Modelling and optimisation of the internal quantum efficiency of Si-based LEDs

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***Abstract*—A new model for a 1D Si-based light-emitting p-i-n diode (LED) is presented, describing DC electrical characteristics and the internal quantum efficiency (η_{IQE}) as a function of the applied bias, showing good agreement with the simulation results. An optimization scheme, based on the model, shows improved η_{IQE} for engineered heterojunctions by reducing the diffusion current.**

I. INTRODUCTION

Silicon LED's are regarded as a potential solution for the anticipated interconnect bottleneck [1]. In literature, so far modelling the light emission in silicon have been minimal [2]–[4]. In this paper we study the 1D p-i-n LED in forward bias mode, as schematically shown in Fig. 1. The band diagram indicates that inside the active (or intrinsic) region of the LED holds that (1) the electron (E_{FN}) and hole quasi-Fermi levels (E_{FP}) are constant, (2) that the full applied voltage (V_{D}) is across this region. Consequently, for the pn-product in the active region holds:

$$pn = n_{\mathrm{i}}^2 \cdot \exp\left(\frac{E_{\mathrm{FN}} - E_{\mathrm{FP}}}{u_T}\right) = n_{\mathrm{i}}^2 \cdot \exp\left(\frac{V_{\mathrm{D}}}{u_T}\right), \tag{1}$$

where u_T is the thermal voltage, and n_{i} is the intrinsic carrier concentration. The pn-product is quite important in understanding the radiative recombination.

II. DC CURRENT MODEL AND EFFICIENCY OF SI-BASED LED

The total DC current flowing through the LED can be regarded as the sum of diffusion current J_{Diff} and the recombination current inside the active region of width W. The recombination current is found by integrating the Radiative (R_{Rad}), Shockley-Reed-Hall (R_{SRH}) and Auger (R_{Auger}) recombination rates [5] through the active region times the elementary charge q :

$$J_{R,\mathrm{Rad}} = \int_0^W q \cdot R_{\mathrm{Rad}}\, dx = qWn_{\mathrm{i}}^2 B_{\mathrm{Rad}} \left[\exp\left(\frac{V_{\mathrm{D}}}{u_T}\right) - 1\right], \tag{2}$$

$$J_{R,\mathrm{SRH}} = \int_0^W q \cdot R_{\mathrm{SRH}}\, dx = \frac{qWn_{\mathrm{i}}}{2\tau_{\mathrm{eff}}} \left[\exp\left(\frac{V_{\mathrm{D}}}{2u_T}\right) - 1\right], \tag{3}$$

$$J_{R,\mathrm{Auger}} = \int_0^W q \cdot R_{\mathrm{Auger}}\, dx = qWn_{\mathrm{i}}^3 (C_p + C_n) \left[\exp\left(\frac{3V_{\mathrm{D}}}{2u_T}\right) - \exp\left(\frac{V_{\mathrm{D}}}{2u_T}\right)\right] \tag{4}$$

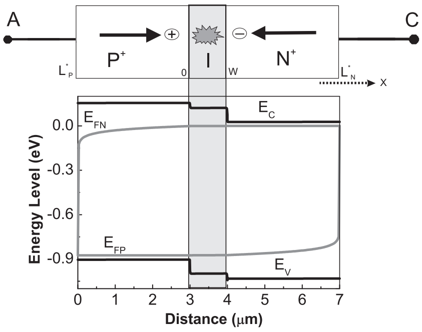

Fig. 1. A schematic drawing of a 1D p-i-n diode showing the principle of light emission (top figure). Its simulated band diagram at forward applied bias is also shown (bottom figure). The carriers are injected from the heavily doped injector regions into the active (or intrinsic) region. Their recombination results in light emission. In the band diagram, E_{C} and E_{V} are the conduction and valence band energies.

Where, B_{Rad} is the radiative recombination coefficient. τ_{eff} is the effective SRH life time and C_p and C_n are the Auger parameters. Now the total current is given by:

$$J_{\mathrm{Total}} = J_{\mathrm{Diff}} + J_{R,\mathrm{Rad}} + J_{R,\mathrm{SRH}} + J_{R,\mathrm{Auger}}. \tag{5}$$

To find η_{IQE} it is essential to find the radiative component of the diffusion current ($J_{\mathit{Diff},\mathrm{Rad}}$) as well. Using continuity equations and applying the correct boundary conditions :

$$J_{\mathit{Diff},\mathrm{Rad}} = \frac{qL_n n_{\mathrm{i}}^2}{N_{\mathrm{A}}\tau_{n,\mathrm{Rad}}} \frac{\left[\exp\left(\frac{V_{\mathrm{D}}}{u_T}\right) - 1\right]}{\left[1 - \exp\left(\frac{-L_p^*}{L_n}\right)\right]} + \frac{qL_p n_{\mathrm{i}}^2}{N_{\mathrm{D}}\tau_{p,\mathrm{Rad}}} \frac{\left[\exp\left(\frac{V_{\mathrm{D}}}{u_T}\right) - 1\right]}{\left[1 - \exp\left(\frac{-L_n^*}{L_p}\right)\right]} \tag{6}$$

where L_n^* and L_p^* are the physical lengths of the injector regions. N_{A}, N_{D} are the acceptor and donor impurity concentrations. $\tau_{n,\mathrm{Rad}}$, $\tau_{p,\mathrm{Rad}}$, are the radiative life times of the electrons and holes. $L_{n,p} = \sqrt{D_{\mathrm{n,p}} \cdot \tau_{\mathrm{n,p}}}$ is the diffusion length found applying Mathiessen's rule. $J_{\mathit{Diff},\mathrm{SRH}}$ and $J_{\mathit{Diff},\mathrm{Auger}}$ are found by changing the radiative life times in Eq. (6) with respective SRH and Auger life times. $J_{\mathit{Diff},\mathrm{Auger}}$ dominates diffusion current J_{Diff} . Now, η_{IQE} can be found analytically by :

$$\eta_{\mathrm{IQE}} = \frac{J_{R,\mathrm{Rad}} + J_{\mathit{Diff},\mathrm{Rad}}}{J_{\mathrm{Total}}} \cdot 100\%. \tag{7}$$

III. SIMULATION RESULTS

The model derived for η_{IQE} is validated through Sentaurus device simulations [6]. For the calculations W was taken as 1 μm. The p+ and n+ injector regions are uniformly doped

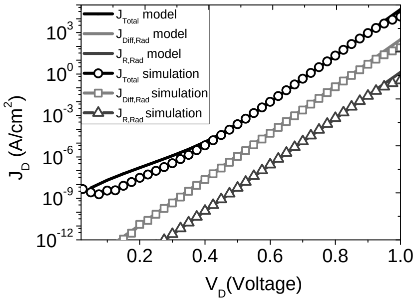

Fig. 2. Simulated (open symbols) and modelled (drawn lines)J-V Curves of a 1D silicon p-i-n diode (W=1 μm, $L_p^* = L_n^* = 3\,\mu$m). The total current density J_{Total} and the radiative current components $J_{Diff,\text{Rad}}$ and $J_{R,\text{Rad}}$ are only plotted. $J_{Diff,\text{Rad}} > J_{R,\text{Rad}}$, indicates more light from the injector regions.

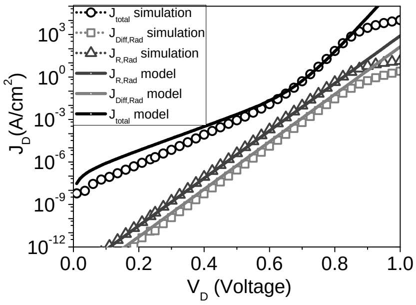

Fig. 3. Simulated (open symbols) and modelled (drawn lines) J-V Curves of a 1D $\text{Si}_{1-x}\text{Ge}_x/Si$ diode. The SiGe layer was asssumed to be 260 nm 21% Ge was used here with a band gap of 0.96 eV (W=0.6 μm, L_p^*=L_n^*=7 μm). The total current density J_{Total} and the radiative current components $J_{Diff,\text{Rad}}$ and $J_{R,\text{Rad}}$ are only plotted. $J_{R,\text{Rad}} > J_{Diff,\text{Rad}}$, increasing the η_{IQE}.

with 10^{19}cm^{-3}. The following Si parameters were used: $B_{\text{Rad}} = 10^{-14}\,\text{cm}^3\text{s}^{-1}$ [7], $\tau_{\text{eff}} = 2.5 \cdot 10^{-5}$ s, $C_n = 1.83 \cdot 10^{-31}\text{cm}^6\text{s}^{-1}$ and $C_p = 2.81 \cdot 10^{-31}\text{cm}^6\text{s}^{-1}$ [8]. Fig. 2 shows the J-V characteristics of the LED. J_{Total} ,$J_{R,\text{Rad}}$,$J_{Diff,\text{Rad}}$ found by the model is in good agreement with the simulations.

IV. OPTIMISATION

Several figures-of-merit could be optimised. First, for increasing the light intensity inside the active region $J_{R,\text{Rad}}$ should be increased. When we employ SiGe in the active region (See Fig. 3), for a given on-current density J_{ON}, the on-voltage V_{ON} drops, but the increase in n_{i} increases the light intensity (at a greater wavelength). In the case of wide band gap injectors, e.g. the $\text{Si}_{1-x}\text{C}_x/Si/\text{Si}_{1-x}\text{C}_x$ LED (See Fig. 4), J_{Diff} drops since n_{i} drops in the injector regions and consequently V_{D}=V_{ON} increases. This simply increases the pn-product and hence the light intensity (Eq. (1), Eq. (2)).

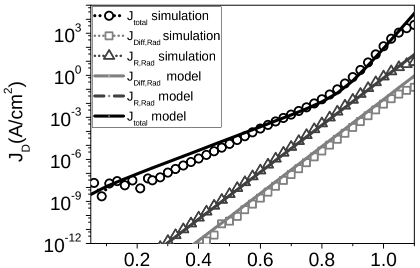

Fig. 4. Simulated (open symbols) and modelled (drawn lines) J-V Curves of a 1D $\text{Si}_{1-x}\text{C}_x/Si/\text{Si}_{1-x}\text{C}_x$ diode. $\text{Si}_{1-x}\text{C}_x$ band gap=1.4 eV, with 35% C [9]. W=0.6 μm, L_p^*=L_n^*=7 μm. The total current density J_{Total} and the radiative current components $J_{Diff,\text{Rad}}$ and $J_{R,\text{Rad}}$ are only plotted.$J_{R,\text{Rad}} > J_{Diff,\text{Rad}}$, increasing the η_{IQE}.

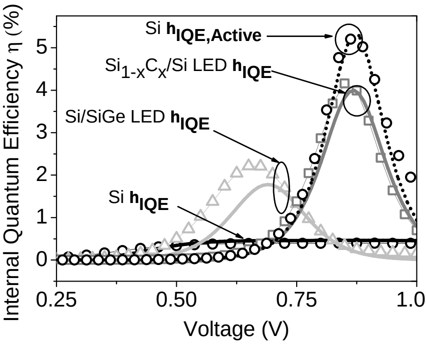

Fig. 5. The simulated (symbol) and modelled (lines) η_{IQE} values for all LEDs studied. The $\eta_{\text{IQE,Active}}$ of Si is also plotted. Using heterojunctions like SiC/Si (dark grey) or Si/SiGe (grey) the η_{IQE} of the Si-based LED can be improved.

Second parameter to be optimised is η_{IQE}. The reduction in J_{Diff} ($\approx J_{Diff,\text{Auger}}$) increases the efficiency. A p-i-n structure in a "wide-narrow-wide" band gap configuration increases the η_{IQE}. When properly tuned, J_{Total} will be determined only by the recombination current inside the active region, and in such a case, the η_{IQE} will be optimal and equal to the (ideal) efficiency of the active region ($\eta_{\text{IQE,Active}}$). The η_{IQE} which can be found according to Eq. (7), is plotted for our Si, SiGe/Si and SiC/Si LED's in Fig. 5. The maximum η_{IQE} of the Si LED is around 0.6% only. However, $\eta_{\text{IQE,Active}}$ in Si reaches upto 5.0%. By reducing the J_{Diff} (or by making it less important), the efficiency η_{IQE} can be increased up-to $\eta_{\text{IQE,Active}}$.

V. CONCLUSION

In summary, we have developed a dc current model describing the J-V and internal quantum efficiency of a 1D Si-based LED. Using the same model, we have also described the optimisation of a 1D Si-based LED . An un-optimised Si LED gives an η_{IQE} of 0.6% which could be increased towards 5% by reducing the diffusion current density.

ACKNOWLEDGMENT

This work is partially funded by the Dutch Ministry of Economic Affairs in the framework of the MEMPHIS project.

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