Efficient Fully-Coupled Electro-Optical Simulation Framework for Large-Area Planar Devices

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***Abstract*—Ongoing progress in optoelectronic devices necessitates computational tools that self-consistently account for both electronic charge carrier and photon dynamics and interactions. In this paper, we introduce an efficient simulation framework, using the concepts of nonlinear transmission lines, to study fully-coupled charge and photon transport in planar devices. Within the developed framework, the drift-diffusion equations for charge transport are self-consistently coupled with the radiative transfer equation for photon transport and a separate lateral transport model, to obtain a realistic picture of the electro-optical device behaviour. The model allows the detailed study of large-area devices with full access to the wavelength and angle dependent features. It also accounts for photon recycling, providing deeper insight into the complex nature of optical energy transfer and losses in planar multi-layer structures. The efficiency of the framework is illustrated by applying it to study intracavity diode structures, which are intended for exploring high-power electroluminescent cooling in III-V light-emitting diodes.**

I. Introduction

Optoelectronic devices impact many areas of modern society, from highly-efficiency solid-state lighting to new green energy technologies and global optical fibre networks [1], [2]. However, obtaining quantitative insight on the relevant optical and electrical transport effects in many emerging and established devices is generally challenging due to the complex interplay of optical emission, absorption, interference and electronic charge transport. In particular, the ability to fully account for the propagation direction, emission and absorption spectra, and related photon recycling and charge transport effects is extremely important e.g. for detailed description of solar cells and light-emitting diodes (LEDs). There are several methods to describe the electrical and optical properties of such structures separately (see e.g. Ref. [3]), but developing fully self-consistent approaches to model these features in real structures has remained a challenge. In this paper, we present our approach to an efficient electro-optical simulation framework for modeling planar large-area three-dimensional (3D) structures involving e.g. LEDs or photodetectors (PDs), combining the power of the radiative transfer equation (RTE) [4] and the drift-diffusion (DD) charge transport model.

II. The Electro-Optical Transport Solver

Fig. 1 shows a schematic illustration of the framework, as applied to planar large-area multi-layer structures, represented in a form that resembles a (non-linear and planar) transmission line. The approach separates the most complex transport effects, described using a vertical one-dimensional (1D) charge-photon transport model (normal to the layer interfaces), from the more straightforward two-dimensional (2D) charge transport description in the lateral direction. This provides a very good approximation when the lateral dimensions are much larger than the vertical ones, as is typical for solar cells and LEDs. Electro-optical coupling in the vertical dimension is achieved by solving self-consistently the DD-RTE equations, in which the RTE and the DD equations are coupled by the absorption and emission terms, as well as the electron and hole quasi-Fermi levels from the DD solution [4]. Hence, and unlike the models based on the Beer-Lambert (BL) approximation, the transfer matrix method and the rigorous coupled wave analysis [3], the RTE model fully accounts even for local photon recycling effects, as photons are emitted or absorbed within the layers, providing deeper insight into optical energy transfer and losses in the structures. Current transport along the lateral direction is modelled by solving the 2D drift equations while accounting for the current sinking and sourcing due to the vertically-flowing net currents.

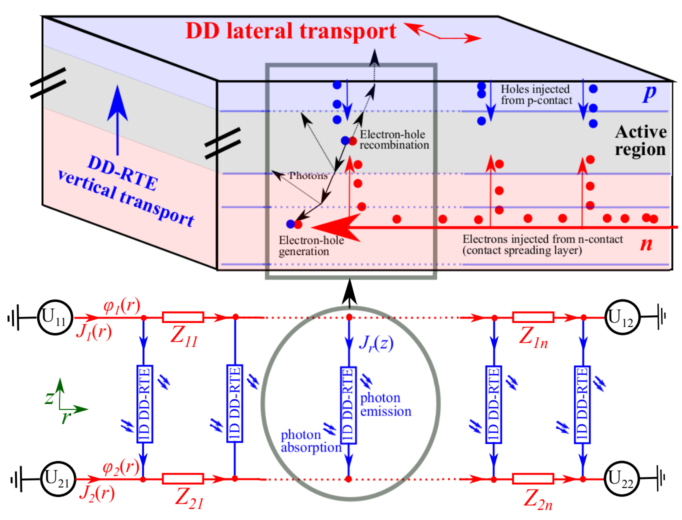

Fig. 1. Illustration of the nonlinear transmission line framework, for multi-layer structures. The RTE and DD equations are documented in Ref. [4].

III. Example Application: The DDS

Recently, there has been a renewed interest in III-As devices, due to their potential in optical cooling [5], [6]. Here, we use the framework to study the double diode structure (DDS) [7], introduced to explore high-power electroluminescent cooling (ELC) in III-As LEDs. The DDS incorporates a III-As LED and a PD within the same epistructure; LED photon emission is guided towards the PD, and the direct measurement of the LED (I_{LED}) and PD (I_{PD}) currents gives the amount of absorbed light. The DD-RTE framework is particularly suited for this type of structure, combining LEDs and PDs. Fig. 2 shows the DDS equivalent circuit dissecting the main components of the simulator. Since the DDS is cylindrically symmetric, we only need to study a 2D section, from the cylinder center ($r = 0$) to the edge ($r = L$), to capture both the electrical transport in the lateral direction, as well as the coupled optoelectronic phenomena in the vertical direction.

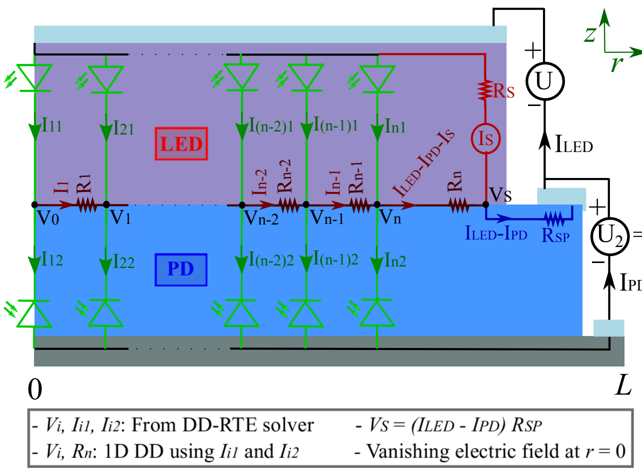

Fig. 2. The equivalent circuit model for the DDS, where the lateral size (mesa diameter) is more than a hundred times larger than the total layer (vertical) thickness. The surface recombination current ($I_S(U)$) and resistance (R_S), and the spreading resistance (R_{SP}) can be directly extracted e.g. from measured LED currents.

IV. Results, Discussion and Conclusions

Figure 3(a) shows the measured and simulated $I-V$ curves, the coupling quantum efficiency (CQE), $CQE = I_{PD}/I_{LED}$, the DDS power conversion efficiency (PCE), $PCE = CQE \times E_{ph}/qU$, and the LED PCE, $PCE_{LED} = IQE \times E_{ph}/qU$, for the DDS from Ref. [7]; U is the LED bias, q is the elementary charge, E_{ph} is the photon energy ($\sim$ emitter bandgap $E_g =$ 1.42eV), and IQE is the LED internal quantum efficiency. Excellent agreement is obtained with experiments. In particular, the LED PCE exceeds 100% at high biases, indicating local cooling of the LED, thanks to the small non-radiative recombination rates in GaAs [8]. In contrast, the DDS PCE peaks only at 70% due to high PD losses. Figure 3(b) compares the net recombination ($recombination - generation$) rates across the DDS layers for $U = 1.4$V, from both the RTE and BL models. The figure shows that the microscopic details of the recombination profiles differ considerably, especially in the PD GaAs layers (position $< 4\mu$m), because the BL model cannot self-consistently account for photon recycling or emission saturation. Figure 3(b) hence highlights the need for sophisticated charge-photon transport models to gain detailed understanding of the microscopic trends in energy transport.

To conclude, we presented a quasi-three-dimensional model for planar optoelectronic devices, self-consistently coupling charge and optical transport using the RTE formalism, and enabling the description of very large structures. The model can be readily applied to various structures with strong electro-optical coupling, ranging from LEDs and solar cells to lasers.

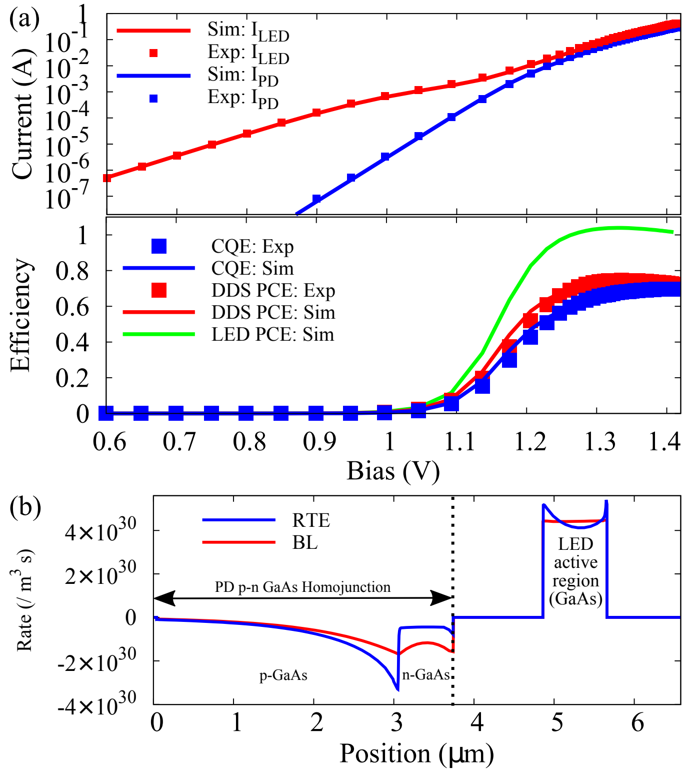

Fig. 3. (a) Measured (points) and simulated (lines) $I - V$ curves, CQE and PCEs. (b) Simulated net recombination rates across the layer structure, along the vertical direction, for $U = 1.4$V, from the full RTE and BL models.

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