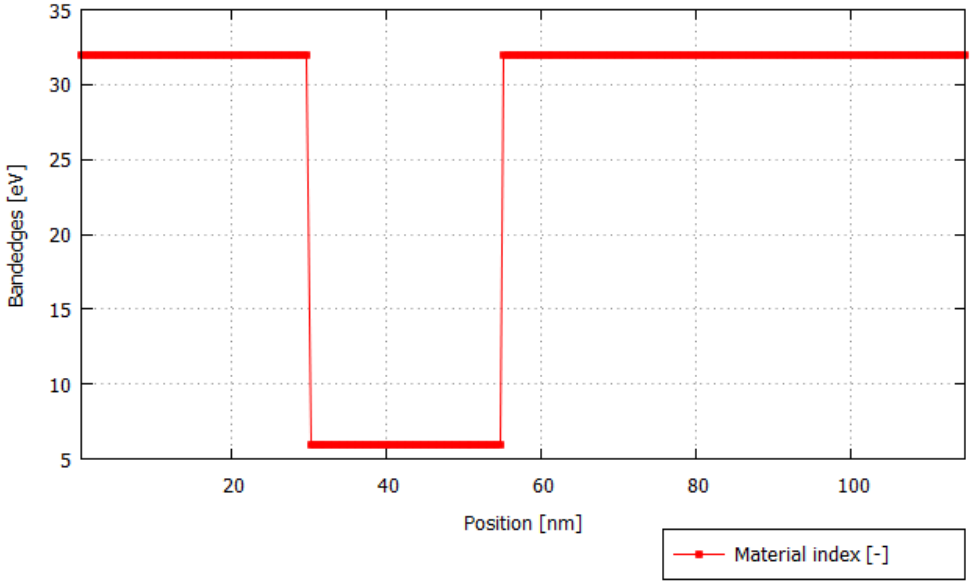
Optics tutorial (Simple)

This simple tutorial shows a simple simulation studies for absorption of semiconductor devices.

Structure

The structure is a simple AlGaAs Quantum well, which can be seen on the following figure.



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
```

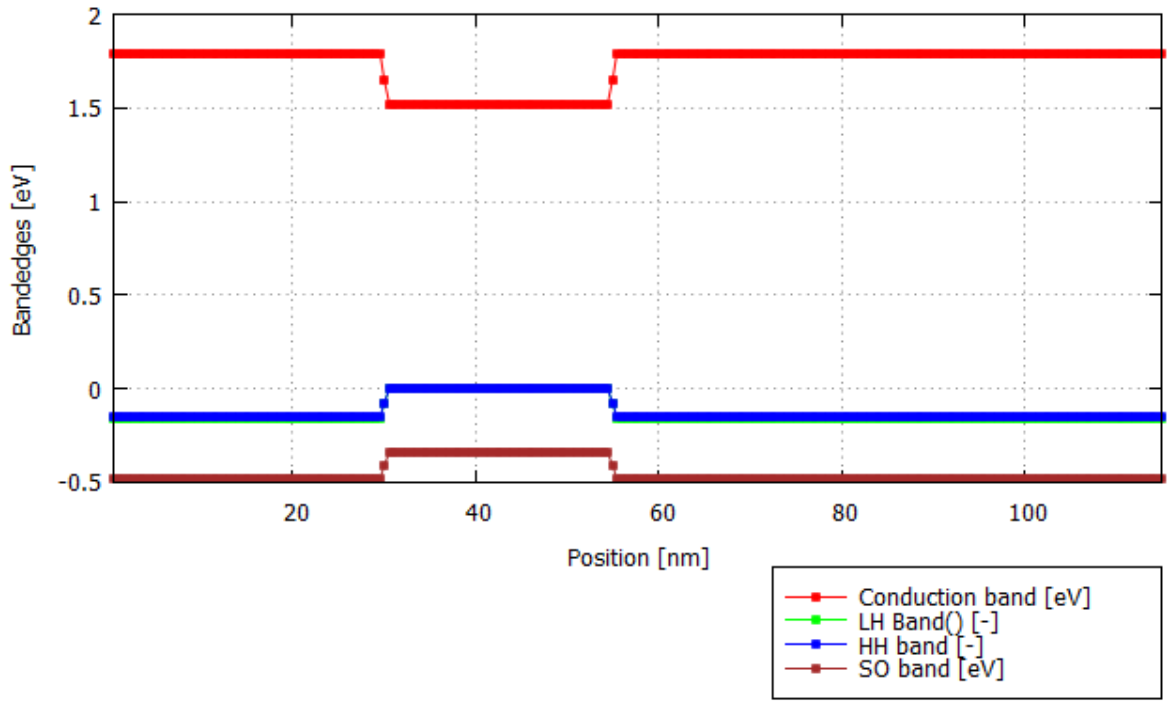
```
    k_integration{
      num_points = $NUM_INTEGRATION_KPOINTS
      num_subpoints = $NUM_INTEGRATION_INTKPOINTS
      symmetry = 1
          relative_size = $RELATIVE_INTEGRATION_KSPACE
    }
}
```

- `interband`, `intraband` Initalizes, should it calculates the intra/interband transitions 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` t, `transition_threshold` The minimum value of the (energy,
- `occupation`, `transition intensity`) of the transition which should be calculated.
- `energy_min`, `energy_max` Borders of the calculated energy spectra.
- `energy_resolution` The 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 it has calculated the strain, it calculates the the bandedges of the structure which can be seen on the figure:



In the quantum well region it can be seen that the bandedge 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 definied in the line:

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

It means how many electron and hole states should be calculated. The wavefunctons are plotted on the following figure:

Optics

Absorption

For each definied polarization it calculates the transition matrix element between the states(Integrationing the wavefunctions in k space). Than 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 in the function of the energy of the incoming field:

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

Im(ϵ)

It imaginary part of the permittivity (related to the conductivity), could be calculated from the the absorption coefficient, with the following formula, if the absoprtion 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 files `imepsilon`.

Transitions

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