Self-Consistent Wigner Monte Carlo Simulations of Current in Emerging Nanodevices: Role of Tunneling and Scattering

Viktor Sverdlov, Hans Kosina, Tibor Grasser and Siegfried Selberherr

Institute for Microelectronics, TU Wien, Gußhausstraße 27–29/E360, 1040 Wien, Austria
{sverdlov|kosina|grasser|selberherr}@iue.tuwien.ac.at

Abstract. Quantum effects determine transport in emerging nanoelectronic devices. At the same time, scattering is still important and may control current at room temperature. A Wigner function based approach, which accounts for the interplay between coherent quantum effects and dissipative scattering effects, is presented. The Wigner equation is solved by means of an advanced Monte Carlo technique. Influence of scattering, tunneling, and space charge effects on the electrical characteristics of single- and double-barrier nanoscale devices at room temperature is investigated.

Keywords: Device simulation, quantum transport, Wigner equation, Monte Carlo method
PACS: 72.10.Bg, 73.40.Qv, 85.30.De, 85.30.Mn, 85.30.Tv, 85.35.-p

INTRODUCTION

Quantum effects play a major role in determining transport in emerging nanoelectronic devices. There are, however, growing evidences that scattering still controls the current [1]. Recent studies demonstrate that the crossover from diffusive to ballistic transport in Si nanowire transistors occurs at approximately 2 nm [2], a much shorter distance than previously anticipated. Transport model for nanoelectronic devices must account for quantum mechanical and dissipative effects. The Wigner function formalism can handle both quantum effects and dissipation simultaneously. Realistic scattering processes are embedded into the Wigner equation via Boltzmann-like scattering integrals [3].

WIGNER MONTE-CARLO METHOD

The solution of the Wigner equation by Monte Carlo methods is hampered by the fact that the Wigner function is not positively defined and cannot be interpreted as a probability distribution. This so-called negative sign problem leads to exponentially growing variances of the Markov Chain Monte Carlo method [4]. We have developed a novel particle Monte Carlo strategy to control the variances. The Wigner potential operator is treated as a generation term [4]. It generates two numerical particles with opposite weights. Two particles stored at the annihilation mesh are chosen such that the weights in the related mesh elements are minimized. The weight sign of the particle continuing the trajectory is the same as the incoming one. To resolve the negative parts of the Wigner function, a certain fraction of negative trajectories has to be introduced. This computation strategy conserves current exactly and minimizes the weight stored. Several numerical methods have been improved to render the Wigner MC technique more robust, including the separation of a classical force, discretization of the Wigner potential. A self-consistent iteration scheme with the Poisson equation is introduced.

RESULTS

We apply the Wigner function formalism to demonstrate the role of tunneling, scattering, and space charge effects on the electrical characteristics of single and double barrier devices, considering *n-i-n* structures, double gate field-effect transistors, and resonant tunneling diodes as examples.

In order to estimate the tunneling component of current Wigner Monte Carlo simulations were carried out for a MOSFET with a gate length of 10 nm in the coherent mode. Good agreement to the results obtained from a Schrödinger solver is observed Fig. 1. The difference between quantum ballistic and semiclassical simulations is due to the additional contribution from electrons tunneling through the potential barrier.

Next, self-consistent Wigner Monte Carlo calculations for Si *n-i-n* structures with an intrinsic region of length W ranging from 20 nm to 2.5 nm were performed. Relative differences between I_{WIG} and the current I_{BALL} computed for a "ballistic" device with scattering inside the intrinsic region turned off is shown in Fig. 2. For W = 2.5 nm the relative differences in current due to quantum effects and scattering in the barrier are still of the order of 25% and cannot be neglected.

Finally, a typical output characteristic of a GaAs resonant tunneling diode, with and without space-charge ef-

CP893, *Physics of Semiconductors, 28th International Conference*
edited by W. Jantsch and F. Schäffler

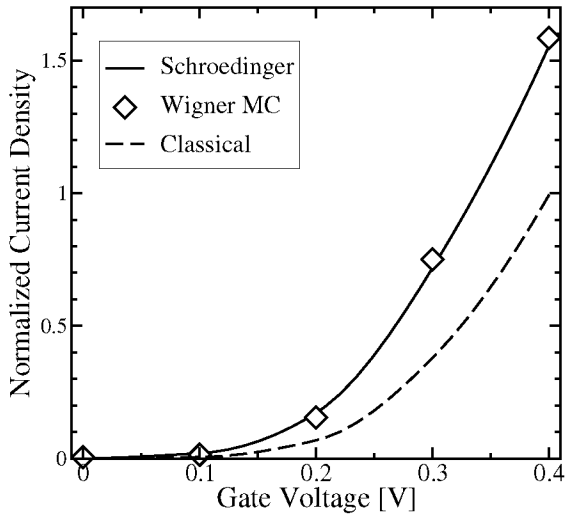

FIGURE 1. Normalized classical ballistic current density and relative quantum mechanical current density obtained with the Wigner Monte Carlo (open symbols). Wigner data are in good agreement with the current density found from the solution of the Schrödinger equation. Additional source-to-drain tunneling current component is clearly visible.

fects taken into account, is shown in Fig. 3. Scattering with polar optical phonons as well as Coulomb scattering in the contacts is considered. A region of negative differential resistance common to transport via a resonant level is clearly visible after the resonance peak at 250 mV applied voltage. A self-consistent solution of the Wigner

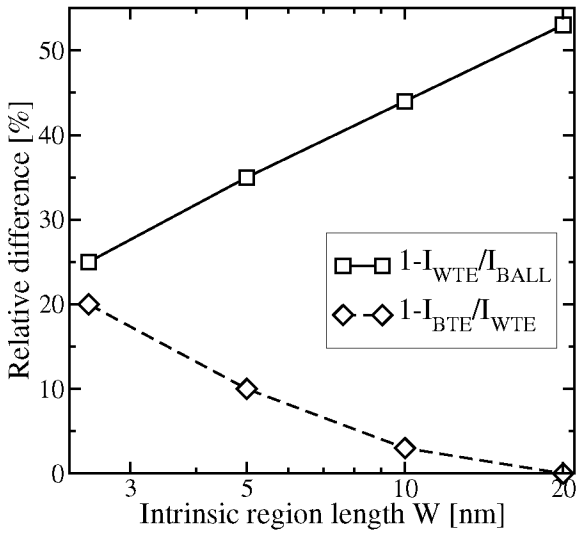

FIGURE 2. Relative difference between currents calculated with the Wigner and Boltzmann Monte Carlo methods (diamonds) and calculated with the Wigner MC for an *n-i-n* structure, with and without scattering in the intrinsic region.

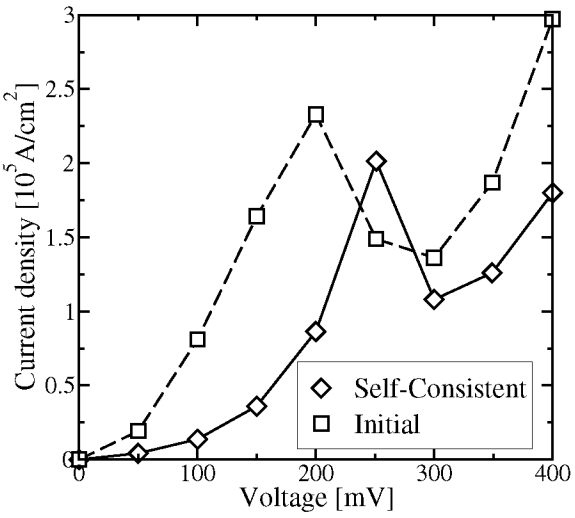

FIGURE 3. Typical *IV* curve of RTD, calculated self-consistently (solid line), contrasted against a non self-consistent characteristics.

and Poisson equation is mandatory for the correct determination of the resonance position.

CONCLUSIONS

The Wigner function approach is a comprehensive method to address simulation needs of emerging nanoelectronic devices. It treats tunneling and realistic scattering mechanisms on equal footing. The method applied to single- and double-barrier nanostructures demonstrates the importance of both quantum-mechanical and scattering effects in emerging nanodevices.

ACKNOWLEDGMENTS

We gratefully acknowledge financial support from the Austrian Science Fund FWF, project P17285-N02.

REFERENCES

1. P. Palestri, D. Esseni, S. Eminente, C. Fiegna, E. Sangiorgi, and L. Selmi, *IEEE Trans.Electron Devices* **52**, 2727–2735 (2005).
2. M. Gilbert, R. Akis, and D. Ferry, *J.Appl.Phys.* **98**, 094303–1–8 (2005).
3. W. Frensley, *Reviews of Modern Physics* **62**, 745–791 (1990).
4. H. Kosina, and M. Nedjalkov, *Handbook of Theoretical and Computational Nanotechnology*, American Scientific Publishers, Los Angeles, 2006, vol. 10, chap. Wigner Function Based Device Modeling, pp. 731–763, (in print).