Full optoelectronic simulation of nanowire LEDs: Effects of temperature

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***Abstract*—Nanowires (NWs) have potential to enable new types of light-emitting diodes (LEDs), which also entail challenges for the development of improved full device simulation models. In this work we calculate the extraction efficiency and emission enhancement in NW array LEDs at different temperatures and couple the results to carrier transport simulations. Our results show that the extraction efficiency of NW LEDs can be strongly temperature-dependent, which complicates the measurement of the internal quantum efficiency of NW LEDs. Through this work we demonstrate the need for full optoelectronic modeling tools in studying and developing new NW-based LEDs.**

I. Introduction

Nanowires (NWs) have potential to enable new functionalities and application areas for light-emitting diodes (LEDs) [1]. For example, strain relaxation in epitaxial NW growth enables a wider range of possible material compositions than what is available in traditional planar growth [2]. This makes NWs especially interesting as light sources in silicon photonics, where integration of direct-bandgap semiconductors with silicon remains a major obstacle [3]. In addition, NW LEDs have been developed for novel display applications, and they could find new use even in, e.g., optical antenna applications and biophotonics. Finally, NW light emitters have potential for quantum technologies in the form of dot-in-a-wire single-photon emitters and detectors [4].

The small size of NWs presents new challenges for device modeling. For example, recent works have demonstrated how the added availability of optical modes in NW structures enhances the spontaneous emission rate of NWs over traditional planar LEDs [5, 6]. However, this emission enhancement is usually not considered in full-device simulations, where a constant spontaneous emission coefficient is typically used for calculating the radiative recombination rate. In this work we develop full optoelectronic device models for NW array LEDs and carry out the simulations at different temperatures. To illustrate how the wave optics of NWs affect the LED characteristics, we show that the light extraction efficiency (LEE) of NW LEDs can be strongly temperature-dependent, complicating the use of conventional methods to estimate the internal quantum efficiency (IQE) of NW LEDs [7].

We carry out our study by simulating the NW array LED shown in Fig. 1. The NWs stand on a p-type substrate in a square array with a pitch of 600 nm, and they contain n- and p-doped GaAs transport layers and an axial InGaAs quantum well (QW) emitting infrared light. We have chosen to model an axial QW to reduce the effect of photon recycling (see, e.g., Ref. [8]), which is not accounted for in the present model. The InGaAs QW is tuned to emit at 1310 nm at room temperature, a wavelength suitable for optical communications.

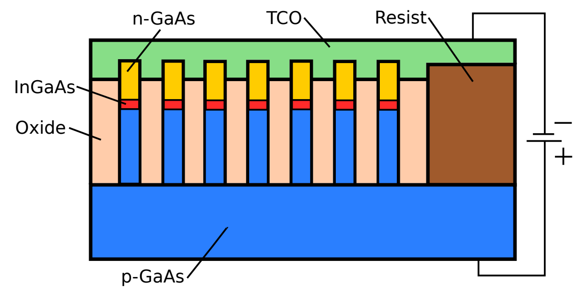

Fig. 1. Nanowire array LED structure simulated in this work, including the processing layers and contacts. (TCO = Transparent conducting oxide)

II. Theoretical model

In our model, we calculate the LEE to the upper half-space and towards the substrate (both semi-infinite) as well as the local Purcell (emission enhancement) factor from Maxwell's equations [6]. The LEE and Purcell factor are calculated by solving for the scattering of incoming monochromatic plane waves from each incidence angle and taking advantage of the Lorentz' reciprocity to obtain the emissivity from the scattering. Note that in such a way the modeling can be done by only solving for the scattering of incoming waves using a real-valued refractive index without calculating light absorption/emission. Using periodic boundary conditions in the in-plane direction of the array, the modeling can be restricted to a single unit cell including only one NW. The oxide and transparent contact shown in Fig. 1 are not considered in the present optical model, and more details can be found in Ref. [6].

Once the local Purcell factor is calculated, the position of the QW within the NW is chosen based on where the emission enhancement towards the top side is largest, and this is done for selected NW diameters. The carrier dynamics and recombination are then simulated for a single NW using the drift-diffusion model [9], where the bulk radiative recombination coefficient is multiplied with the Purcell factor from optical modeling. We solve the optical properties and carrier transport at different temperatures (especially focusing on room temperature and liquid N_2 temperature, 77 K) with

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the low-temperature drift-diffusion simulations carried out following Ref. [10].

To account for thermal effects, we calculate the bandgap (and emission wavelength) as a function of temperature using the Varshni equation given by $E_g(T) = E_g(T = 0) - \lambda T^2/(T + \beta)$, where $E_g(T = 0)$ is the bandgap at 0K and α and β are the Varshni parameters [11]. We also account for the temperature dependency of the refractive index, even if it changes much less as a function of temperature than the bandgap [12, 13]. The temperature dependency of the SRH recombination is taken from Ref. [14], and the radiative and Auger recombinations depend on temperature as in Ref. [8]. Finally, the carrier mobility as a function of temperature is obtained from Ref. [15].

III. Results

Figure 2(a) shows the LEE (towards the top side) averaged over the NW volume at four different temperatures as a function of the NW diameter. With large diameters, the NWs in the array have almost merged to a planar layer and the LEE consequently approaches the corresponding escape cone limit. With small diameters, on the other hand, light does not couple efficiently to substrate modes that have a large lateral k vector, and consequently the LEE increases. The peak in the LEE at a diameter of approx. 200 nm is caused by resonant modes in the NW that couple strongly to freely propagating modes at the top side of the NW array. Due to the strong wavelength dependence of these resonances and the temperature dependency of the emission wavelength, the LEE is strongly temperature-dependent around the diameter of 200 nm, indicating that the conventional method to determine the IQE with variable temperature measurements is not valid [7].

Figure 2(b) shows the Purcell factor averaged over the whole NW at four different temperatures, including emission towards the substrate. Values over 1 indicate emission enhancement as compared to a planar structure. At the large diameter limit, the Purcell factor approaches unity, as the NWs merge to form a planar layer. On the other hand, the Purcell factor peaks at values larger than 1 roughly at wavelengths of 300 and 450 nm due to resonant modes in the NW. Interestingly, the Purcell factor decreases strongly at diameters of roughly 250 nm and below as light no longer couples as efficiently between the substrate and the NW. Comparison to Fig. 2(a) shows that the LEE reaches its maximum value at these small diameters. Similarly as with the LEE, the resonant peaks of the Purcell factor have a strong temperature dependency. The position-dependent Purcell factor is used in the carrier transport modeling to simulate the effects of carrier leakage and other electrical losses on the overall device efficiency at different temperatures. Our results demonstrate the importance of including nano-optical effects in the modeling of NW LEDs.

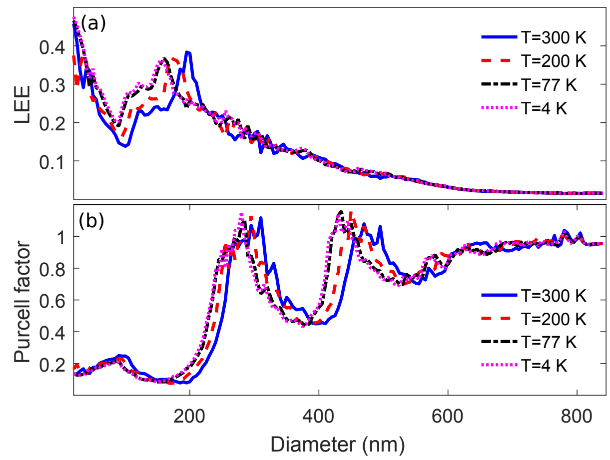

Fig. 2. (a) Light extraction efficiency (LEE) and (b) Purcell factor, both calculated as averages over the NW volume.

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