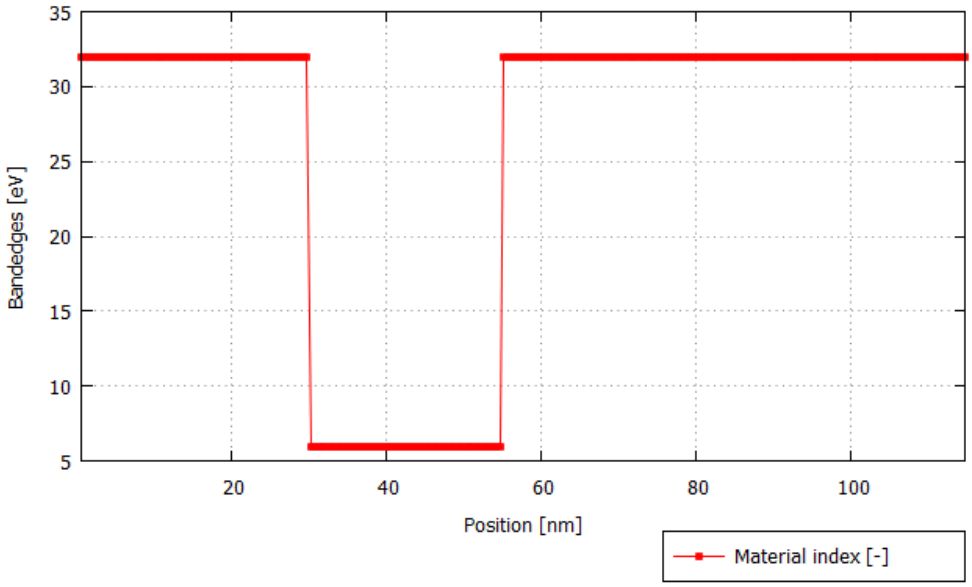
Optics tutorial (Simple)

This simple tutorial shows a simple simulation studies for absorption of semiconductor devices. (It seems that this tutorial is based on the file AlGaAs_QW_Frankenberger_nnp.in which has been documented here: Optics tutorial)

Structure

The structure is a simple AlGaAs quantum well which can be seen in the following figure.



<caption>The structure of the simulated device</caption>

The barriers are made from AlGaAs, and the well is GaAs.

Optics

The optics feature initialization looks like this:

```
optics{
        name = "all"
    debuglevel = 2

    interband = $INTERBAND # yes
    intraband = $INTRABAND # no

        polarization{ name="y_plus_iz"  re = [0,1,0] im = [0,0,1] }
    polarization{ name="y_minus_iz" re = [0,1,0] im = [0,0,-1] }
    output_transitions = $TRANSISITONS #yes
    occupation_threshold = $MIN_OCCUPATION
    energy_threshold = 1E-8
```

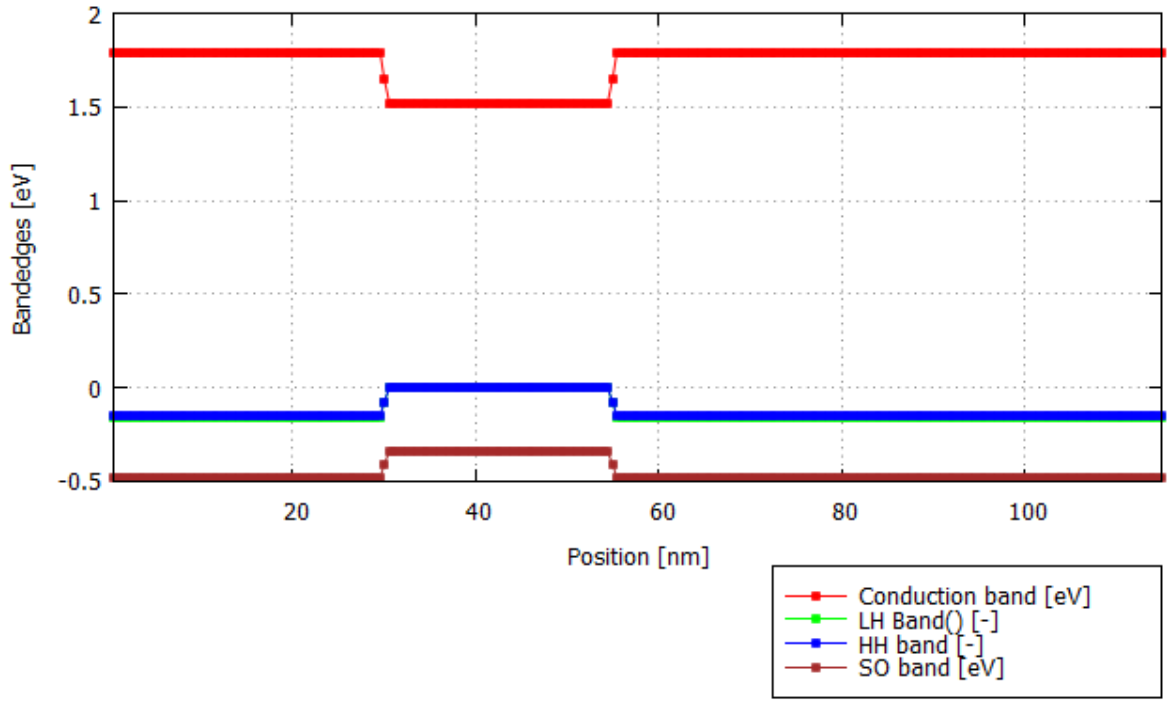
```
    transition_threshold = $MIN_TRANSISTION
    energy_min = $ENERGY_MIN
    energy_max = $ENERGY_MAX
    energy_resolution = $ENERGY_RESOLUTION
    k_integration{
      num_points = $NUM_INTEGRATION_KPOINTS
      num_subpoints = $NUM_INTEGRATION_INTKPOINTS
      symmetry = 1
          relative_size = $RELATIVE_INTEGRATION_KSPACE
    }
}
```

- `interband`, `intraband` Initalizes if intra/interband transitions should be calculated or not.
- `polarization` describes the polarization direction of the electric field. (When there is an 'i' it means it is circulary polarized)
- `output_transitions` Calculation of the transition matrix elements (`yes`/`no`)
- `occupation_threshold`, `energy_threshold`, `transition_threshold` The minimum value of the energy, occupation and transition intensity of the transition which should be calculated.
- `energy_min`, `energy_max` Boundaries of the calculated energy spectra.
- `energy_resolution` The energy grid spacing of the calculated points in the energy space.
- `k_integration` defines the points for integrating in the k space

The output

Bandedges in the sample

After the strain has been calculated, the bandedges of the structure are determined which can be seen in the figure:



<caption> The bandedges in the sample: Conduction band, heavy hole, light hole and split-off hole band edges </caption>

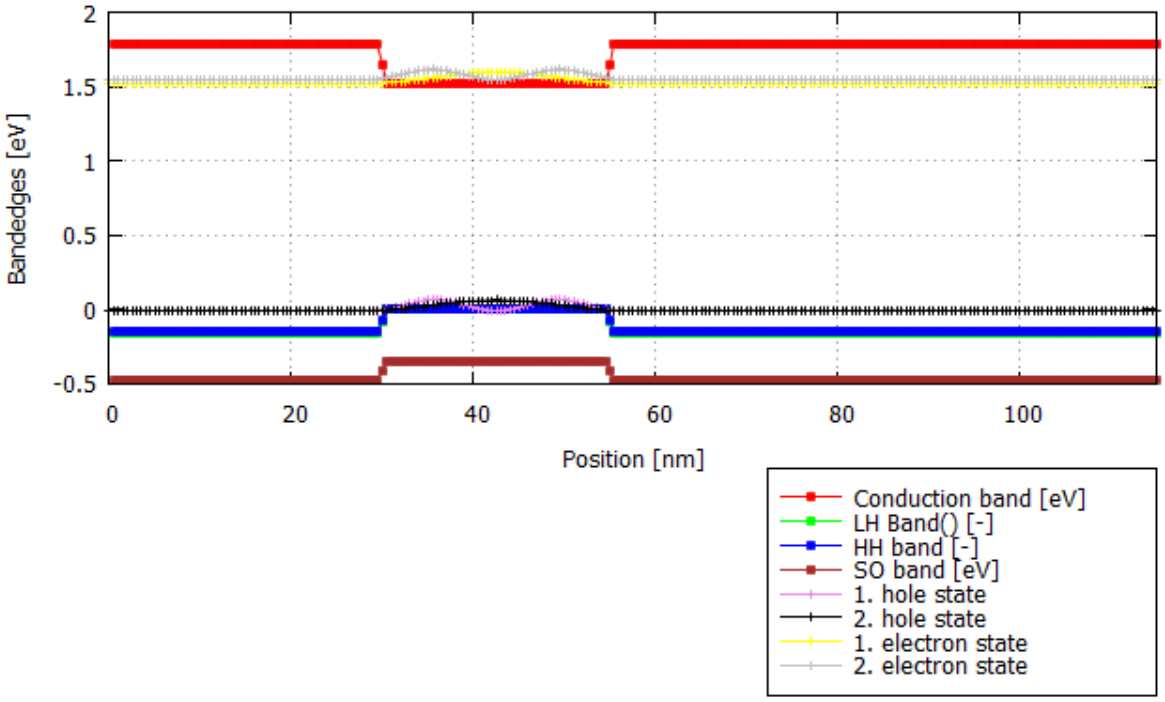
In the quantum well region it can be seen that the bandedge is smaller, and the valence band edge is close to the Fermi level. That is the reason why the valence band is populated and interband transition could happen.

Quantum Mechanics

From the bandedges the program calculates the wavefunctions in each band which is defined in the line:

```
num_electrons=$NumE
num_holes=$NumH
```

Here you can specify how many electron and hole states should be calculated. The wavefunctons are plotted on the following figure:

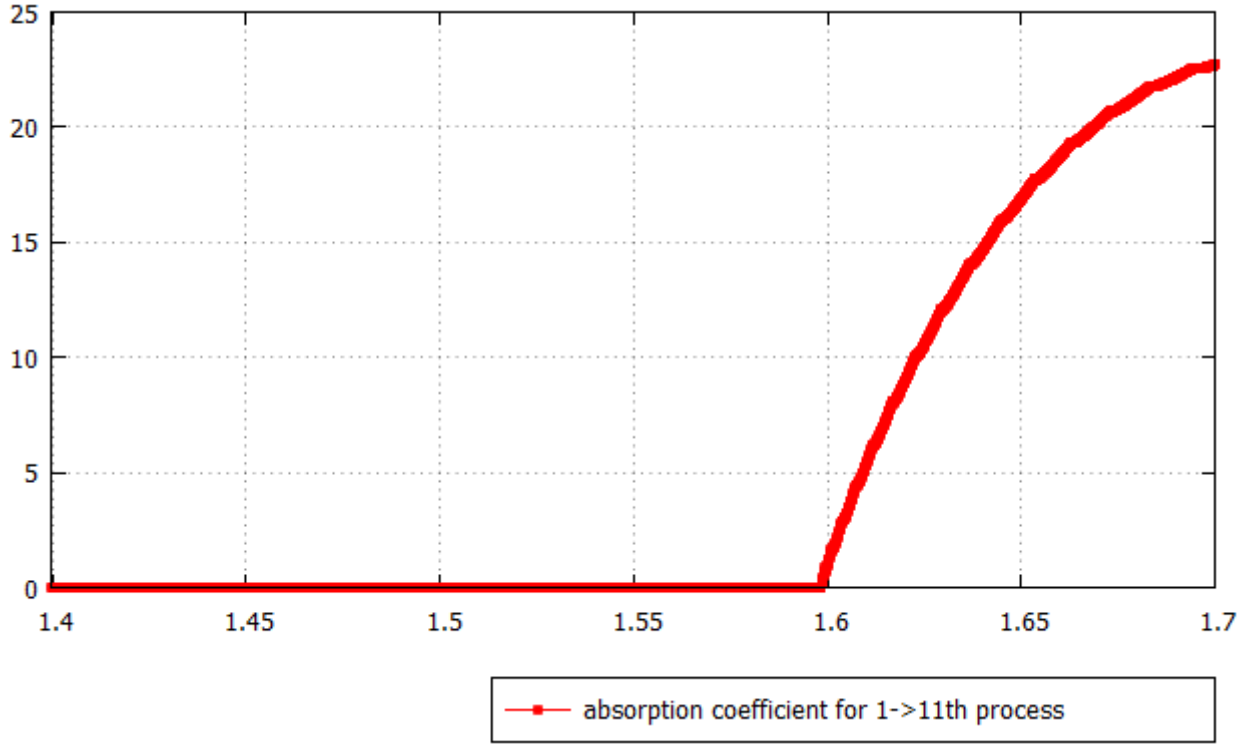


<caption>The wavefunction probabilities for each band</caption>

Optics

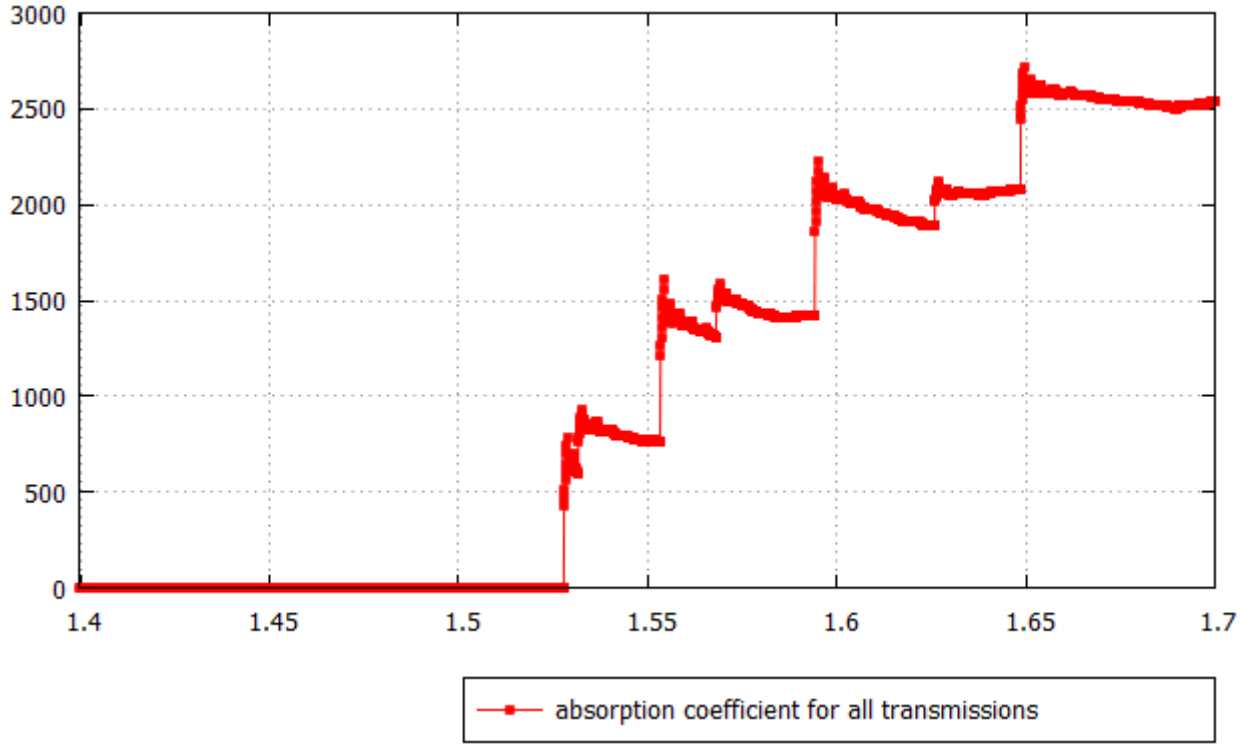
Absorption

For each defined polarization the program calculates the transition matrix elements between the states (integration of the wavefunctions in k space). Then it calculates the absorption coefficient (1/mucm) per one transition (it should consider the population of the states). For example one absorption coefficient can be seen as a function of the energy of the incoming field:



<caption>The absorption coefficient between the 1st and the 11th eigenstate of the system as a function of energy</caption>

The overall absorption coefficient of the system is the sum of the partial absorption coefficients of each transition.



<caption>The overall absorption coefficient as a function of energy</caption>

Im(ϵ)

Its imaginary part of the permittivity (related to the conductivity) could be calculated from the absorption coefficient with the following formula if the absorption is small.

$\alpha= \frac{\omega}{n_r c} \cdot \frac{\epsilon_2}{\epsilon_0}$

The values of the imaginary part of the permittivity function is in the files `imepsilon*.dat`.

Transitions

The summary of the transitions have been saved in the “transitions_all.dat” files, together with the intensity, and the rate of the transition.