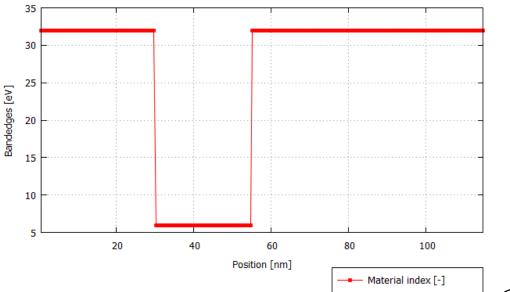
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# **Optics tutorial (Simple)**

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.



<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
```

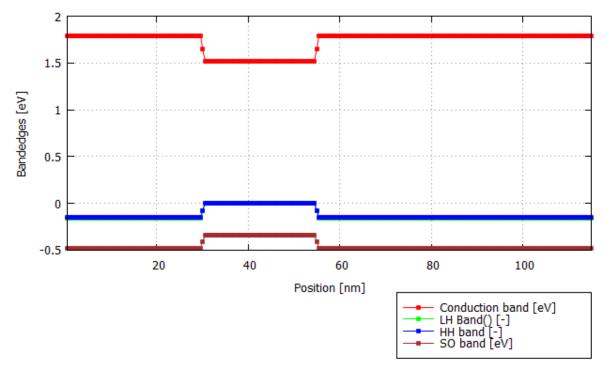
```
energy_max = $ENERGY_MAX
energy_resolution = $ENERGY_RESOLUTION
k_integration{
   num_points = $NUM_INTEGRATION_KPOINTS
   num_subpoints = $NUM_INTEGRATION_INTKPOINTS
   symmetry = 1
       relative_size = $RELATIVE_INTEGRATION_KSPACE
}
```

- interband, intraband Initalizes, 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 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

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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 absorption coefficients of each transition.

#### Im(\$\epsilon\$)

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

 $\alpha = \frac{n_r c}{\operatorname{n_r c} \cdot \frac{\operatorname{n_2}{\operatorname{n_s}}}{\operatorname{n_r c}}}$ 

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.

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