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P:18 Multi-scale nonequilibrium green's function method for LEDs: Balance of thermalization and tunneling

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GaN/InGaN multi-quantum-well (MQW) structures are the core technology of most mid-to-high power blue light-emitting diodes (LED). Their optimization requires a quantitative understanding of the nanoscale carrier flow. Typical LEDs are characterized by high carrier density regions such as n-GaN/p-GaN leads and InGaN quantum wells (QW). The charge transport is based on both tunneling and thermionic emission. In this work, a multi-scale quantum transport model for efficient and quantitative modeling of a commercial LED is applied [1,2] and augmented to include nonlocal quantum effects. This method is based on the nonequilibrium Green's function (NEGF) formalism to compute the dynamics (states) and the kinetics (filling of states) in the entire extended complex device. The model results agree with experimental I-V curves quantitatively. In this work, we provide a quantitative assessment of long-range tunneling in LEDs. II.

The methodology is based on carrier scattering versus carrier tunneling oriented partitioning of the device as shown in Fig. 1. The n-GaN/p-GaN layers and QWs have extremely high carrier densities. Since the carrier scattering is very strong in these regions, they are considered local equilibrium carrier reservoirs with local quasi Fermi levels. In each reservoir, an imaginary optical potential (η = 0.1eV according to photoluminescent (PL) measurements [3]) is included in the diagonal of the Hamiltonian [4] to mimic the scattering. Current conservation is ensured by self-consistently solving the local Fermi levels [2]. Figure 1 shows all current paths through barrier #4 as an example. In the previous work, all the current paths coupling more than two QW were not considered. In this work, the model is expanded to allow for transport current coupling multiple QWs. 'Hot carrier' formation is allowed in this way. III.

The model is applied to simulate a commercial GaN/InGaN blue LED (see Fig. 1). Figure 2 plots the electron and hole densities with band diagrams and local Fermi levels. Electrons are well transported across the MQW, as indicated by low Fermi level drop (∼25meV) and well spread-out carrier distribution. In contrast, the hole Fermi level drop (∼180meV) is much larger and as a result the hole distribution is skewed towards the p-side. A realistic (0.1eV) and a reduced (0.01eV) η value were simulated and compared. For each η, two sets of simulations were performed. The first set (denoted as 'short') includes only nearest neighbor QW currents. The second set (denoted as 'long') includes all transport components across different QWs. Larger η leads to higher thermionic emission due to more broadened states. The majority of current conduction occurs below the barriers, and decays significantly with longer coupling range. Figure 3 and 4 compares the I-V and internal quantum efficiency (IQE) for different η values and coupling ranges. For larger η, the IQE droops became worse. This is because higher scattering reduces the mobility in the QWs, which leads to more holes piling up at the p-side (see Fig. 2) and thus increases nonradiative losses. The I-V at 0.1eV agrees quantitatively with experimental results. The effect of long-range coupling is only observable at low scattering case (η=0.01eV). Realistic thermalization in LEDs prevent the hotcarrier formation.

An efficient, multi-scale NEGF based transport model was applied on a commercial LED structure. Complete thermalization in the LED QWs has been confirmed. Reducing the scattering rate by 1 order of magnitude, however, allows for the formation of 'hot carriers' due to long range tunneling.

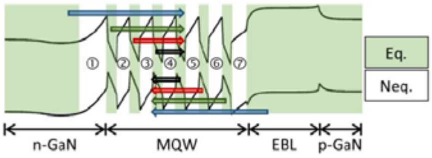

Fig. 1. LED structure considered in this work. Equilibrium (eq - green) and non-equilibrium (neq - white) regions are highlighted. As an example, various tunneling paths through barrier #4 are illustrated with arrows of different colors.

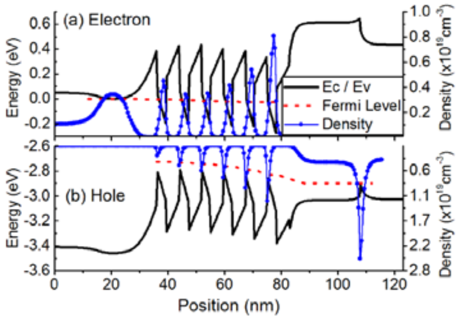

Fig. 2. (a) Conduction band profile with electron density and (b) valance band profile with hole density for η=0.1eV. Note that local Fermi levels (red dashed lines) are only defined in the equilibrium regions of Fig. 1 only. The Fermi level lines are meant to guide the eye.

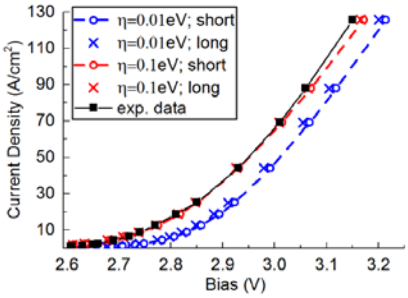

Fig. 3. I-V characteristics with different scattering strengths (η) and tunneling ranges (short vs. long). Larger η suppresses long-range tunneling and long range tunneling can be neglected. The simulated I-V at η = 0.1eV agrees quantitatively with experimental results (black squares).

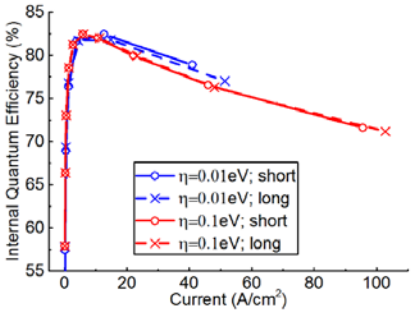

Fig. 4. Internal quantum efficiency (IQE) with different scattering strengths (η) and tunneling ranges. Carriers become more thermalized at higher values of η. This yields charge accumulation at p-side and causes the efficiency droop.

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