From Semiclassical to Quantum Transport Modeling Including Carrier Recombination and Generation

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The non-equilibrium Green function (NEGF) method is capable of nanodevice performance predictions including coherent and incoherent effects. Typically, treating incoherent scattering, carrier generation and recombination in NEGF is computationally very expensive since it involves several nonlinear and highly dimensional integro-differential equations [1]. In contrast, drift-diffusion (DD) [2] models, with or without quantum corrections [3] have been the industrial standard for TCAD due to their efficiency. The Büttiker-probe model represents a good compromise between the accuracy of NEGF and the efficiency of heuristic thermalization models. In this work, the charge self-consistent NEGF Büttiker-probe model is expanded to include carrier recombination and generation effects. Several highlights are achieved with this method. First, atomic resolved recombination/generation effects such as Shockley-Read-Hall, radiative, and Auger recombination are incorporated into NEGF. Second, an alteration of the Büttiker-probe convergence criterion carefully satisfies the continuity equations – also in the presence of carrier recombination and generation. Note that atomically, energy and/or momentum resolved observables that give deep insight into the nanodevice physics and represent an important feature of NEGF are available just like with expensive self-consistent Born models. The new method is first benchmarked against charge self-consistent DD. A standard 20 nm GaN pn diode with $10^{20}/cm^3$ doping is constructed with 2 bands tight binding parameters from NEMO5's tool suit [4] and semiclassical parameters from Silvaco's Atlas tool suit. Current-voltage characteristics (Fig.1), bandstructures (Fig.2), density (Fig.3), and recombination profiles (Fig.4) compare very well. When carrier confinement effects are added to the pn junction with an $In_{0.13}Ga_{0.87}N$ quantum well, quantum transport capabilities are needed to cover the device behavior (Fig.5). These confinement effects enhance the recombination current as shown in Fig.6.

[1] J. Charles, et al., "Incoherent transport in NEMO5: realistic and efficient scattering on phonons," *J. Comput. Electron.*, vol. 15, no. 4, pp. 1123–1129, 2016.
[2] Y.-R. Wu, et al. , "Analyzing the physical properties of InGaN multiple quantum well light emitting diodes from nano scale structure," *Appl. Phys. Lett.*, vol. 101, no. 8, p. 83505, 2012.
[3] J. Geng, et al. , "Quantitative Multi-Scale, Multi-Physics Quantum Transport Modeling of GaN-Based Light Emitting Diodes," *Phys. Status Solidi*, vol. 1700662, p. 1700662, 2017.
[4] S. Steiger, et al., "NEMO5: A parallel multiscale nanoelectronics modeling tool," *IEEE Trans. Nanotechnol.*, vol. 10, no. 6, pp. 1464–1474, 2011.

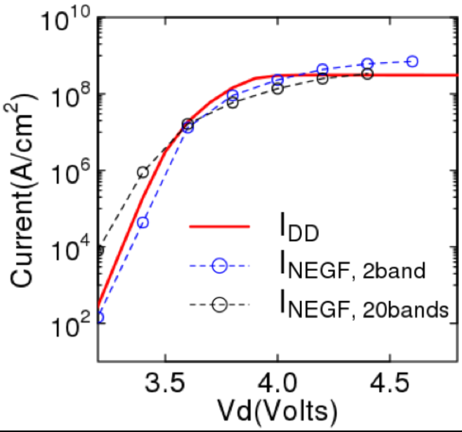

Fig.1: Current-voltage characteristics predicted within quantum transport of NEMO5 and drift diffusion(DD). The current densities match well in a two band model. The better resolution of the 20band results of NEMO5 yield more pronounced deviations.

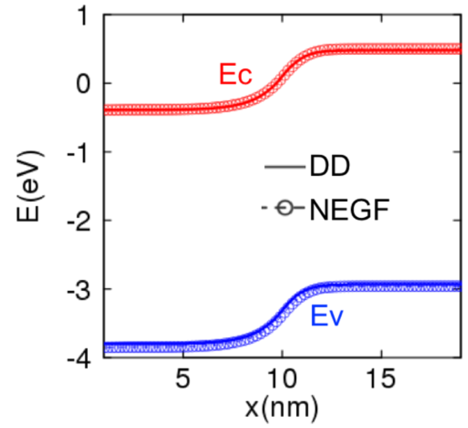

Fig.2: Band diagram (Ec, Ev) comparison between drift diffusion(DD) and NEGF at Vd=3V. Excellent agreement between the two models is observed.

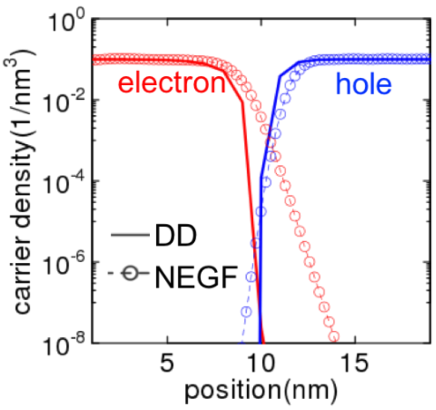

Fig.3: Hole and electron density comparison between drift diffusion(DD) and NEGF at Vd=3V. NEGF predicts a higher minority carrier concentration, presumably since NEGF avoids local equilibrium assumptions.

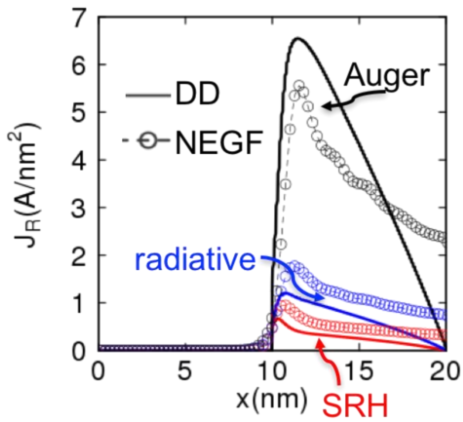

Fig.4: Recombination rates at Vd=3.6V for quantum transport (NEMO5) and drift diffusion(DD). The good agreement is consistent with the carrier comparison of Fig.3.

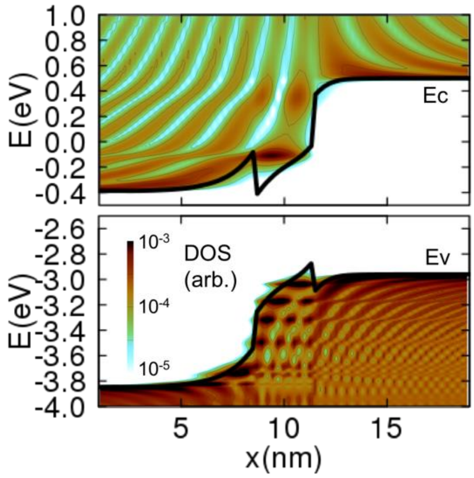

Fig.5: Energy resolved density of states (contour) and band edges (lines) of the pn junction with a quantum well at Vd=3V at the Gamma point. Confined states illustrate the need for quantum transport in nanodevice predictions.

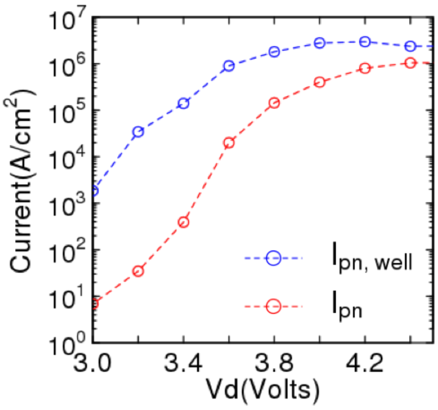

Fig.6: IV curve comparing the standard pn diode case with the same diode added by a quantum well (pn, well). A larger recombination induced by additional carriers in the well increases the total current.