



Tutorial

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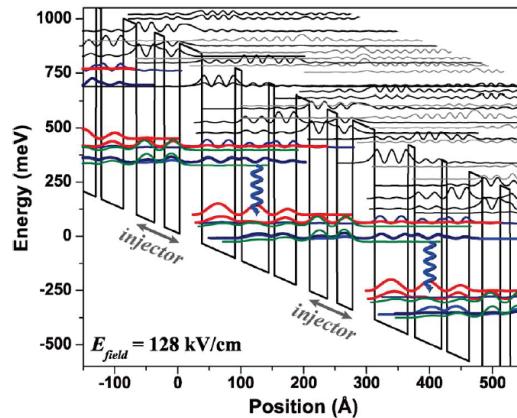
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ErwinJr Tutorial

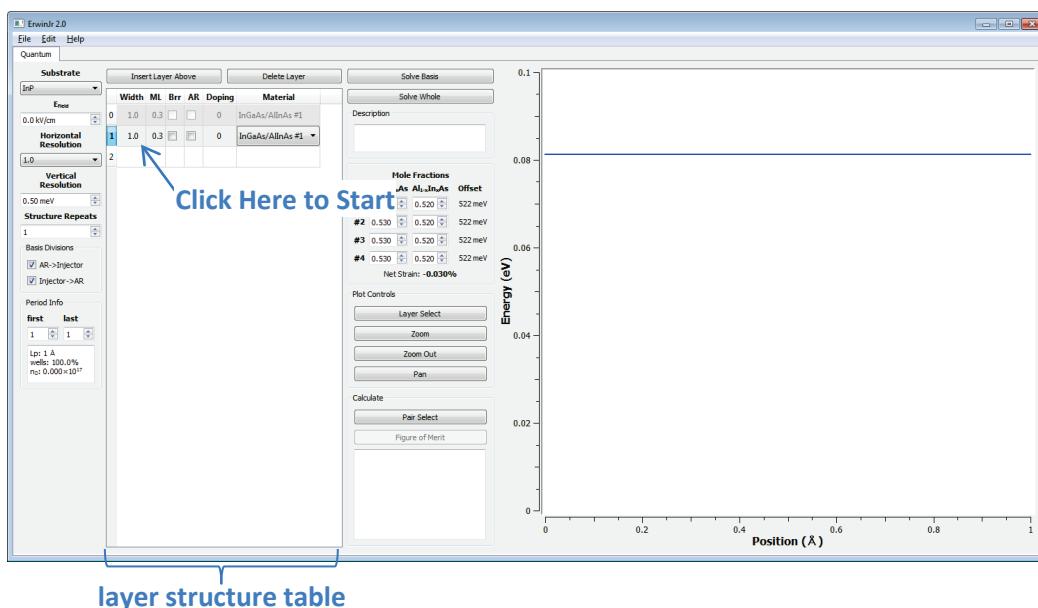
Creating a Simple QCL Structure

To start our tour, we will re-create the simple, 5 well QC laser as published in [K.J. Franz et al., IEEE J. Quantum Electron. 46, 591 \(2010\)](#). The text describes the layer structure and band diagram as described below. (This tutorial assumes you understand the meaning of the below text.)

The total QC period length $L_p = 274.5 \text{ \AA}$, for a design field $E_{\text{field}} = 128 \text{ kV/cm}$. As shown in the Fig. 7 conduction band diagram, the layer sequence is, in angstroms, starting from the injection barrier, **35/53/10.5/43/8.5/35/21/28.5/15.5/24.5**, where $\text{Al}_{0.710}\text{In}_{0.290}\text{As}$ layers are in bold type, $\text{In}_{0.638}\text{Ga}_{0.362}\text{As}$ layers are in plain type, and layers Si-doped $n = 1.4 \times 10^{17} \text{ cm}^{-3}$ are underlined;



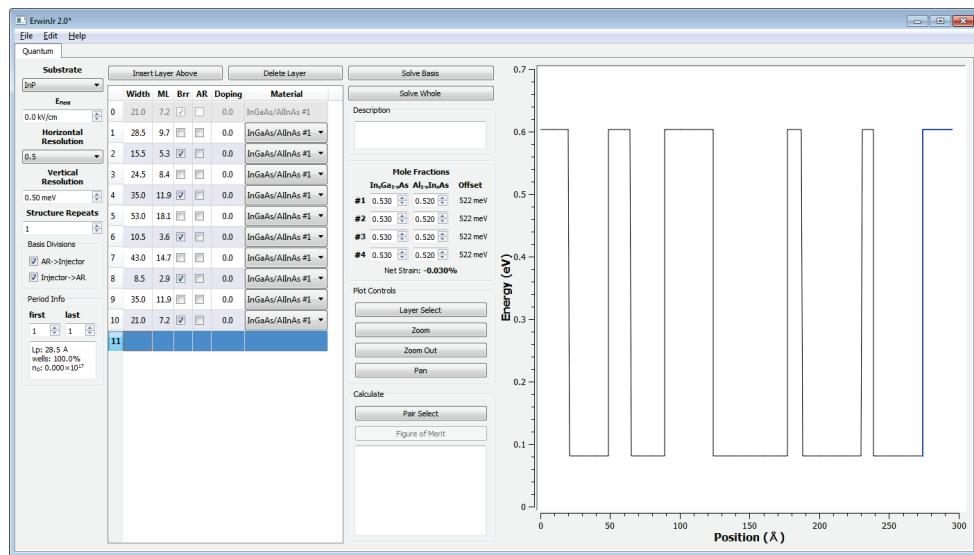
To start, open *ErwinJr*, and create a new file [File | New]. Select the Width column in row 1 of the layer structure table. The layer structure table lets you set many parameters for each layer in your QC structure. Specifically, the layer structure table contains for each QC layer: width (or width by monolayer, ML), whether or not the layer is a barrier (Brr), whether or not the layer is an “active region” (AR) layer, the doping of the layer (in units of 10^{17} cm^{-3}), and the layer material.



Let's start entering some numbers. For a reason that will become clear soon, I'm going to start with the layer of width 28.5. Enter 28.5 in the Width column of row 1, then press enter. Next, select row 2 in the Width column; enter 15.5; press enter. Several things just happened:

- The layer was automatically set to Barrier (because the previous layer was a well);
- The figure on the right was updated with the current layer structure;
- Because row 2 is the last row of the structure, the layer width 15.5 was automatically put into row 0; and
- The cursor position was automatically moved to row 3 for the next input.

Now, the rest of the layer structure can be entered. Press enter after entering each of the following: 24.5, 35, 53, 10.5, 43, 8.5, 35, 21. Your window should now look something like this:

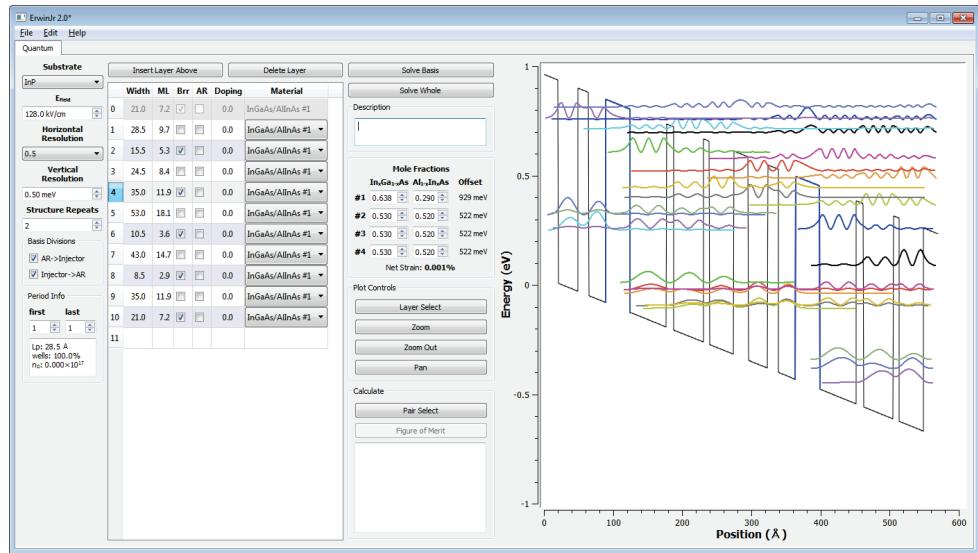


In general, I like for the first and last layers of the structure to be barriers. Therefore, I have created a layer "0," which is a repeat of the last layer of the stack. It is also my personal preference to have the injector region precede the active region.

Now click on layer 4, which is the injection barrier. In the plot on the right, a blue outline shows you which layer you have selected. If you wanted, you could make this layer a well layer by unchecking the box under the Brr (Barrier) column.

There are a few other items we need to input to complete the structure. In the E_{field} box, highlight the contents and type 128 to set the field to 128 kV/cm. The material compositions were specified as In_{0.638}Ga_{0.362}As and Al_{0.710}In_{0.290}As. In the Mole Fractions area, set the row #1 box under In_xGa_{1-x}As to the x fraction value 0.638; set the row #1 box under Al_{1-x}In_xAs to the x fraction 0.290. Notice that the calculated net strain is near 0%. Finally, since this is such a simple structure, solving one period would be boring. Set the Structure Repeats box to 2.

Click the Solve Whole button. Was that fast enough? Your window should now look like this:

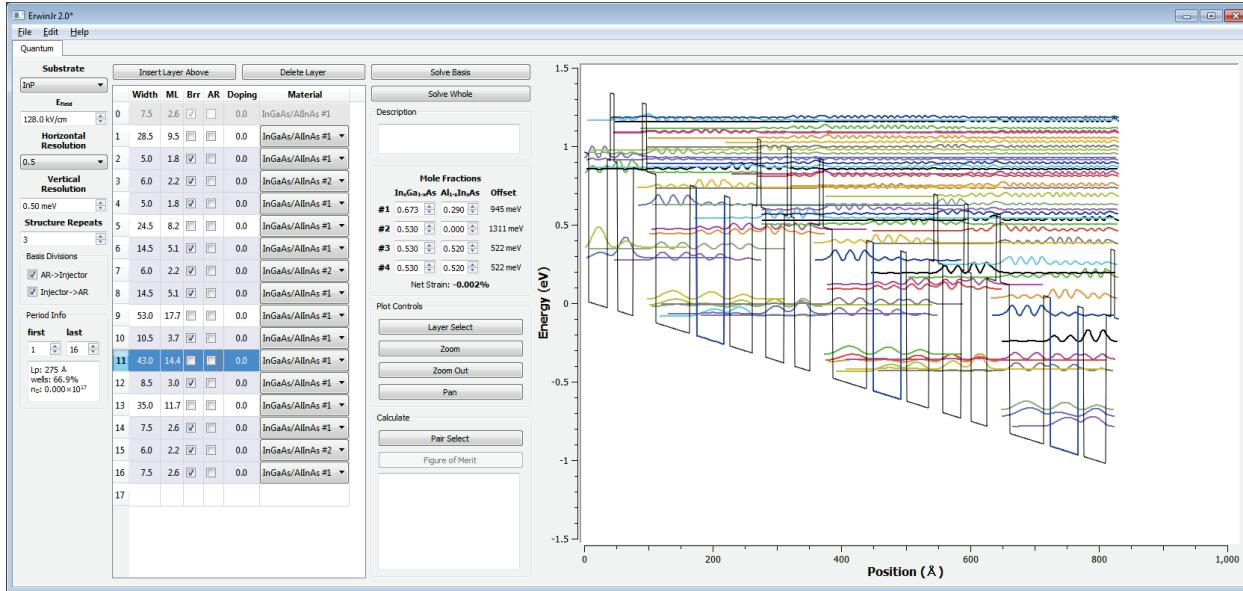


Flexing ErwinJr's Muscles: Creating a more complex QCL structure

Say we want to add AlAs barrier layers into our structure. Specifically, we want to insert 6 Å AlAs layers into the extraction barrier, the middle injector barrier, and the injection barrier (the 21, 15.5, 35 Å barrier layers, respectively). We want to replace these single layers with layers that look something like

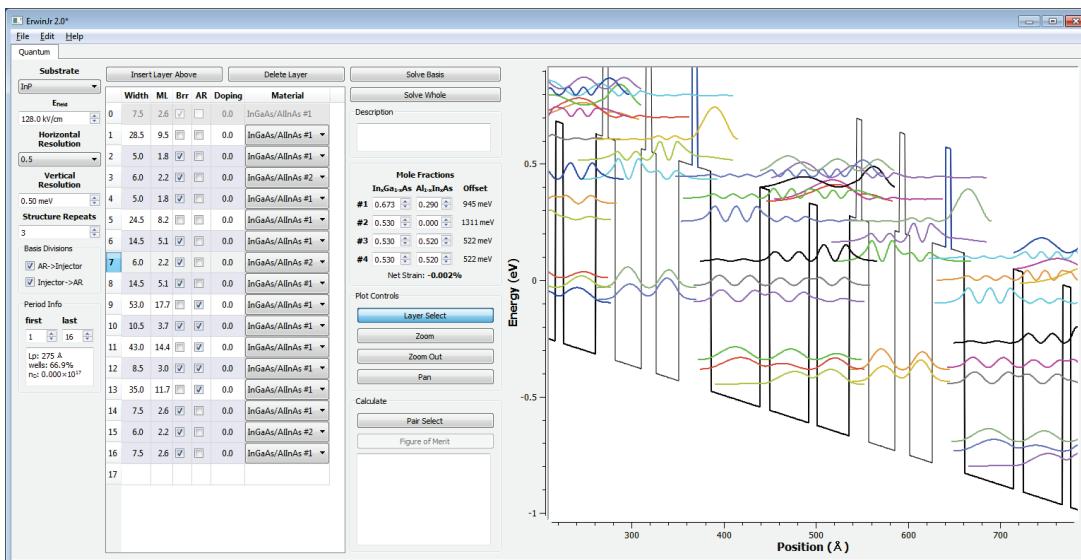
- 21 → 7.5, **6**, 7.5
- 15.5 → 5, **6**, 5
- 35 → 14.5, **6**, 14.5

where the layers in normal font are $\text{Al}_{0.710}\text{In}_{0.290}\text{As}$ and the bold layers are AlAs. To do this, the first step we can take is setting, in the Mole Fractions box, the row #2 column $\text{Al}_{1-x}\text{In}_x\text{As}$ box to 0. This means that the barrier layer of the “InGaAs/AlInAs #2” material will be $\text{Al}_{1.00}\text{In}_{0.00}\text{As}$ or AlAs. Next, highlight row 10 in the layer structure table; click the Insert Layer Above button. Now, change the widths in rows (10, 11, 12) to (7.5, 6, 7.5) and make sure the barrier box is checked in each of these rows. Finally, for row 11, change the material from “InGaAs/AlInAs #1” to “InGaAs/AlInAs #2.” Repeat this procedure of inserting rows and modifying the layer structure for the 15.5 and 35 Å barriers. We can balance the strain by changing the Mole Fractions box row #1 $\text{In}_x\text{Ga}_{1-x}\text{As}$ column to 0.673. Finally, for effect, change the number of structure repeats to 3, and click the Solve Whole button. Your window should look like this.

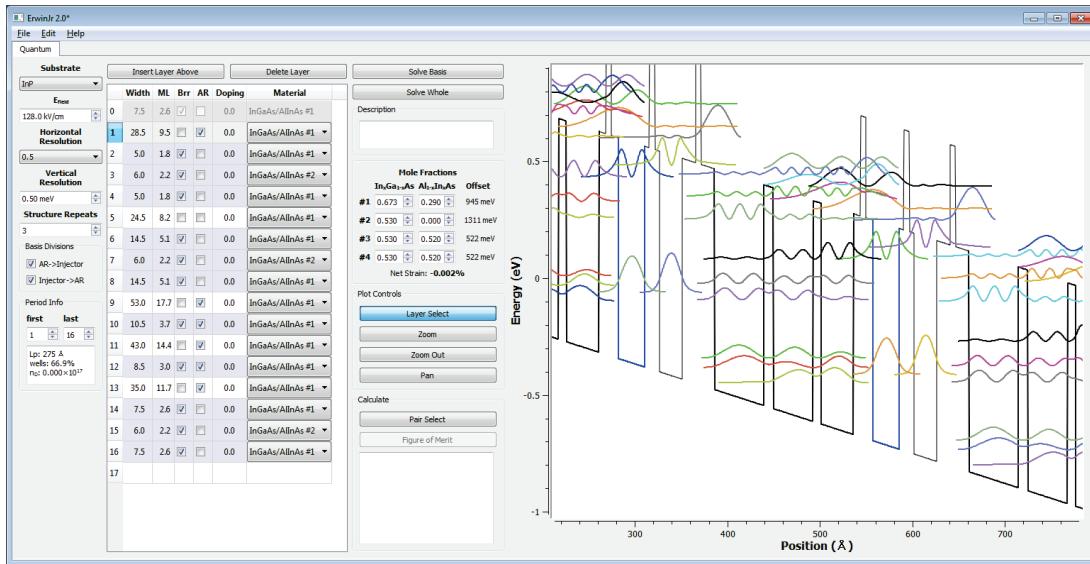


The Plot Controls box contains four buttons: Layer Select, Zoom, Zoom Out, and Pan. Let's click Zoom and drag a box around an area we want to zoom in to on the right conduction band diagram. The Zoom Out button will bring us back to the original, full zoom. The Pan button moves the plot around when under zoom. Clicking the Layer Select button will allow you to choose a layer to edit the width of: after clicking Layer Select, click a layer on the conduction band diagram. The layer is highlighted in the layer structure table and the width column is active.

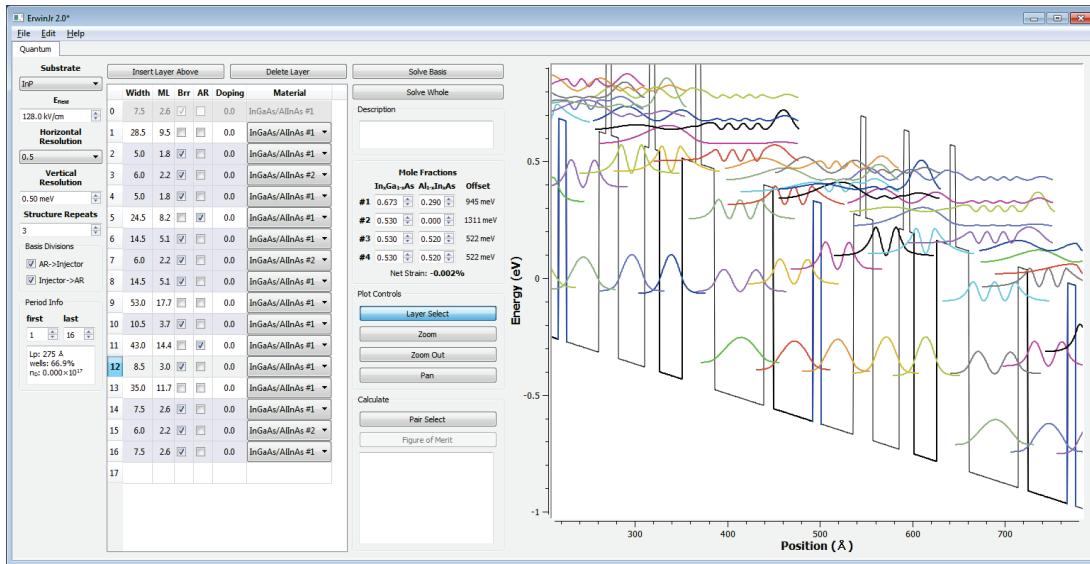
Now let's explore the capabilities of defining the active region. Click the checkbox in the AR column for layers 9 through 13. You'll notice that the conduction band outline for these wells and barriers is now thicker. The AR feature also allows you to define basis states for solving the structure. Click Solve Basis. The *ErwinJr* window (with a zoomed in band diagram) should look like this.



You'll notice that the active region now has solutions that are "separate" from the injector region. Say we want to solve each injector region well state separately. Check the AR box for layer number 1; then click **Solve Basis**. The window looks like this.



Notice, now, that each of the two states in the injector region is solved individually, with no coupling between the two. One rule you'll need to follow when setting basis states this way is that the group of states should both begin and end with a well layer. For example, to solve *each well individually*, only layers 5 and 11 (or, alternately, layers 1, 9, and 13) should have the AR box checked in this structure.

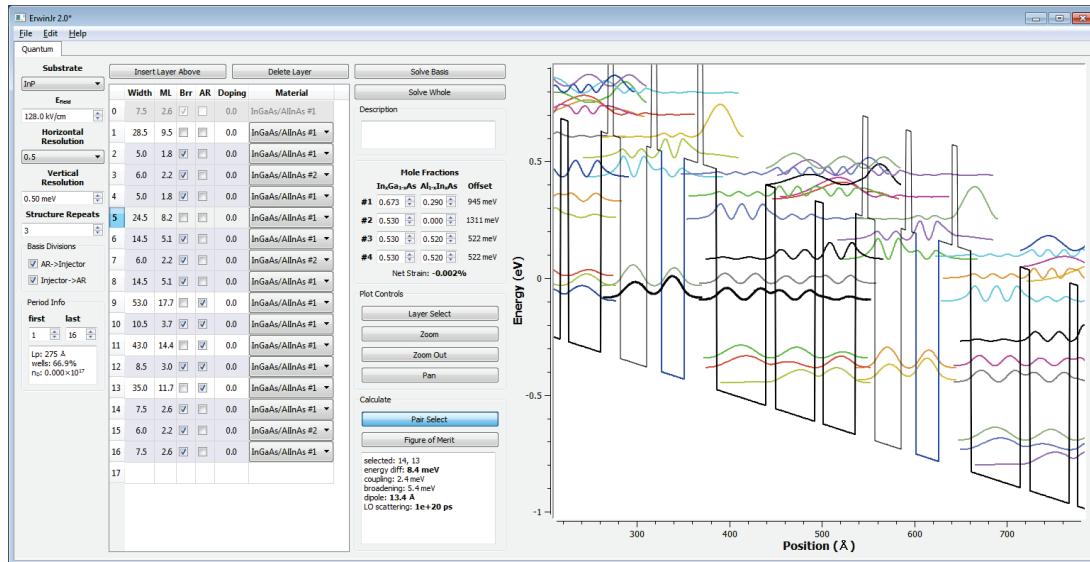


Calculations in ErwinIr

Let's go back to the structure where we have defined the active region with the AR checkboxes (*i.e.* the AR box for layers 9 through 13 is checked, all other AR boxes are unchecked). The Period Info box gives

us some useful information about the structure. We can define the set of layers to consider; by default, the first layer (1) and last layer (16) are chosen. The box tells us that the period length L_p between layers 1 and 16 is 275 Å. The composition of the layers 1-16 region is 66.9% well material. If we had input doping values into the layer structure table, the average doping for the defined region would be reported as n_D .

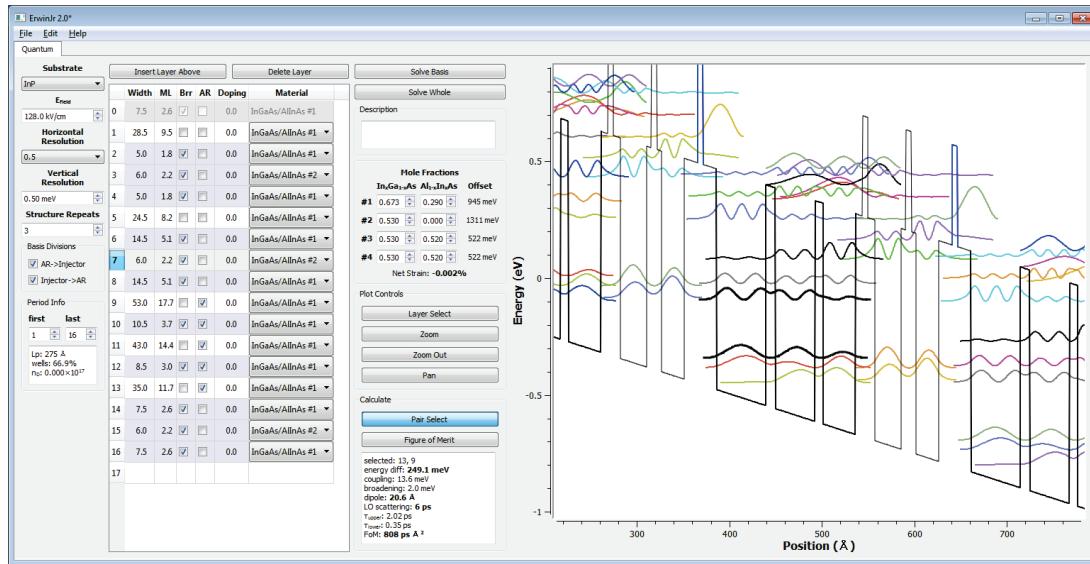
Now to the Calculate box. The basic functionality here works when two energy states are selected. Then, data is calculated and reported based on those two states. Click the **Pair Select** button; next click very near to an injector ground state and then click near the adjacent upper laser state. Once selected, each state turns bold and black. After the second state is selected, information is reported in the white Calculate box.



The given information is as follows:

- “selected: 14, 13”: indicates that states number 13 and 14 (counting from the first state at the bottom of the structure) are used in the calculations
- “energy diff: 8.4 meV”: indicates that the energy difference between the selected states is 8.4 meV
- “coupling: 2.4 meV”: indicates that the coupling energy between the selected states 2.4 meV
- “broadening” 5.4 meV”: indicates that the interface roughness broadening energy between the selected states is 5.4 meV
- “dipole: 13.4 Å”: indicates that the optical dipole matrix element between the selected states is 13.4 Å
- “LO scattering time: 1e+20 ps”: indicates the LO scattering time between the selected states in units of picoseconds. In this case, the energy between the selected states is less than the LO phonon energy, so no LO phonon scattering exists at the Γ point, indicated by the 1e+20 ps time.

Clicking the Pair Select button a second time will clear the selected states, however, this is not necessary; the calculation will be done for every second state selected. Now select the upper laser state and the lower laser state in the same active region. Click the Figure of Merit button.



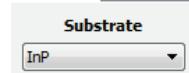
Additional information is given in the Calculate dialog box.

- “ τ_{upper} : 2.02 ps”: gives the overall LO phonon lifetime of the selected energy state of highest energy
- “ τ_{lower} : 0.35 ps”: gives the overall LO phonon lifetime of the selected energy state of lowest energy
- “FOM: 808 ps Å²”: Gives the figure of merit calculated as $\tau_{\text{upper}} * (1 - \tau_{\text{lower}}/\tau_{\text{upper-lower}}) * \text{dipole}^2$

Navigating and Working in *ErwinJr*

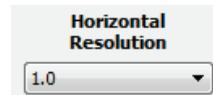
Now, let's work in a systematic order to explore some of the features and functionality of *ErwinJr*.

Substrate



ErwinJr is designed to be used with different materials systems. By default, *ErwinJr* uses InGaAs/AlInAs on an InP substrate. InAsSb/AlGaSb on a GaSb substrate is also currently programmed. In the future, I envision adding more materials systems, such as systems for II-VI materials along with systems for GaAs and III-nitride substrates. Material parameters for each substrate are largely taken from [I. Vurgaftman, et al., J. Appl. Phys. 99, 5815 \(2001\)](#).

Horizontal Resolution



The Horizontal Resolution box sets the resolution of the horizontal (Position) axis in angstroms. A value of 1 (\AA) will give the “coarsest” solution, but it will also give the fastest solution. In general, at a minimum, should be such that dividing each layer width by the horizontal resolution results in an integer. For example, if your structure has a layer of width 5.5 (\AA), the minimum horizontal resolution should be 0.5 (\AA); if you structure has a layer of width 8.7 (\AA), the minimum horizontal resolution should be 0.1 (\AA).

Vertical Resolution



A screenshot of a software interface showing a vertical resolution input field. The field is labeled "Vertical Resolution" and contains the value "0.50 meV". Below the input field are two small, semi-transparent square buttons with upward and downward arrow symbols, used for incrementing or decrementing the value.

The Vertical Resolution box sets the minimum spacing in energy (meV) that the solver uses to find eigenvalues (*i.e.* energy states). Thus, if two or more energy states exist in the system with an energy separation of less than the vertical resolution, the solver will only find one of those energy states. A smaller vertical resolution will result in an increased solve time.

Structure Repeats



A screenshot of a software interface showing a structure repeats input field. The field is labeled "Structure Repeats" and contains the value "3". Below the input field are two small, semi-transparent square buttons with upward and downward arrow symbols, used for incrementing or decrementing the value.

The Structure Repeats box contains the number of times the entire QC structure is repeated in the energy diagram on the right of the window. When plotting (and solving, etc.) the energy diagram, layer 0 is ignored in all cases except for the very first layer.

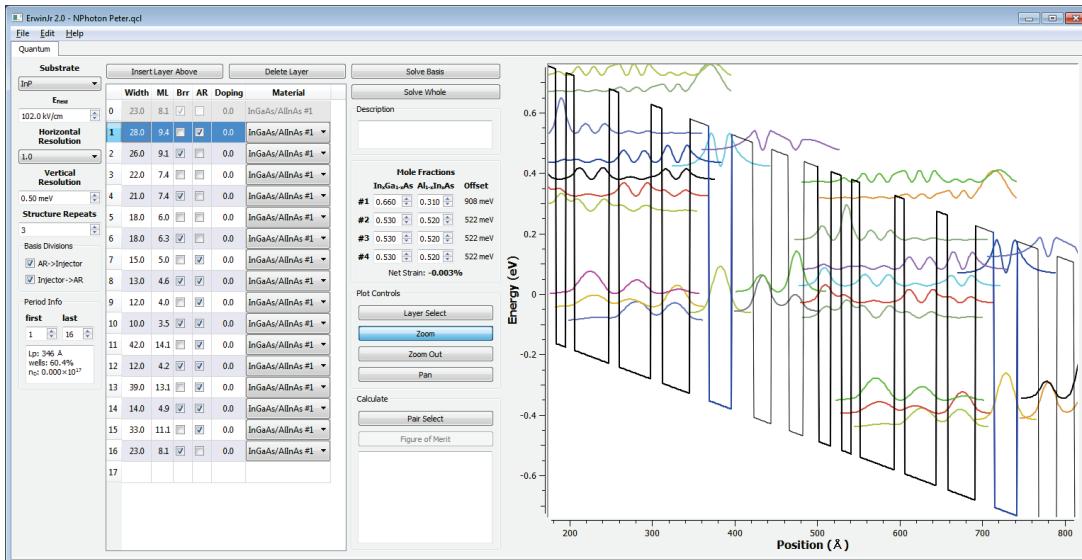
Basis Divisions Box



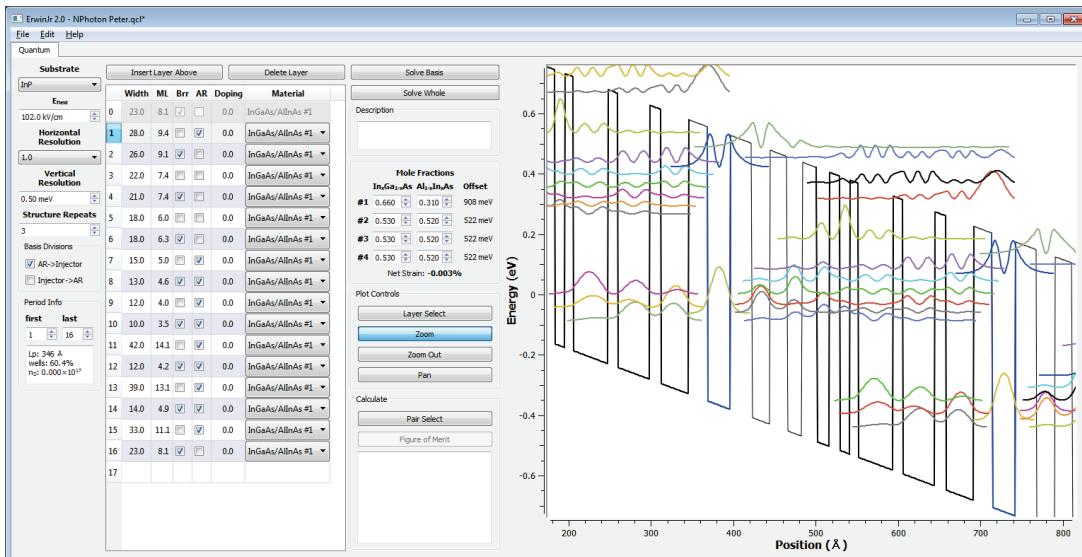
A screenshot of a software interface showing a basis divisions checkbox group. The group is labeled "Basis Divisions" and contains two checkboxes: "AR->Injector" and "Injector->AR", both of which are checked (indicated by a blue checkmark). There are also two small, semi-transparent square buttons with upward and downward arrow symbols, used for selecting other checkboxes.

The Basis Divisions box allows customization of where bases are divided when the Solve Basis button is used. Checking the AR->Injector checkbox creates basis divisions at transitions between an AR layer and a non-AR layer. Checking the Injector->AR box creates basis divisions at transitions between a non-AR layer and an AR layer. In all cases, divisions are made at the boundary of a structure repeat; for example, with neither AR->Injector or Injector->AR checked, there will be basis divisions only for each period of the QC structure.

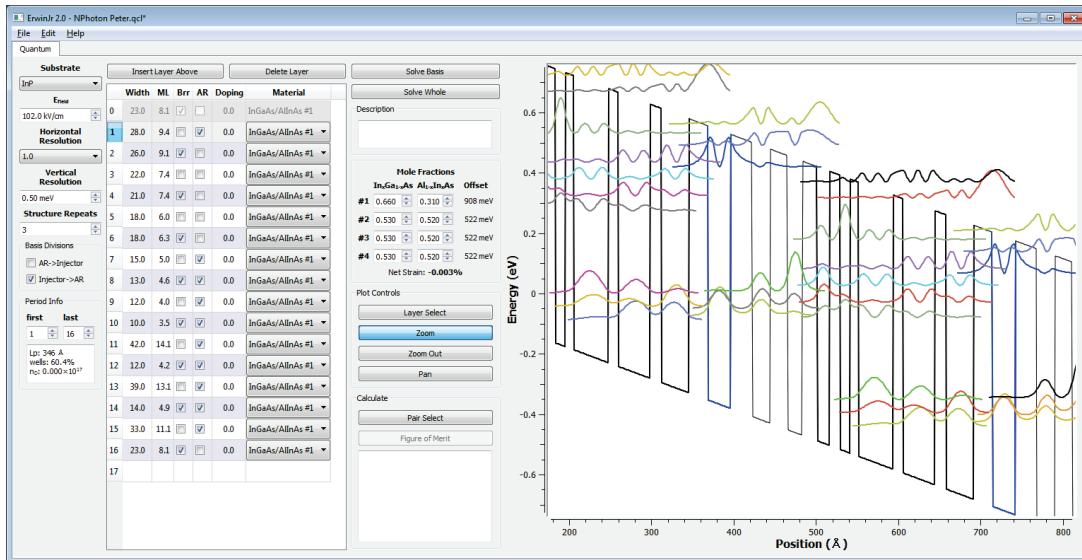
Compare the following three figures as an example where both checkboxes are checked, and where one or the other checkboxes is checked.



Both AR->Injector and Injector->AR are checked.



Only AR->Injector is checked.



Only Injector->AR is checked.

Period Info Box



The Period Info box gives specific information about your QC structure for a range of layers defined by the “first” box and the “last” box. The numbers in “first” and “last” correspond to the layers in the Layer Structure Table. Most of the time, the boxes will have the actual first and last layers of your structure as the default settings. Three data items are reported:

- L_p: the total length of layers inclusive of the first and last; in the example given, the thickness of the stack of QC layers from layer 1 to layer 22 is 501 Å
- wells: reports the percent of the material composition that is designated as well material between and including the first and last layers; in the example given, the structure contains 54.3% well material
- n_D: reports the average doping concentration for the range of layers inclusive of the specified first and last layer in units of cm⁻³; in the example given, the average doping level for the structure is 0.201×10¹⁷ cm⁻³.

Layer Structure Table

	Width	ML	Brr	AR	Doping	Material
1	26.0	8.7	<input type="checkbox"/>	<input checked="" type="checkbox"/>	0.0	InGaAs/AlInAs #1
2	21.0	7.3	<input checked="" type="checkbox"/>	<input type="checkbox"/>	0.0	InGaAs/AlInAs #1
3	25.0	8.4	<input type="checkbox"/>	<input checked="" type="checkbox"/>	0.0	InGaAs/AlInAs #1
4	21.0	7.3	<input checked="" type="checkbox"/>	<input type="checkbox"/>	0.0	InGaAs/AlInAs #1
5	23.0	7.7	<input type="checkbox"/>	<input checked="" type="checkbox"/>	0.0	InGaAs/AlInAs #1
6	23.0	8.0	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1.5	InGaAs/AlInAs #1
7	21.0	7.0	<input type="checkbox"/>	<input checked="" type="checkbox"/>	1.5	InGaAs/AlInAs #1
8	23.0	8.0	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1.5	InGaAs/AlInAs #1
9	20.0	6.7	<input type="checkbox"/>	<input checked="" type="checkbox"/>	0.0	InGaAs/AlInAs #1
10	25.0	8.7	<input checked="" type="checkbox"/>	<input type="checkbox"/>	0.0	InGaAs/AlInAs #1

The Layer Structure Table lets you set many parameters for each layer in your QC structure. Each row represents one layer in the QC stack. The Layer Structure Table contains for each QC layer:

- layer width in Å,
- layer width by monolayer (ML),
- whether or not the layer is a barrier (Brr),
- whether or not the layer is an “active region” (AR) layer,
- the doping of the layer (in units of 10^{17} cm^{-3}), and
- the layer material.

The Insert Layer Above and Delete Layer buttons can be used to manipulate the QC layer stack. The Material dropdown box for each layer represents the material number as defined in the Mole Fractions Box.

The last row in the table is blank; by entering a number in the width column of the last row, a new layer is appended with your specified width. The layer is automatically set as barrier (Brr) if the previous layer is a well layer, and the layer is automatically set as a well layer if the previous layer is a barrier.

Insert Layer Above

The Insert Layer Above button adds a QC layer (a row) above the layer currently selected in the Layer Structure Table.

Delete Layer

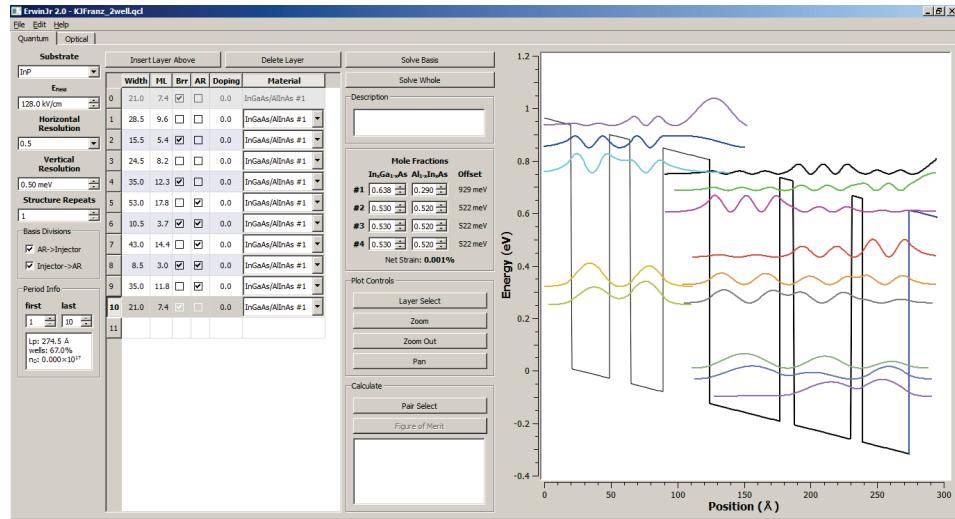
The Delete Layer button removes the selected QC layer (row) in the Layer Structure Table.

Solve Basis

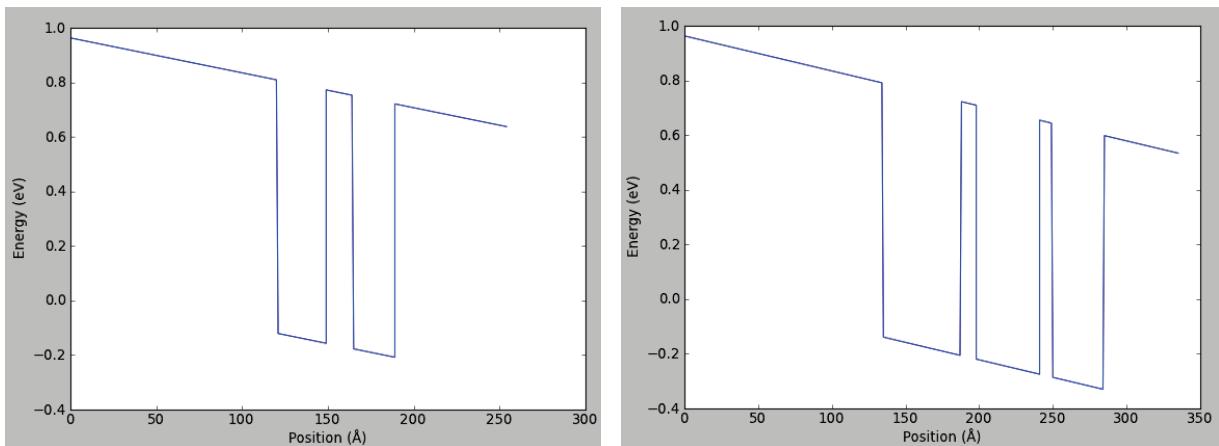
The Solve Basis button allows the user to acquire structure solutions where the structure is divided into “sections” or bases. Bases are defined by use of the active region (AR) feature in conjunction with the Basis Divisions Box. The boundaries of a basis state are identified by a transition from AR->Injector or a

transition from Injector->AR. Once a set of basis wells is identified, the solver places a 100 Å barrier layer on the left (higher potential) side of the structure, a 30 Å barrier layer on the right (lower potential) side of the structure, and then infinite barriers to enclose the structure.

Take for example the two-well structure given in the tutorial: 28.5, **15.5**, 24.5, 35, 53, 10.5, 43, 8.5, 35, 21, where $\text{Al}_{0.710}\text{In}_{0.290}\text{As}$ barrier layers are in bold font, $\text{In}_{0.638}\text{Ga}_{0.362}\text{As}$ layers are in normal font, and active region (AR) layers are underlined. When Solve Basis is used, *ErwinJr* shows a window that looks like this:



In this case, *ErwinJr* is solving two separate structures; the conduction band edges for the two structures are shown below. Infinite barriers are placed on either ends of the structures shown below.

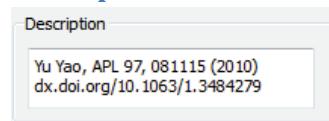


Solve Whole

The Solve Whole button solves the entire QC structure as viewed in the zoomed out version of the band diagram plot. For the solution, infinite barriers are placed at 0 Å and at the end point of the structure.

The solution method is described in chapter 2 my PhD thesis, available at www.kalefranz.com/publications.

Description Box



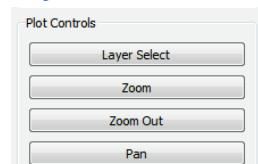
The description box holds optional, user-defined text about the current QC structure.

Mole Fractions Box

Mole Fractions		
	In _x Ga _{1-x} As	Al _y -In _{1-y} As
#1	0.673	0.342
#2	0.530	0.520
#3	0.530	0.520
#4	0.530	0.520
Offset		
#1	865 meV	
#2	522 meV	
#3	522 meV	
#4	522 meV	
Net Strain: 0.000%		

The Mole Fractions box defines the material compositions for the materials given in the dropdown box in each layer of the Layer Structure Table. Each row number in the Mole Fractions box corresponds to a material option given in the Layer Structure Table. The conduction band offset for each material is given in units of meV. The overall net strain for the whole structure as defined in the Layer Structure Table is given in units of percent.

Layer Select

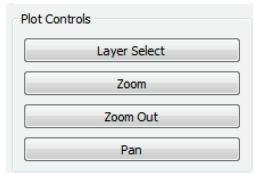


The Layer Select button in the Plot Controls box allows the user to navigate through and edit the QC structure by using the mouse to click on a layer in the band diagram plot. When the Layer Select button is active (depressed), clicking on or near a layer in the band diagram plot will:

- highlight that layer in blue on the band diagram plot,
- make active the selected layer in the Layer Structure Table, and
- set the width column for the selected layer as active and ready for editing.

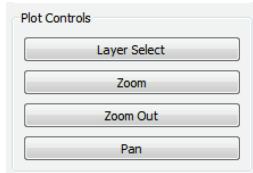
The feature is designed so that editing layer thicknesses is as easy as “point, click, change.”

Zoom



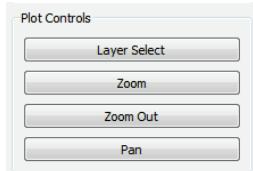
The Zoom button makes a crosshair indicator for the mouse position on the conduction band diagram plot. The structure can be zoomed in by drawing a box around the desired feature to be zoomed in on. The zoom can be taken back to the previous zoom by clicking the right mouse button.

Zoom Out



The Zoom Out button sets the zoom level to the full extent of the current structure in the conduction band diagram plot.

Pan



The Pan button allows the user to move or “pan” the structure as displayed in the conduction band diagram plot when under zoom.

Pair Select

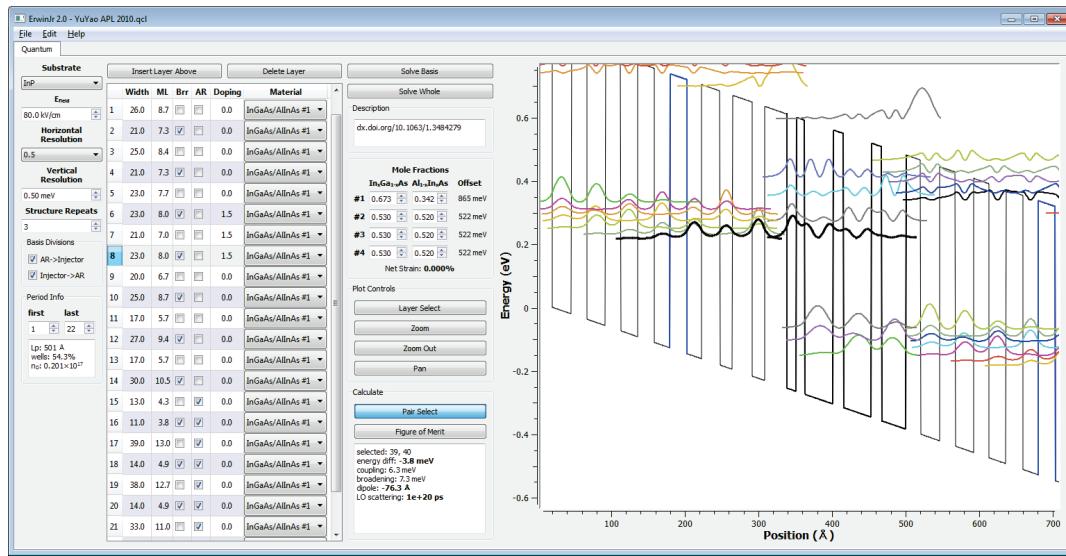
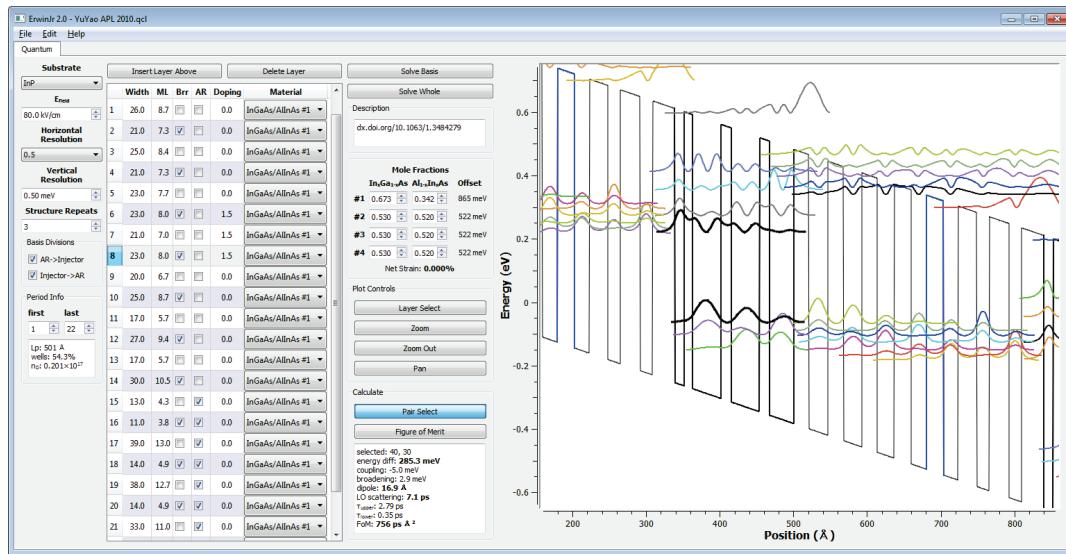


Figure of Merit



Beyond the information described for the Pair Select button, the Figure of Merit button calculates the following:

- “ τ_{upper} : 2.79 ps”: gives the overall LO phonon lifetime of the selected energy state of highest energy
- “ τ_{lower} : 0.35 ps”: gives the overall LO phonon lifetime of the selected energy state of lowest energy
- “FOM: 756 ps \AA^2 ”: Gives the figure of merit calculated as $\tau_{\text{upper}} * (1 - \tau_{\text{lower}}/\tau_{\text{upper-lower}}) * \text{dipole}^2$

File | Export Band Diagram Data

Export Band Diagram Data under the File menu creates a two comma-separated value (CSV) files. The first file (filename appended with “_CB”) has as its first column the position values array and the second column the conduction band edge. The second file (filename appended with “_States”) has as its first column the position values array and the remaining columns the squared moduli of the wavefunctions offset by the wavefunction energy.

File | Export Band Diagram Image

Export Band Diagram Image under the File menu creates a portable network graphics (PNG) image of the band diagram as it is in its present state.

Edit | Bump First Layer

Bump First Layer under the edit menu moves layer 0 to layer 1, and then replaces layer 0 with the last layer of the QC stack. This feature improves compatibility between the Matlab version of *ErwinJr* and the Python version of *ErwinJr*.

Edit | Copy Structure

Copy Structure under the Edit menu copies the layer widths of the QC stack to the clipboard.