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Simulation of photon transport in resonant double-diode structures

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ABSTRACT

The optical and electrical properties of planar optoelectronic devices are well known, but their fully self-consistent modeling has remained a serious challenge. At the same time, the improving device fabrication capabilities and shrinking device sizes make it possible to reach higher efficiencies and develop totally new device applications. Success in this context, however, requires sophisticated device modeling frameworks, such as fully self-consistent models of optical and electrical characteristics. In this article, we explore the predictions provided by the recently introduced interference radiative transfer (IRT) model and apply it to a simplified double-diode structure presently used to study the possibility of electroluminescent cooling. The purpose of this proof-of-principle study is to show that the IRT model is straightforward to implement once one has access to the dyadic Green's functions, and that it produces solutions that satisfy the more general quantized fluctuational electrodynamics framework. We examine the photon numbers, propagating optical intensities and net radiative recombination rates from the IRT model solved by assuming a constant quasi-Fermi level separation in the active region. We find that they behave qualitatively as expected for the chosen device structure. However, the results also exhibit wave-optical characteristics, as e.g. the propagating intensity depends non-monotonously on the propagation angle due to constructive and destructive interferences. Based on the results, the IRT model offers a promising way to self-consistently combine the modeling of photon and charge carrier dynamics, also fully accounting for all interference effects.

Keywords: Radiative transfer, Drift-diffusion model, Dyadic Green's functions, Fluctuational electrodynamics, Electroluminescent cooling

1. INTRODUCTION

Optoelectronic devices form one cornerstone of modern society, as they enable new clean energy technologies, high-efficiency solid-state lighting, and global optical fibre networks that power today's information society.¹⁻³ Sustained technological progress over several decades has also resulted in the possibility to fabricate highly sophisticated device structures with a large control over their properties. This is allowing new possibilities in (1) studying the basic physics of optical, electrical and thermal processes in semiconductor optoelectronic devices, and (2) pursuing new device applications that require both excellent fabrication capabilities and detailed understanding of the underlying physics. One such application is electroluminescent (EL) cooling, where the aim is to make photons transfer heat away from an externally biased light-emitting diode (LED, see e.g. Ref. 4 for more information).

Our approach to study and develop EL cooling is based on using a so-called double-diode structure (DDS), where an LED and a photodiode (PD) are integrated within the same layer structure, where they also share one common contact.⁴ The LED is biased with a voltage slightly smaller than the one corresponding to the bandgap energy, and the objective is to make most of the photons to be absorbed within the PD with a high carrier collection efficiency by the contacts. Achieving this requires detailed understanding of both the carrier dynamics in the LED and the PD as well as the optical transport in the full device structure. In terms of modeling, one should be able to calculate the local emission and absorption rates self-consistently with the charge carrier dynamics, and as the layer thicknesses are made smaller, the optical modeling should also take into account interference effects.

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Figure 1. The optically relevant material layers of the simplified double-diode structure simulated using the IRT model. The 4 μm thick GaAs layer on the left acts as a photodiode absorbing light emitted by the 300 nm thick GaAs layer on the right. To solve the IRT model, the bias voltage (or quasi-Fermi level separation) is set to a constant 1.4 V in the 300 nm thick GaAs layer, and zero elsewhere. The metal contact on the right reflects back almost all incident radiation, as specified in the main text.

The recently introduced quantized fluctuational electrodynamics (QFED) framework (see e.g. Ref. 5) provides a general framework for studying the full wave-optical properties of absorption and emission in connection with the electrical properties, but it has so far remained challenging to implement it self-consistently with charge carrier dynamics due to the nonlocal nature of the emission-absorption cycles. In this paper, we take a concrete step towards full electro-optical simulation of arbitrary planar resonant devices by combining our recent formulation of the dyadic Green's functions based on the optical admittance method⁶ and the so-called interference radiative transfer (IRT) model.⁷ We show that the IRT model provides the solutions that satisfy the QFED and moreover, it gives a straightforward way to include the quasi-Fermi level separation from carrier dynamics simulations in the emission term, eventually enabling self-consistent electro-optical simulations of planar optical resonators.

In more concrete terms, here we implement the IRT model for the somewhat simplified DDS conceptually similar to the one in Ref. 4 and specified in Fig. 1. We analyze the position-dependent damping and scattering coefficients and show that using them in a full IRT calculation produces the optical properties that match the full QFED calculation. In this paper, we solve the IRT model without full electro-optical self-consistency by assuming that the quasi-Fermi level separation is 1.4 eV in the GaAs layer on the right and zero elsewhere. The total emission-absorption rates calculated with the IRT model account directly for the Purcell effect, other interference effects such as the internal reflections, and photon recycling as determined by Maxwell's equations. To provide a proof-of-principle calculation using the IRT model, we show that by using the position-dependent damping and scattering coefficients of the IRT model, one obtains direction-resolved photon numbers, Poynting vectors, and net recombination rates that satisfy the more general QFED framework.

2. THEORY

The IRT model studied in this paper describes the emission, propagation and absorption of photons fully according to the QFED framework. In QFED, emission arises from fluctuating electric (and magnetic) current terms of the inhomogeneous Maxwell's equations. The propagation and absorption of photons is then governed by the homogeneous Maxwell's equations with complex permittivities (and permeabilities). In this work we consider only nonmagnetic materials with $\mu = 1$ everywhere. In general terms, the QFED framework makes use of dyadic Green's functions and local (LDOS), nonlocal (NLDOS) and interference (IFDOS) densities of states to calculate rightward- and leftward propagating photon number expectation values as⁵

$$\langle \hat{n}_{\pm, \sigma}(z, K, \omega) \rangle = \frac{1}{\rho_{\sigma}(z, K, \omega)} \int_{-\infty}^{\infty} \rho_{NL\pm, \sigma}(z, K, \omega, z') \langle \hat{\eta}(z', K, \omega) \rangle dz'. \quad (1)$$

Here $\pm$ refers to rightward and leftward propagating photon numbers, z is the position as in Fig. 1, K is the wavevector component in the plane perpendicular to z , ω is the angular frequency, $\sigma \in \{\text{TE/TM}\}$ is the

polarization, ρ_σ is the LDOS, $\rho_{NL\pm,\sigma} = \rho_{NL,\sigma} \pm \rho_{IF,\sigma}$ is the NLDOS for rightward and leftward photons calculated from the full NLDOS $\rho_{NL,\sigma}$ and the IFDOS $\rho_{IF,\sigma}$, and $\langle\hat{n}\rangle$ is the expectation value of the source-field operator, which for electrically or optically excited semiconductors is given by the modified Bose-Einstein distribution $1/[e^{(\hbar\omega - eU)/(k_B T)} - 1]$, where e is the elementary charge, U is the local quasi-Fermi level separation, k_B is Boltzmann's constant, and T is the lattice temperature.⁸

The total photon number $\langle\hat{n}_\sigma\rangle = \langle\hat{n}_{+,\sigma}\rangle + \langle\hat{n}_{-,\sigma}\rangle$, separated into the rightward and leftward propagating components defined above, can be used to calculate the local net emission rate at any point of the device. The net emission rate $\langle Q_\sigma(z)\rangle$ is defined as the derivative of the Poynting vector $\langle S_\sigma(z)\rangle$, and they can be calculated from the rightward and leftward propagating photon numbers as⁵

$$\langle Q_\sigma(z)\rangle_\omega = \frac{\partial \langle S_\sigma(z)\rangle_\omega}{\partial z}, \quad \langle S_\sigma(z)\rangle_\omega = \frac{\hbar\omega c}{n(z,\omega)} \rho_\sigma(z,\omega) (\langle\hat{n}_+\rangle - \langle\hat{n}_-\rangle). \quad (2)$$

Here c is the speed of light in vacuum, $n(z,\omega)$ is the real part of the refractive index, and the subscript ω indicates that $\langle Q_\sigma(z)\rangle$ has to be integrated over the angular frequency to obtain the total net emission rate. Also, it is noteworthy that the total net emission rate is the sum of the TE and TM rates. In this paper we demonstrate the alternative and potentially more simple calculation of $\langle\hat{n}_{\pm,\sigma}\rangle$ by using the recently introduced IRT model, where the rightward and leftward propagating photon numbers are governed by a generalized radiative transfer equation of the form⁷

$$\begin{aligned} \frac{d}{dz} \langle\hat{n}_{\pm,\sigma}(z,\omega,K)\rangle = & \mp \alpha_{\pm,\sigma}(z,K,\omega) [\langle\hat{n}_{\pm,\sigma}(z,K,\omega)\rangle - \langle\hat{n}(z,\omega)\rangle] \\ & \pm \beta_{\pm,\sigma}(z,K,\omega) [\langle\hat{n}_{\mp,\sigma}(z,K,\omega)\rangle - \langle\hat{n}(z,\omega)\rangle], \end{aligned} \quad (3)$$

where $\alpha_{\pm,\sigma}$ and $\beta_{\pm,\sigma}$ are the damping and scattering coefficients, which can be calculated from the dyadic Green's functions as specified in Ref. 7, and which account for the local photon absorption and transfer of photons between rightward and leftward modes due to internal reflections. The α parameter therefore has a contribution both from the absorption by the material and from the transfer of photons to the reverse-propagating mode, and therefore it is called a damping coefficient instead of simply an absorption coefficient. Equation (3) can be compared with the conventional radiative transfer equation, which would only include the term multiplied by $\alpha_{\pm,\sigma}$, which would in that case be a piecewise constant absorption coefficient.⁹ After solving Eq. (3), its right-hand side terms can be directly used for the derivative of the Poynting vector to calculate the local net emission rate using Eq. (2) (either for each K separately or integrated over K). The derivative of the LDOS required in Eq. (2) can be calculated as instructed in the supplemental material of Ref. 7.

Equation (3) is straightforward to integrate with carrier dynamics models to obtain a fully self-consistent electro-optical simulation. To pave the way for them, here we solve Eq. (3) numerically as a proof-of-principle study for the geometry shown in Fig. (1), assuming a constant positive quasi-Fermi level separation in the GaAs layer on the right. To show that the IRT model can indeed be used to solve the full QFED problem, we compare the result with the one obtained by calculating the integral of Eq. (1) and show that the results are exactly the same. This encourages the use of the IRT model in full-device studies especially in more complex geometries, where carrying out the integral (1) at all points of the device would be impractical self-consistently with the chosen carrier dynamics model. To obtain $\alpha_{\pm,\sigma}$ and $\beta_{\pm,\sigma}$ as well as the transmission matrices of interfaces (see supplemental material of Ref. 7), we use the optical admittance formulations of the Green's functions and densities of states presented in Ref. 6.

3. RESULTS & DISCUSSION

The IRT model is used to calculate the damping and scattering coefficients, rightward and leftward propagating photon numbers and power flows, and total net emission rates in the geometry shown in Fig. 1. The wavelength and photon energy are fixed in the calculations to 867 nm and 1.43 eV, respectively, corresponding roughly to the bandgap energy of GaAs. The corresponding relative permittivities of GaAs and AlGaAs are respectively $13.31 + 0.826i$ and $10.24 + 0.01i$ in accordance with Refs. 10–12. We assume the quasi-Fermi level separation to be 1.4 V in the 300 nm thick GaAs layer and zero elsewhere. To maximize the omnidirectional reflection from

Figure 2. IRT model parameters for TE modes as a function of position and lateral wave number normalized by k_0 : (a) damping coefficient α_+ for rightward propagating modes, (b) damping coefficient α_- for leftward propagating modes, (c) scattering coefficient β_+ for rightward propagating modes and (d) scattering coefficient β_- for leftward propagating modes.

the rightmost AlGaAs outer interface, we include in the IRT calculation a contact structure including SiN, Ti, and Au layers with their respective permittivities 4, $-2.09+0.10i$, and $-37.55+1.91i$ obtained from Refs. 13–15. In this paper, we only note that the chosen contact structure reflects over 95 % of the incoming reflection back towards the device at all angle, with a direction-averaged power reflection of almost 99 %. The contact structure is included in the calculations but not in the following figures that only show photon numbers and other relevant quantities within the actual semiconductor device.

Figure 2 shows (a) the damping coefficient for rightward modes, (b) the damping coefficient for leftward modes, (c) the scattering coefficient for rightward modes, and (d) the scattering coefficient for leftward modes, all normalized by k_0 . The damping and scattering coefficients are presented only for TE modes, but the calculation of TM modes proceeds in a completely similar way using the equations for TM (see supplemental material of Ref. 7), and they are qualitatively very similar to the ones for TE for the structure studied here. In Figs. 2(a)–(b), it can be seen that as expected, especially at smaller K values, the damping coefficient is generally larger in the GaAs layers, as they have a larger ε_i and thereby a stronger absorption or emission than the AlGaAs layers for the photon energy considered here. On the other hand, at larger K values, all α and β coefficients in Figs. 2(a)–(d) exhibit oscillations due to interference effects in the internal reflections and Purcell effect. Also, it is of note that both α and β exhibit negative values at some positions and K values. The position dependence of both α and β is remarkable, considering that conventionally α is taken as a piecewise constant parameter. However, in the coming paragraphs we show that using these coefficients in the simulations nonetheless produces the expected optical characteristics that satisfy the QFED framework.

The damping and scattering coefficients in Fig. 2 and the corresponding coefficients for TM can now be used to solve the IRT model. Figure 3 shows (a)–(d) the rightward and leftward photon numbers for TE and TM and (e)–(f) the Poynting vector values for TE and TM. Focusing first on the rightward photon numbers for TE and TM in Figs. 3(a)–(b), we see that they are practically zero until the intermediate AlGaAs layer where they start showing positive values at the larger K values due to leftward modes reflecting rightwards from the GaAs-AlGaAs interface in a nonlocal fashion. The rightward-propagating photon numbers increase at all K values at the biased GaAs layer at 5 μm due to positive net emission. Figures 3(c)–(d) show the leftward propagating photon numbers for TE and TM, which are larger than zero already at the contact on the right side due to a reflection of over 95 %. Note that this reflection is directly included in the IRT model through its damping and scattering coefficients and interface transmission matrices, so that it does not need to be set as an additional angle-dependent boundary condition. The leftward photon numbers in Figs. 3(c)–(d) increase again

Figure 3. Optical propagation characteristics calculated with the IRT model: (a) rightward propagating photon number for TE, (b) rightward propagating photon number for TM, (c) leftward propagating photon number for TE, (d) leftward propagating photon number for TM, (e) Poynting vector for TE and (f) Poynting vector for TM.

at the biased GaAs layer due to emission, and they too show an interference pattern in the intermediate AlGaAs layer due to internal reflections. Finally, the leftward modes decay within roughly $1 \mu\text{m}$ in the GaAs layer on the left due to strong absorption.

The Poynting vector calculated from the photon numbers is shown for TE and TM modes in Fig. 3(e)-(f), using Eq. (2) for each K separately. Even if the photon numbers exhibited an interference pattern in the AlGaAs layer, the propagating intensity as described by the Poynting vector is not oscillating as a function of position. On the left side, the Poynting vector is zero as there is no net flow of photons. In the AlGaAs layer on the left, the Poynting vector is negative describing the net flow of photons towards the left. The Poynting vector is roughly zero also in the AlGaAs layer on the right, as the optimized contact reflects almost all the radiation back towards the device. The Poynting vector value changes most notably in the leftmost GaAs layer due to absorption, and in the biased GaAs layer due to emission. Interestingly, the value of the Poynting vector changes non-monotonously as a function of K in the intermediate AlGaAs layer due to resonant cavity effects through constructive and destructive interferences and/or differences in the emission rate resulting from the Purcell effect.

Finally, the photon numbers from the IRT model can be used to calculate the net recombination rate using Eq. (2). This is first done separately for each K value in Figs. 4(a)-(d) for TE and TM modes. To show that the IRT simulation gives the same result as direct calculation of the integral in Eq. (1), the K -resolved net recombination is shown both as calculated from the IRT simulation (Figs. 4(a)-(b)) and by carrying out the integration in Eq. (1) numerically (Figs. 4(c)-(d)). Comparison of Figs. 4(a)-(b) with Figs. 4(c)-(d) makes it clear that the IRT simulation produces the result that satisfies the QFED framework for the present device. Moreover, it can be seen that in Figs. 4(a)-(d), the net recombination rate is largest in the biased GaAs layer as expected due to the quasi-Fermi level separation used there in the calculations. In addition, one can see a clear interference pattern in the recombination rate in the biased GaAs layer due to resonant cavity effects. In the GaAs absorber layer on the left side, the net recombination rate is negative due to the absorption of photons emitted by the biased GaAs layer. To obtain the recombination rate of Eq. (2), the rates in Fig. 4(a)-(d) have

Figure 4. Net radiative recombination rates normalized with their maximum values: (a) K -resolved net recombination rate for TE from the IRT simulation, (b) K -resolved net recombination rate for TM from the IRT simulation, (c) K -resolved net recombination rate for TE based on Eq. (1), (d) K -resolved net recombination rate for TM based on Eq. (1), (e) net recombination rate integrated over K for TE and (f) net recombination rate integrated over K for TM.

to be integrated over K . This is done in Figs. 4(e)-(f), which show the total net emission rates at the single photon energy 1.43 eV. These rates would still need to be integrated over all photon energies to get the total rate per unit volume. The rates nonetheless show the expected behaviour, in which photons are emitted by the biased GaAs layer and mostly absorbed by the GaAs layer on the left. Note that this calculation indeed includes all emission enhancement and suppression effects as well as internal reflections, fully accounting also for constructive and destructive interference.

4. CONCLUSIONS

In this paper, we implemented the recently introduced interference radiative transfer (IRT) model in a simplified double-diode structure aimed at demonstrating electroluminescent cooling. We also compared the results to those calculated directly from the underlying quantized fluctuational electrodynamics (QFED) theory. This comparison showed that the IRT model offers a reliable tool to apply QFED in planar structures and is thus an excellent tool to create self-consistent simulations of photon and charge carrier transport in the future. Specifically, as a proof-of-principle study we examined the photon numbers, propagating optical intensities, and net radiative recombination rates produced by the IRT model. The results exhibited the qualitative characteristics expected for the chosen device structure, including also some clearly visible wave-optical properties. Therefore, the IRT model is a promising tool to create self-consistent models of photon and charge carrier transport, potentially giving interesting possibilities to study and develop new devices with a higher efficiency and new functionalities based on e.g. thin-film technology.

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