Comparison of Numerical Quantum Device Models

H. Kosina, G. Klimeck[†], M. Nedjalkov, and S. Selberherr

Institute for Microelectronics, TU Vienna, Gusshausstrasse 27–29, Vienna, Austria
Phone: +43-1-58801/36013, Fax: +43-1-58801/36099, Email: Hans.Kosina@TUWien.ac.at

[†]Jet Propulsion Laboratory, California Institute of Technology, MS 169-315, 4800 Oak Grove Dr.
Pasadena CA 91109

The Wigner equation and the non-equilibrium Green's functions (NEGF) are two widely used approaches to quantum device simulation. The Wigner equation has been commonly solved by finite difference methods. In this work, however, a recently developed Monte Carlo (MC) method is employed [1] to solve the stationary Wigner equation of the form,

$$(\mathbf{v} \cdot \nabla_r + q\mathbf{E} \cdot \nabla_k)\, f_w = Q[f_w] + \Theta_w[f_w]$$

where scattering processes are treated semi-classically through the Boltzmann collision operator Q. Due to the equation's similarity with the Boltzmann equation the quantum MC method shows various features of the semiclassical MC method. In the underlying particle model the non-local potential operator Θ_w is interpreted as a generation term. Numerical particles of positive and negative statistical weight have to be generated pair-wise. The problem arising from the avalanche of numerical particles has been solved for stationary conditions. Particles of opposite weight and a sufficiently small distance in phase space are continuously removed in the course of a simulation.

In this work a comparison of the Wigner MC solver and NEMO–1D is shown. NEMO–1D is based on NEGF [2] and has served as a quantitatively predictive design and analysis tool for RTDs at room temperature including the dominant effects of bandstructure [3] and at low temperatures including dominant scattering effects[2, 4]. As a benchmark device a double barrier structure from the literature has been chosen [5]. The potential drop is assumed to be linear across the central device, the effective mass is uniform 0.067 and the barrier height is 0.27eV. The barriers have a thickness of 2.825nm and the well has a thickness of 4.52nm. The doping level in the contacts is assumed to be $2 \cdot 10^{18}\mathrm{cm}^{-3}$.

Because of the rather large valley current of this resonant tunneling diode phonon scattering has only little effect on the I/V characteristics. Both simulators predict a slight increase in valley current due to inelastic scattering (Fig. 1). The I/V characteristics without scattering at 77K and 300K are shown in Fig. 2. Compared with NEMO–1D, a somewhat higher peak current and a lower valley current are obtained by Wigner MC. Fig. 3 demonstrates that the coherence length has to be selected carefully in Wigner transport simulations. This comparative study shows that only a sufficiently large value gives realistic results. A too short coherence length leads to an overestimation of the valley current. Fig. 4 shows as an experimentally observable effect a polar optical phonon peak in the valley current of an RTD simulated by NEMO. The barrier thickness is doubled, thereby reducing the off-resonant coherent valley current contribution and the doping is reduced to expose the phonon peak. Advantages of the MC approach with respect to integration into existing simulation codes and advantages of the NEGF approach in its ability to resolve large carrier density differences will be discussed.

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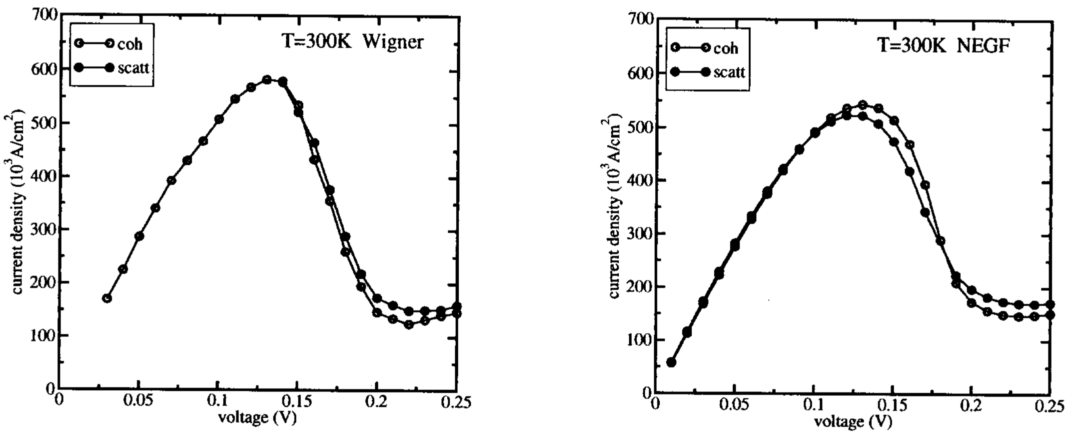

Figure 1: Both simulators predict a small effect of phonon scattering on the I/V characteristics.

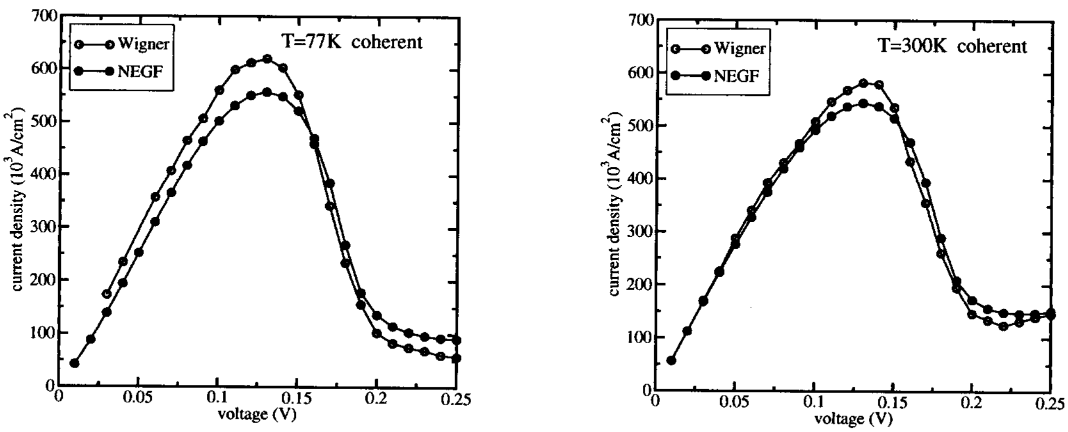

Figure 2: I/V characteristics of the RTD at different temperatures obtained from Wigner MC and NEMO–1D. The valley current increases with temperature, whereas the peak current is only little affected.

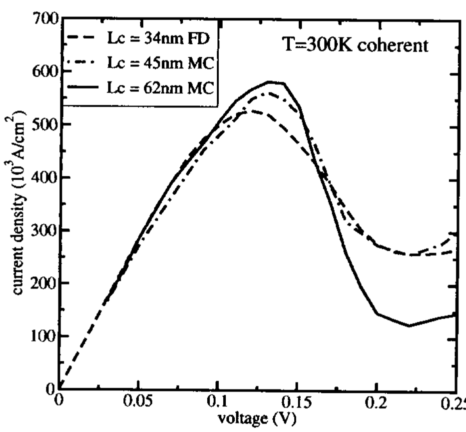

Figure 3: Effect of the coherence length on the I/V characteristics in Wigner simulations. The finite difference (FD) result is taken from [5].

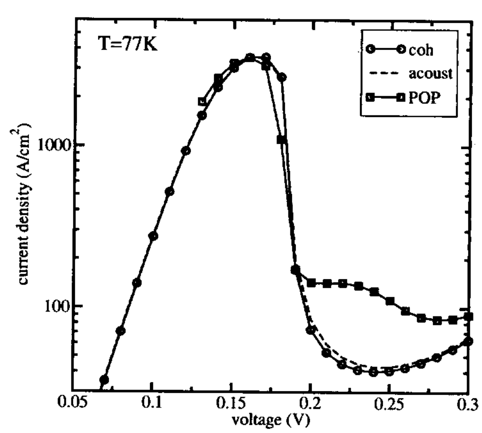

Figure 4: Polar optical phonon peak in the valley current of a RTD with doubled barrier thickness and fivefold reduced doping at 77K. Acoustic phonon scattering alone does not raise the coherent off-resonant current significantly.