Led Simulation

In the following example we are going to show you, how can be the spectra of a Light emitting diode calculated with the **nextano++** software.

Physics model

In a Led the photons are emitted in the radiate recombination process:

$$R_{rad} = c_r (n p - n_i n_i)$$

Where the n, and p correspond the density of the holes and the electrons in the volume element, and n_i is the intrinsic density of the charge carriers. This recombination rate is coupled in the drift-diffusion solver of the **nextnano++**, and it calculates the stationary solution of the problem:

$$\frac{d}{dt}n = 0 $$ $$\frac{d}{dt}p = 0 $$

Spectrum of the emission

According to this simple model, where c_r is just a material constant, the radiation recombination rate, which generates photons on energy E_r could be written in the form:

$$R_{rad}(E_r) = c_r \int n(E_e) \cdot p(E_h) \delta(E_e-E_h-E_r) dE_e dE_h $$

Where the density $n(E_e)$, and $p(E_h)$ the electron and hole densities on the energy niveu 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 model calculates with constant c_r, which is in **QW** structures not correct, and also 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{}
```

```
}
```

In order to get physically valid results we have to calculate with radiative recombinations in the drift diffusion.

```
           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 in
function of energy
    min = -5                     # Integrate from
    max = 5                      # Integrate to
    energy_resolution = 0.05     # Integration Resolution
   }
}<>
```

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 in
function of energy
    min = -5                     # Integrate from
    max = 5                      # Integrate to
    energy_resolution = 0.05     # Integration Resolution
   }
```

Results

The simulated test system was a **p-i-n** diode structure from *pGaAs-pAlGaAs-InGaAs-nAlGaAs-nGaAs* hetero-structure composition. In the center insulator part (*InGaAs*) the Fermi level reaches the band-edges of the Quantum well, which makes population in the well for both electrons, and holes. The applied bias in the drift diffusion equation results the splitting of the hole and electron Fermi levels. It can be seen on the band structure profile on figure 1

Figure 1: Band Structure of the **p-i-n** diode under forward bias

The carrier distribution in the energy can be seen on figure 2. The density is summed for the full device, it results the loss of the position information for the carrier densities.

Figure 2: Energy distribution of carriers for the full device volume

The emission spectrum of the Led is plotted on figure 3. The dependence of the spectrum on the bias voltage can be calculated with voltage sweeps.

Figure 3: Emission spectrum of the **p-i-n** diode structure in arbitrary units.