LED Simulation

In the following example we are going to show how the spectra of a Light Emitting Diode (LED) can be calculated with the **nextnano++** software. This example does not include the Schrödinger equation.

Physics model

In an LED the photons are emitted in the radiative recombination process,

$$R_{\rm sp} = c_{\rm rad} (n p - n_{\rm i}^2),$$

where $R_{\rm sp}$ is the local spontaneous emission rate, n and p correspond to the density of the electrons and the holes in the volume element, and $n_{\rm i}$ is the intrinsic density of the charge carriers. $R_{\rm sp}(x)$ depends on position x because the densities depend on position. The bimolecular recombination coefficient $c_{\rm rad}$ is a material dependent constant and has units ${\rm cm}^3/{\rm s}$. The order of magnitude is around $10^{-10}{\rm cm}^3/{\rm s}$.

This recombination rate is coupled into the drift-diffusion equation and the stationary solution of the problem,

$$\frac{\rm d}{{\rm d}t}n = 0,$$ $$\frac{\rm d}{{\rm d}t}p = 0,$$

is calculated.

Spectrum of the emission

According to this simple model, where $c_{\rm rad}$ is just a material constant, the radiative recombination rate, which generates photons of energy $E_{\rm rad}$ can be written in the form,

$$R_{\rm sp}(E_{\rm rad}) = c_{\rm rad} \int n(E_e) p(E_h) \delta(E_e-E_h-E_{\rm rad}) {\rm d}E_e {\rm d}E_h,$$

where $n(E_e)$ and $p(E_h)$ are the electron and hole densities of the energy level E_e and E_h in the volume element.

In order to get the spectra of the emission the integral should be calculated for each volume element, and integrated over volume. This simple model uses the bulk material constant $c_{\rm rad}$. However, this approach is not correct for **QW** structures. Additionally, the re-absorption of photons is not included.

Input file structure

Drift-Diffusion Calculation

```
currents{
```

```
    mobility_model    = constant
    recombination_model{
      SRH            = no        # Shockley-Read-Hall recombination
      Auger          = no        # Auger recombination
      radiative      = yes       # radiative recombination (direct
recombination)
    }
    output_fermi_levels{}
    output_currents{}
}
```

We have to include radiative recombination in the drift-diffusion equation in order to take into account the spontaneous emission rate.

```
           radiative      = yes       # radiative recombination (direct
recombination)
```

Density Calculation

```
classical{
   Gamma{}
   LH{}
   HH{}
   SO{}

   output_bandedges{ averaged = no }
   output_carrier_densities{}
   output_intrinsic_density{}
   energy_distribution{              # Calculation of carrier densities as a
function of energy
    min = -5.0                   # Integrate from
    max =  5.0                   # Integrate to
    energy_resolution = 0.05     # Integration resolution
        emission_spectrum = yes      # Output classical emission spectrum
(both, photon count and intensity)
   }
}
```

The density has to be calculated in the energy domain, which means we have to define the integration range

```
   energy_distribution{              # Calculation of carrier densities as a
function of energy
    min = -5.0                   # Integrate from
    max =  5.0                   # Integrate to
    energy_resolution = 0.05     # Integration resolution
```

```
        emission_spectrum = yes      #
    }
```

Results

Band structure

The simulated structure is a **p-i-n** diode. The layers of the heterostructure are *p*-GaAs - *p*-AlGaAs - InGaAs - *n*-AlGaAs - *n*-GaAs. The applied bias in the drift-diffusion equation results in a splitting of the hole and electron quasi-Fermi levels. This can be seen in the plot of the band edge profile of figure 1. In the intrinsic InGaAs region in the center, the Fermi levels reach the band edges of the quantum well, which leads to a significant density of electrons and holes in the quantum well (*not shown*).

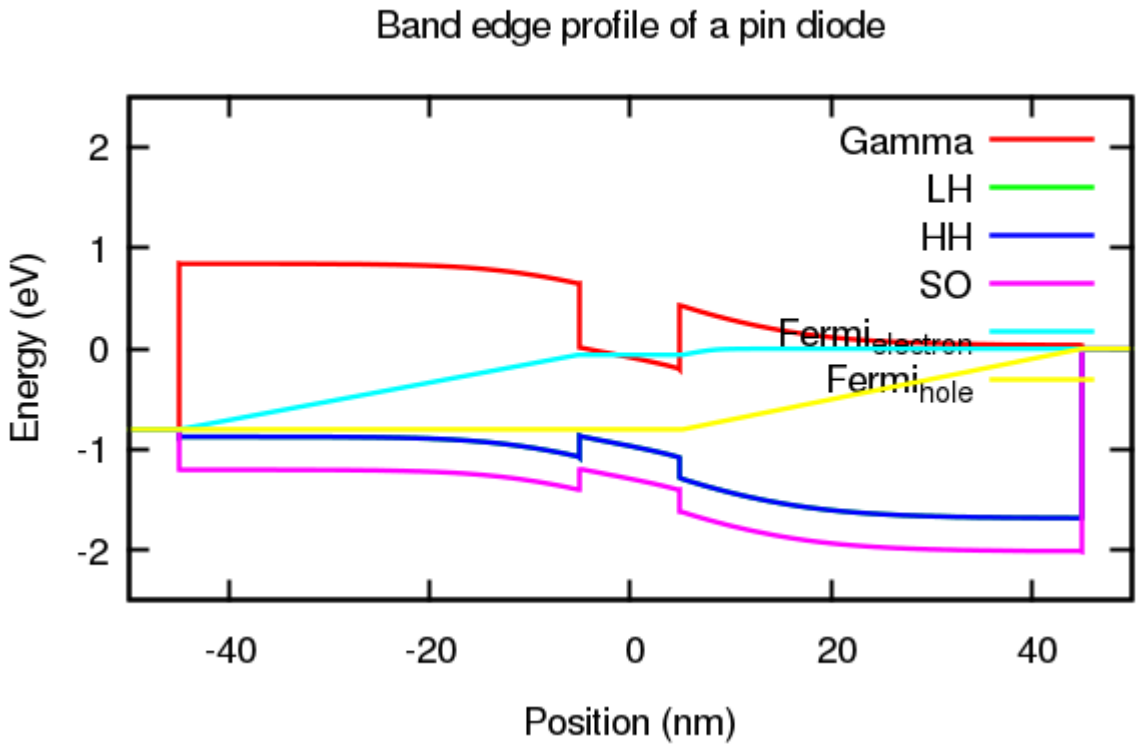

Figure 1: Band edges and quasi-Fermi levels of the **p-i-n** diode under forward bias

Carrier distribution

The carrier distribution with respect to energy ($n(E)$, $p(E)$) can be seen in figure 2. The density is summed up (integrated) for the full device. (This means that the position information of the carrier densities is “lost” in this view).

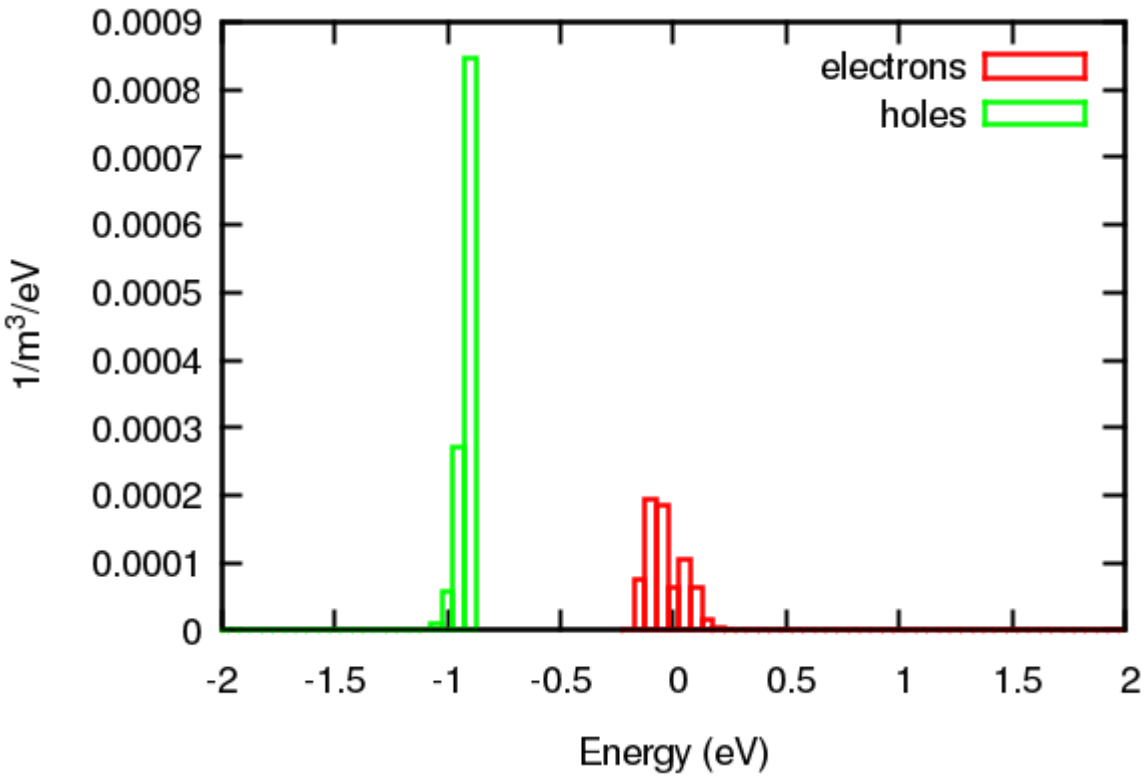

Figure 2: Energy distribution $n(E)$ and $p(E)$ of the electrons and holes for the full device

Emission Spectrum

The emission spectrum of the LED is plotted in figure 3. The dependence of the spectrum on the bias voltage can be calculated using a voltage sweep.

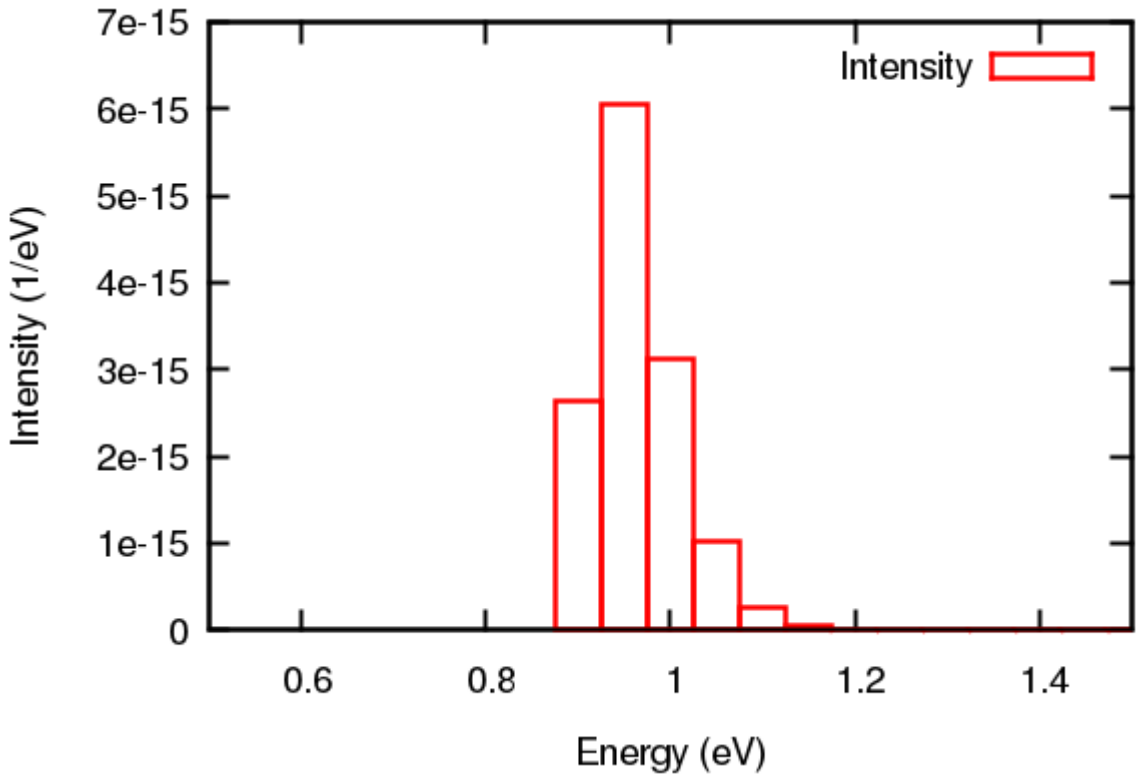

Figure 3: Emission spectrum (intensity) of the **p-i-n** diode structure in units of 1/eV.

The input file can be downloaded from here

From:
https://nextnano-docu.northeurope.cloudapp.azure.com/dokuwiki/ - **nextnano.NEGF - Software for Quantum Transport**

Permanent link:
https://nextnano-docu.northeurope.cloudapp.azure.com/dokuwiki/doku.php?id=nnp:optics:led_simulation

Last update: **2019/06/28 13:56**