

Interference-exact radiative transfer simulations: intracavity transport effects

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Abstract—Electroluminescent (EL) cooling of semiconductors has received increasing attention in recent years. To optimize the performance of devices intended for EL cooling, special care is needed in minimizing electrical losses resulting from e.g. potential barriers, and optical losses resulting from e.g. parasitic absorption. In this work, we introduce and explore a full-device modeling tool for arbitrary planar photonic devices by coupling together the interference-exact radiative transfer equation (IFRTE) of photon transport and drift-diffusion (DD) equations of carrier transport. The IFRTE coupled with DD represents a fully self-consistent model of lossy wave optics and carrier transport, connecting emission and photon recycling with electron and hole dynamics. We deploy the model to study and optimize photon emission and absorption as well as photocarrier collection in double-diode structures for EL cooling.

I. INTRODUCTION

Photonics and optoelectronics have experienced major developments during the last few decades, and today they are disrupting the lighting and energy industries through high-efficiency light-emitting diodes and solar cells [1, 2]. More research is needed even for these basic technologies to reach their full potential, but photonics research is also increasingly focusing on more sophisticated applications where a combined understanding of the optical, electrical and thermal processes is crucial. Examples of this include diverse nanowire-based devices [3], photocatalytic solar fuel production [4], optical on-chip communication using nanostructure optical interconnects on silicon [5], and electroluminescent (EL) cooling [6]. EL cooling was proposed by Tauc [7] and demonstrated experimentally at extremely low voltages by Santhanam *et al.* [8]. We have recently studied the possibility to observe EL cooling at higher powers in double-diode structures (DDS) illustrated in Fig. 1, where photons transfer heat from the emitter part to the absorber part of the device, where the photogenerated carriers are collected [6].

For studying and optimizing the DDS of Ref. 6, it is very important to have detailed understanding and control of where photons are emitted and absorbed, and how the materials and doping levels affect carrier transport and recombination throughout the device. The intertwined nature of carrier and photon transport calls for optoelectronic simulation tools where emission, transport, and absorption of photons is self-consistently coupled with the injection, transport and generation/recombination of carriers. The conventional way to build such a model is to solve the radiative transfer equation (RTE) and couple it with the drift-diffusion (DD)

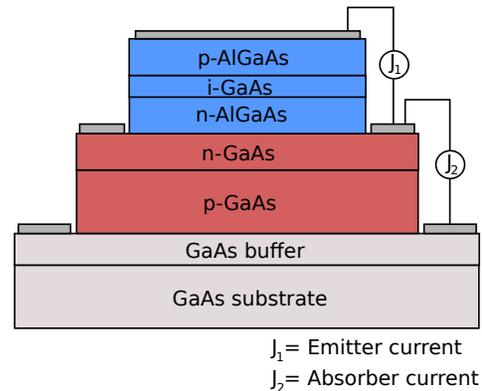


Fig. 1. Schematic illustration of the DDS. The structure is grown on GaAs, and the GaAs pn junction in the middle absorbs photons emitted by the intrinsic GaAs layer on top.

equations of carrier transport [9]. Such a model can already provide extremely valuable insight, but it does not account for interference and other wave-optical effects that need to be considered when optimizing optical transport. Here, we use a coupled RTE-DD solver to study the DDS, and extend the RTE to include interference effects for future studies of devices where the active layer thicknesses are of the order of the emission wavelength.

To include interference in the RTE, we implement the very recently reported interference-exact radiative transfer equation (IFRTE) [10] and couple it with the DD equations. We employ the optical admittance framework [11] to simplify the calculation of the damping and scattering coefficients required for the IFRTE. Solving the photon numbers in all the modes from IFRTE self-consistently with the generation/recombination rates from DD constitutes a fully coupled simulation of semiconductor carrier and wave-optical photon transport, and interaction of carriers and photons.

II. THEORY

In Ref. 10, Partanen *et al.* showed how the quantized fluctuational electrodynamics formalism can be used to define the IFRTE accounting for wave-optical effects. In the IFRTE, the expectation value of the photon number operator $\langle \hat{n}_{\pm, \sigma} \rangle$

in the mode $\sigma \in \{TE, TM\}$ satisfies

$$\begin{aligned} \frac{d}{dz} \langle \hat{n}_{\pm, \sigma}(z, K, \omega) \rangle = \\ \mp \alpha_{\pm, \sigma}(z, K, \omega) [\langle \hat{n}_{\pm, \sigma}(z, K, \omega) \rangle - \langle \hat{\eta}(z, K, \omega) \rangle] \\ \pm \beta_{\pm, \sigma}(z, K, \omega) [\langle \hat{n}_{\mp, \sigma}(z, K, \omega) \rangle - \langle \hat{\eta}(z, K, \omega) \rangle], \end{aligned} \quad (1)$$

where K is the wave vector component in the plane parallel to the layer interfaces, and $\alpha_{\pm, \sigma}$ and $\beta_{\pm, \sigma}$ are the position- and direction-dependent damping and scattering coefficients, which can be calculated from the nonlocal densities of states and interference densities of states [10]. In addition, \pm refers to photons propagating either up or down, and $\langle \hat{\eta} \rangle$ is the source-field photon number operator accounting for the recombination through the fluctuation-dissipation theorem, which can be written using the Bose-Einstein distribution. Note that Eq. (1) is very similar with the conventional radiative transfer model, where β is zero and α only depends on the material. In Ref. 11, we show how the dyadic Green's functions needed for the $\alpha_{\pm, \sigma}$ and $\beta_{\pm, \sigma}$ coefficients can be calculated for an arbitrary planar layer structure using optical admittances [12], which remove the need to formally solve the electromagnetic fields. The photon number expectation values from Eq. (1) are solved with the DD model, which gives the quasi-Fermi level separation throughout the device to be used as the photon chemical potential [13]. Integrating the photon numbers over all propagation directions enables calculating the radiative recombination-generation rate for the DD model.

III. RESULTS AND DISCUSSION

The IFRTE-DD model is used to carry out self-consistent simulations of coupled carrier and photon transport in the DDS shown in Fig. 1. Having evaluated $\alpha_{\pm, \sigma}$ and $\beta_{\pm, \sigma}$ from optical admittances and carrier dynamics from DD, Fig. 2 shows the photon numbers in TE modes resulting from Eq. (1) as a function of the propagation angle and position. The emitter is biased with 1.2 V and the absorber is short-circuited. Figure 2(a) shows the upward-propagating photon number, which is set to zero at the bottom boundary. It is therefore very small below the emitter layer and includes only minor emission from the absorber. At the emitter layer, the upward photon number increases due to spontaneous emission and remains large until the top mirror due to minor absorption in AlGaAs. The angle dependence of the field is clearly visible, as the emitter layer is not sufficiently thick for the field to saturate during a single pass at small angles of incidence. The downward-propagating photon number is shown in Fig. 2(b). One can see that it is large, even above the emitter, due to the reflection of the upward-propagating photons from the top contact. The downward-propagating photon number increases again at the emitter due to spontaneous emission and propagates through the AlGaAs barrier layer before starting to decay strongly in the GaAs absorber layer. Especially in the AlGaAs barrier layer, one can also observe oscillations in the downward propagating photon number. These oscillations arise from the interaction between the photon modes mediated

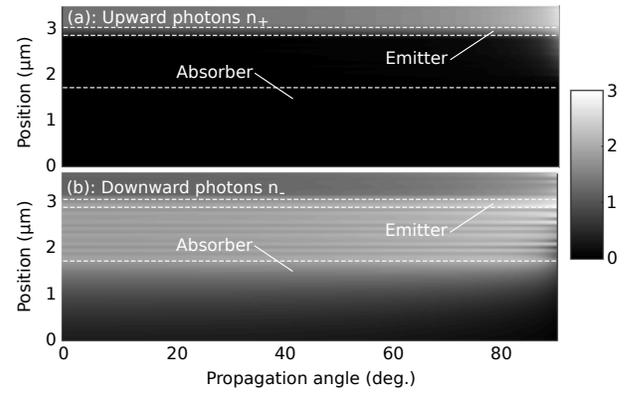


Fig. 2. (a) Upward and (b) downward photon number expectation values in arbitrary units for a wavelength of 867 nm.

through the scattering coefficients, and their significance and physical interpretation will be studied further in the future.

Outlook: Besides EL cooling, the IFRTE-DD model is expected to enable detailed studies of various planar devices such as new thin-film solar cells. In addition, we expect that it can be generalized for nanostructures such as plasmonic gratings and optical antennas using perturbative and/or other approximative techniques.

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