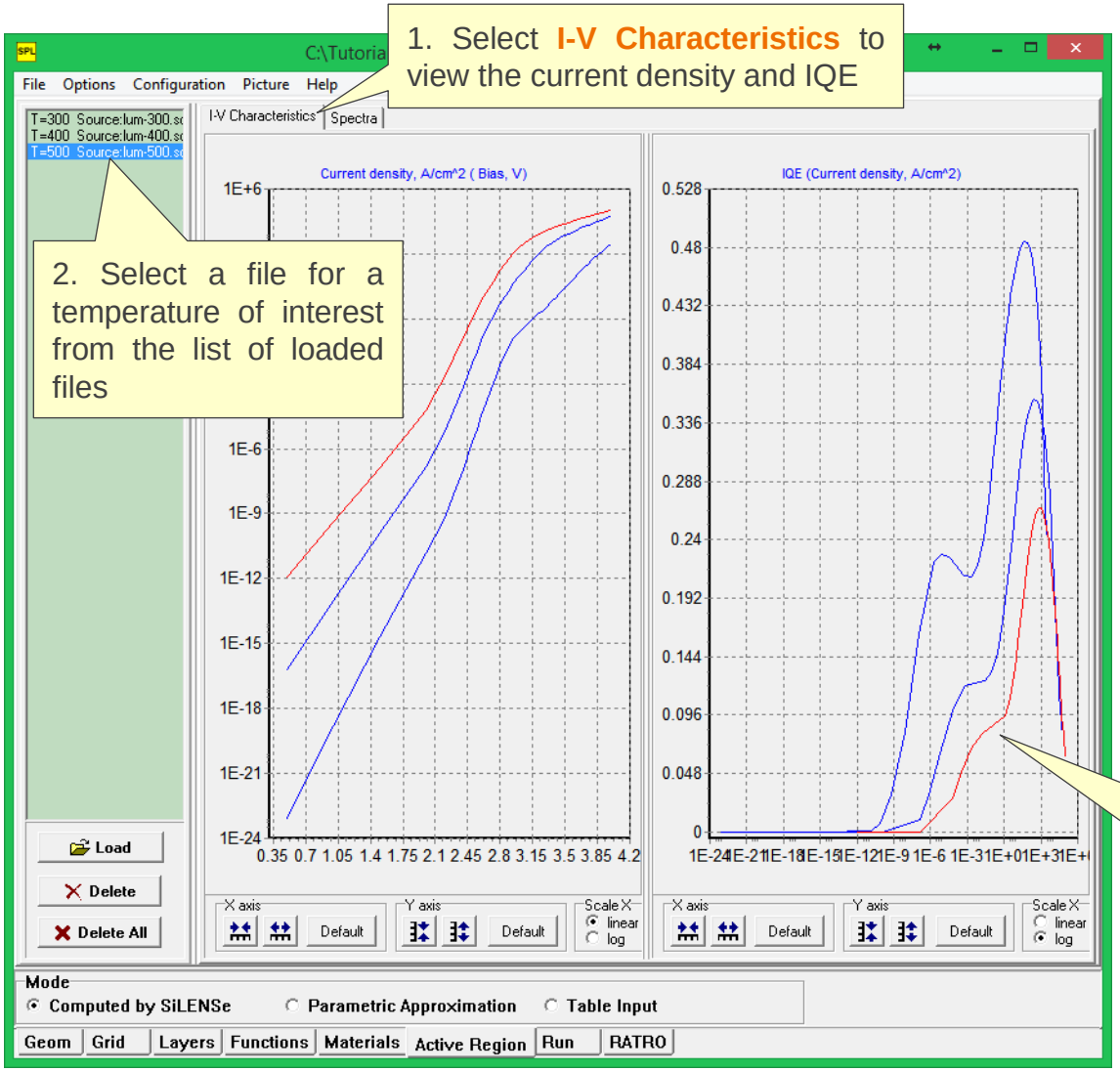


Now, import of the I-V characteristics calculated by SiLENSe tool will be used. Description of specification of parametric dependencies within SpeCLED will be shown later.

4. Load the files ivc-300.sct, ivc-400.sct and ivc-500.sct from Tutorials/IVC directory. These files contain data on active region i-v characteristics for **T = 300°C, T = 400°C** and **T = 500°C,** respectively. Multiple file opening is not available, so you should load the files one after another.

5. After loading the files, you do not have to assign any active region parameters but can view the loaded values (next page)

Step 6 (Continued): Viewing the properties from SiLENSe

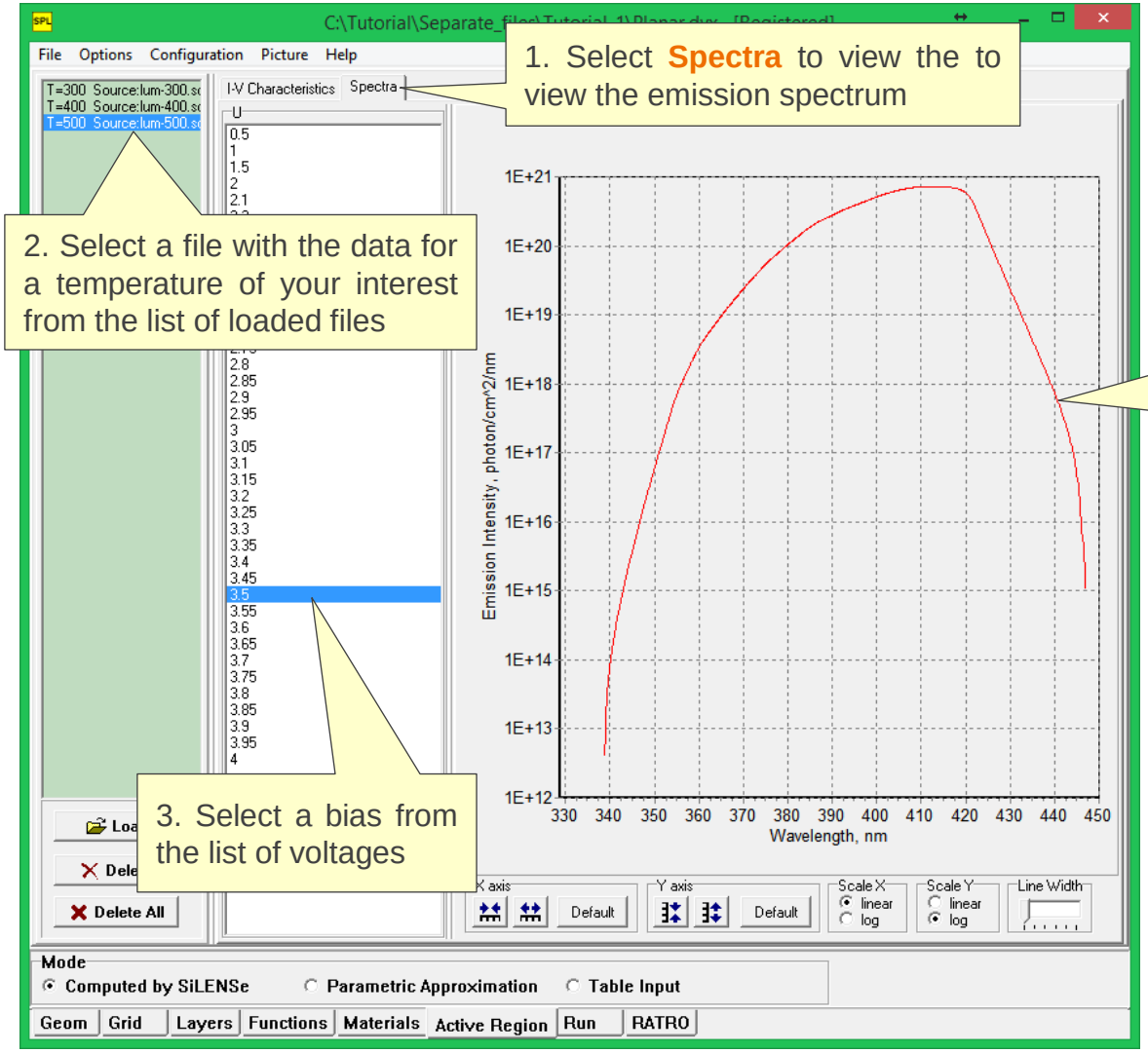


The files imported at the previous stage contain the following data:

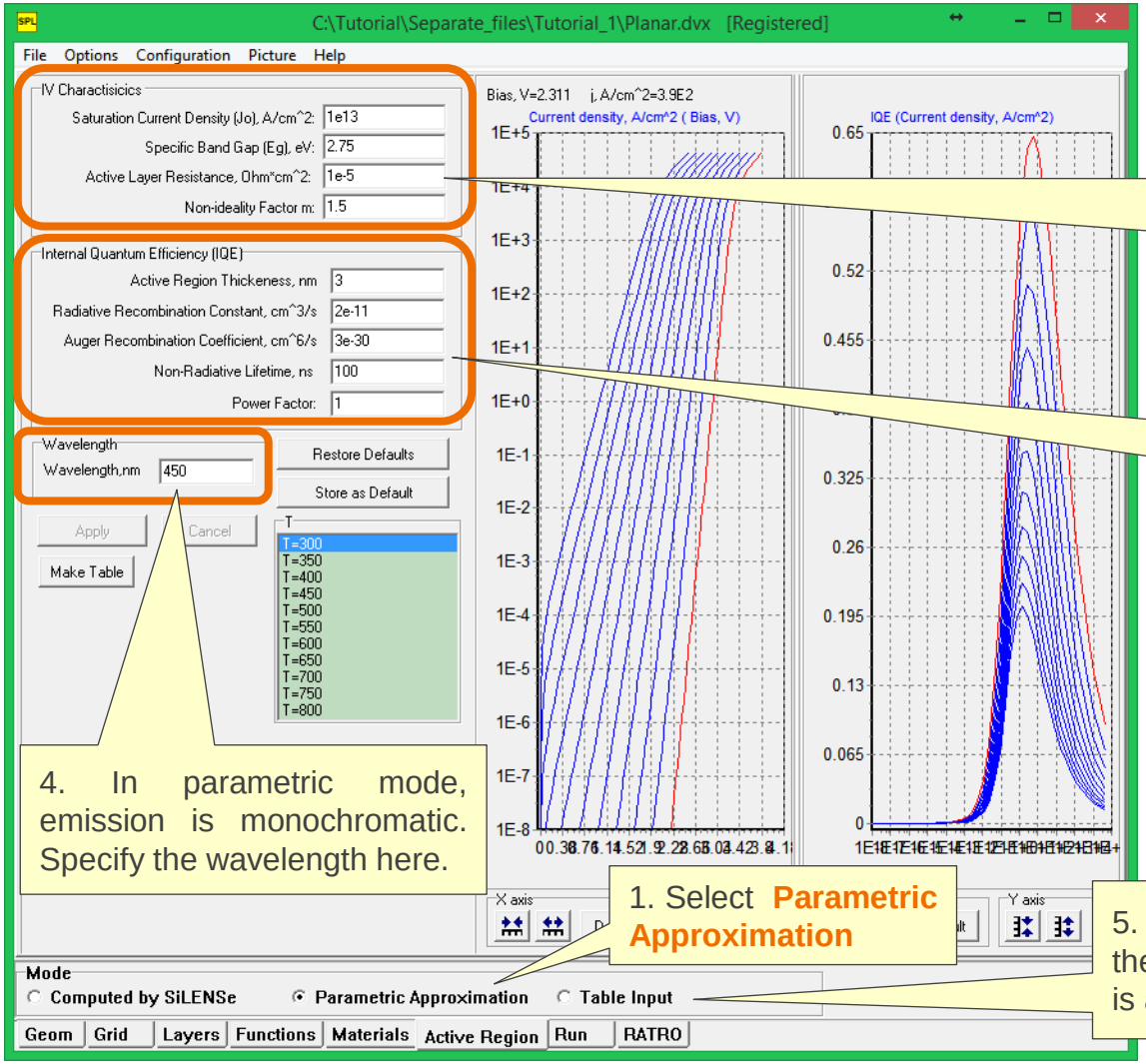
- Current density as a function of the bias
- Internal quantum efficiency as a function of current density
- Emission spectrum for each bias

3. Plots for all loaded files are drawn. The selected plot is drawn in red. The other plots are drawn in blue

Step 6 (Continued): Viewing the spectrums from SiLENSe



Step 6 (Continued): Parametric specification of active region



Parametric approximation can be used to describe the active region properties.

2. These parameters describe the dependence of the p-n junction current density on the p-n junction bias, j(U). Feel free to edit the default set as you wish.

3. Dependence of IQE on the p-n junction current density, IQE(j). Edit the default values as you need.

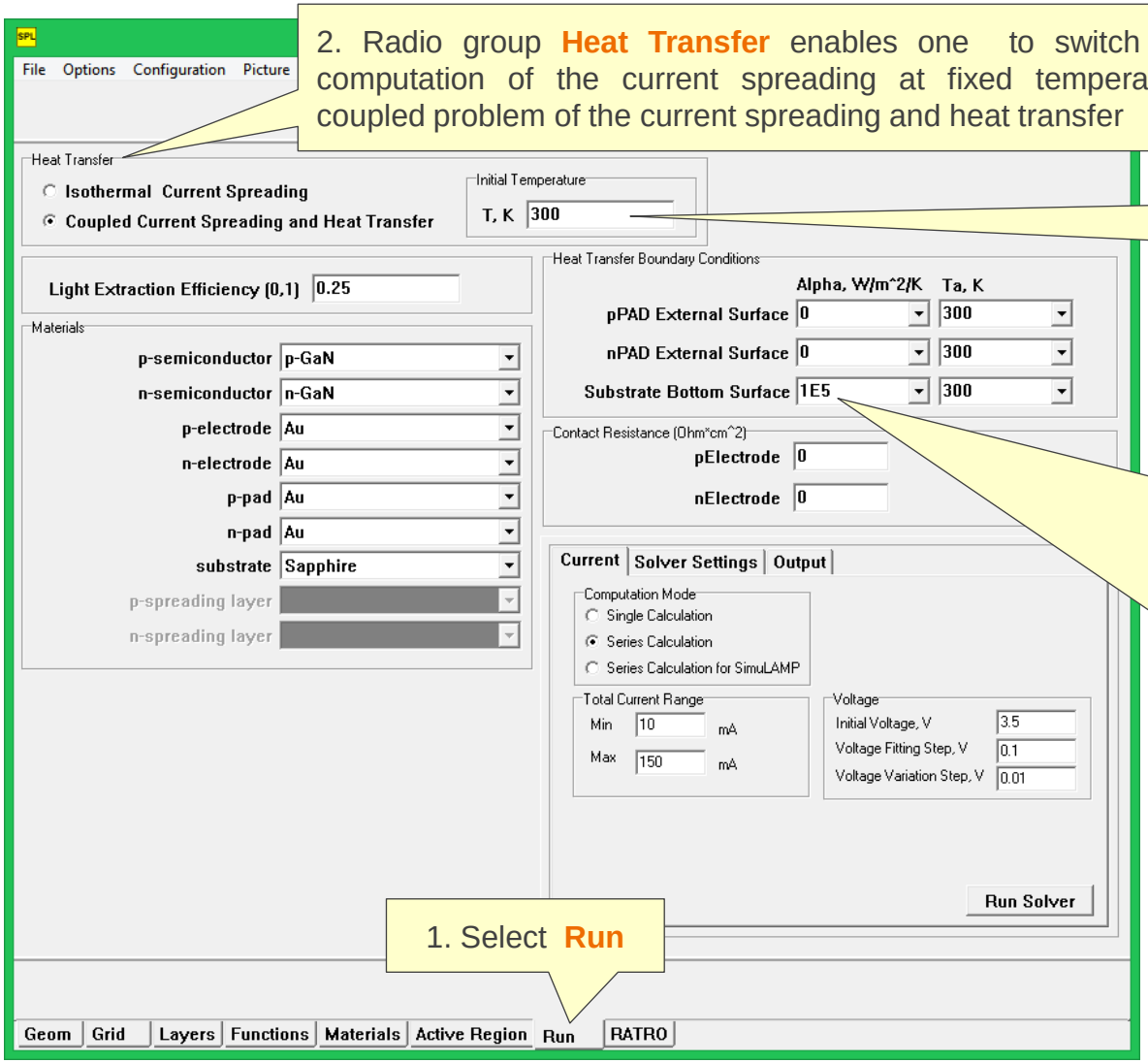
Please, read the manual for details about parametric approximation of j(U) and IQE(j).

4. In parametric mode, emission is monochromatic. Specify the wavelength here.

1. Select **Parametric Approximation**

5. Input of tabulated data for the active region properties is also available

Step 7: Specification of the heat transfer problem



2. Radio group **Heat Transfer** enables one to switch between computation of the current spreading at fixed temperature and coupled problem of the current spreading and heat transfer

3. Input device temperature for isothermal problem. Otherwise, input initial guess for the temperature

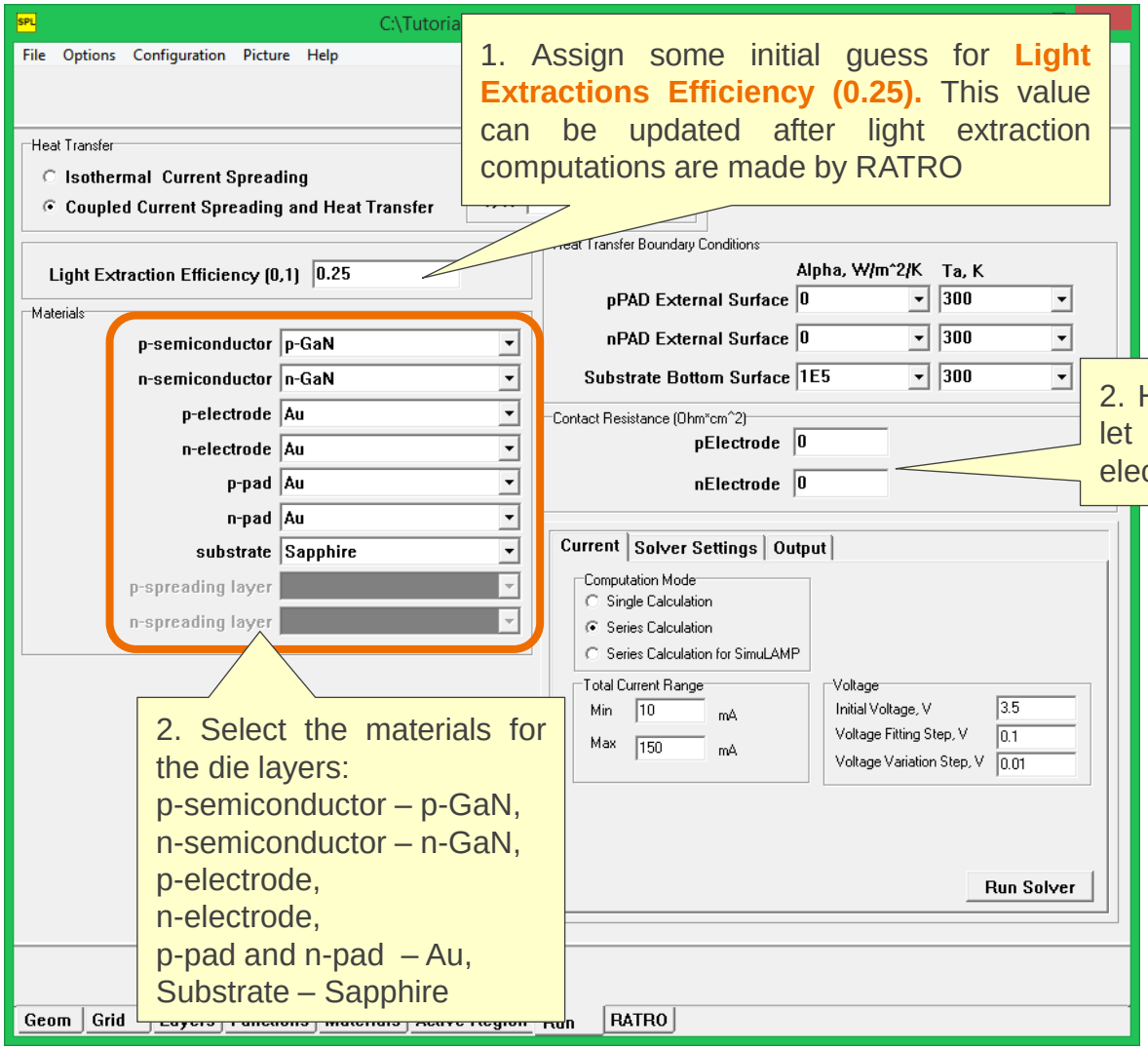
4. Considering the chip where substrate is mounted onto the heat sink, let us specify the heat transfer coefficient for substrate bottom surface only. Reasonable default is 1e5 W/(m^{2}K).

For our case, let us keep zero values for the heat transfer coefficients for pads. On the contrary, for flip-chip mounted LEDs one should specify heat release through the pads.

All other surfaces are always considered adiabatic

1. Select **Run**

Step 7 (Continued): Specification of global parameters



1. Assign some initial guess for **Light Extractions Efficiency (0.25).** This value can be updated after light extraction computations are made by RATRO

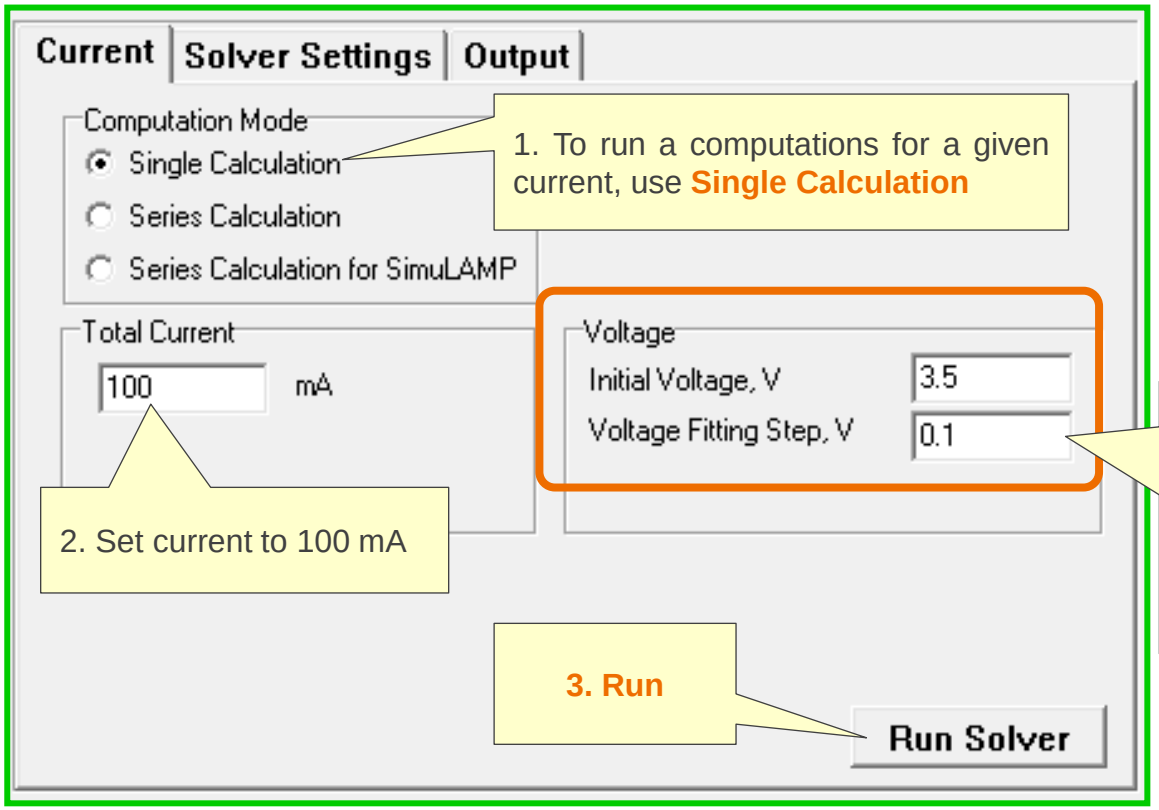
2. Having no additional information, let us keep zero values for the electrode contact resistances

2. Select the materials for the die layers:
p-semiconductor – p-GaN,
n-semiconductor – n-GaN,
p-electrode,
n-electrode,
p-pad and n-pad – Au,
Substrate – Sapphire

Light Extractions Efficiency is used to calculate the external quantum efficiency and wall-plug efficiency. For simulations with self-heating effects, it is also used to determine the heat source related to light absorption in the chip (it is assumed that all absorbed light contributes to the heat source in the active region)

Step 8: Running computations

Before running the computations, do not forget to select the **File -> Save As** … menu item to save the project



The following modes of running computation are available:

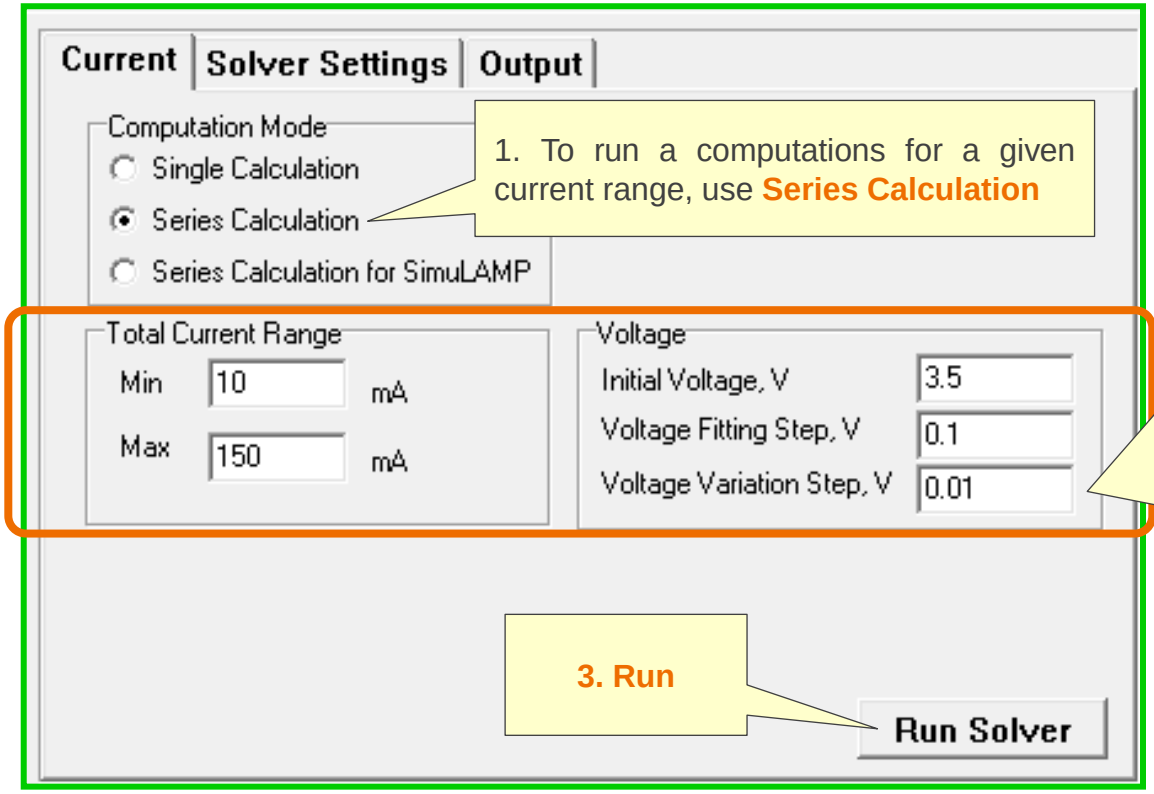
- Single Calculation
- Series Calculation
- Series Calculation for SimuLAMP

3. Set parameters of the current fitting by the voltage variation:

Initial Voltage = 3.5 V

Voltage Step = 0.1 V - a fitting parameter, can be rather high

Step 8 (Continued): Running series computations



2. Specify the following values:

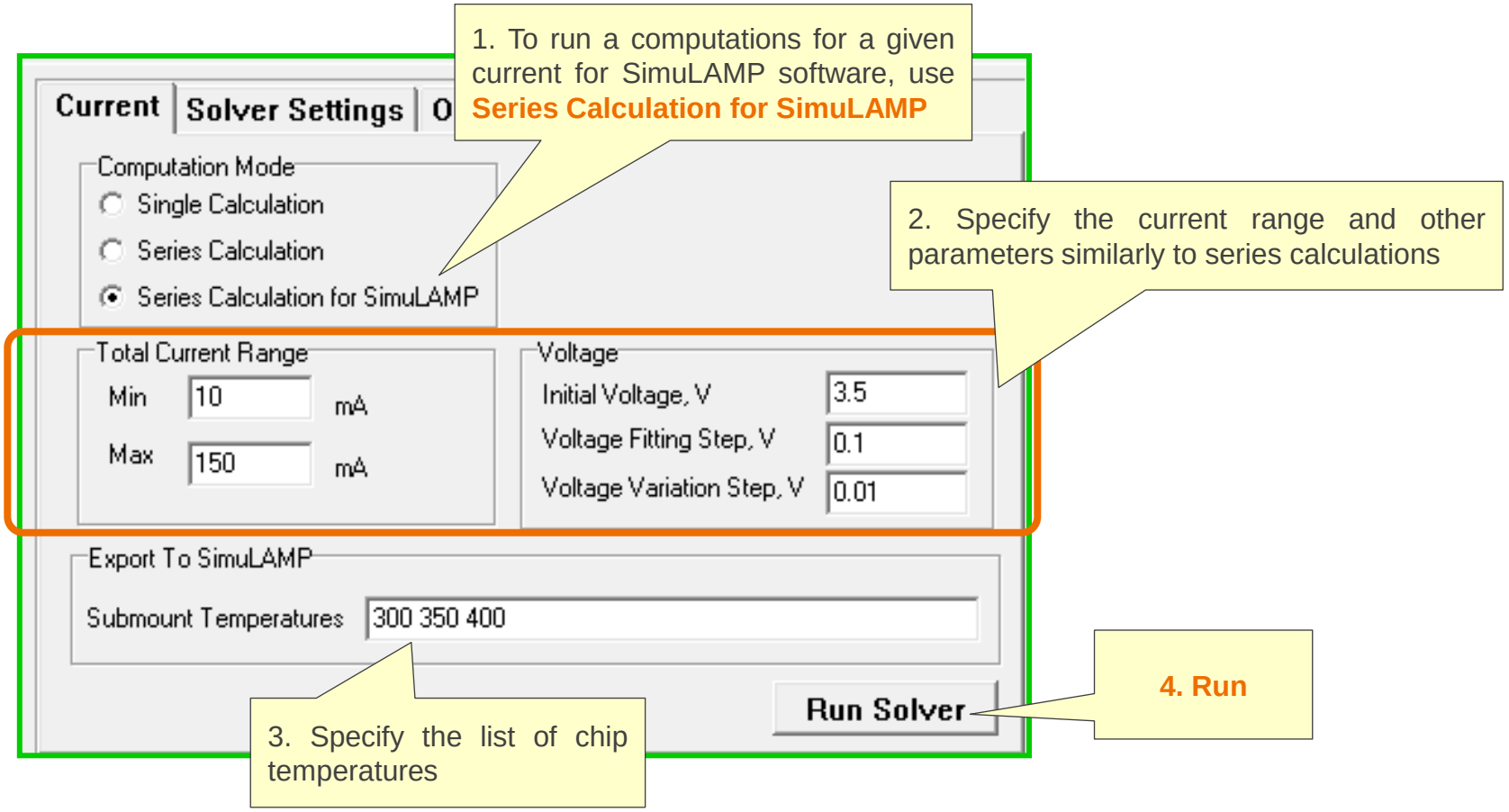
Total Current **Min** 10 mA

Total Current **Max** 150 mA

Initial Voltage 3.5 V - initial voltage is used only for fitting the minimal current (here, 10 mA) by the voltage variation

Voltage Variation Step 0.01 V - step of the I-V characteristics, should be rather small

Step 8 (Continued): Running computations for SimuLAMP



End of Tutorial 3