Scattering and Space-Charge Effects in Wigner Monte Carlo Simulations of Single and Double Barrier Devices

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Due to the aggressive downscaling of MOSFETs the channel length L is rapidly approaching 25 nm and is expected to be further reduced. At these channel lengths quantum effects such as direct source-to-drain tunneling start affecting the device characteristics. At the same time, scattering still controls the current in decananometer devices [1]. An accurate theory of MOSFETs near the scaling limit must therefore properly account for the interplay between coherent quantum and dissipative scattering effects. This mixed transport regime can be treated by the Wigner function formalism which allows for a seamless link between classical and quantum device regions [2]. Early numerical solutions of the Wigner equation were obtained by the finite difference method, assuming simplified scattering models based on the relaxation time approximation [3]. However, for realistic device simulations comprehensive scattering models are required. The Wigner equation including realistic scattering mechanisms can be solved by means of Monte Carlo (MC) techniques [2]. Due to the non-positive kernel, however, Wigner MC simulations require significantly longer computation times than classical MC simulations do.

In this work we demonstrate the role of scattering and space charge effects on the electrical characteristics of single and double barrier devices. Single barrier *n-i-n* structures, double gate field-effect transistors (FET), and resonant tunneling diodes (RTD) are considered. 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, and a particle annihilation algorithm. A self-consistent iteration scheme with the Poisson equation was introduced.

For the lowest sub-band profile of a 10 nm gate length double-gate FET we have compared the quantum ballistic currents computed using Wigner MC and a numerical Schrödinger solver. Fig.1 demonstrates good quantitative agreement and also shows the classical ballistic current for comparison. The quantum ballistic current is higher than the classical one due to carriers tunneling through the potential barrier.

Self-consistent (SC) potentials for *n-i-n* Si diodes with a lengtg W of the intrinsic region ranging from 20 nm down to 2.5 nm have been calculated by Wigner and classical MC simulations (Fig.2.) The transition regions of the doping profile have length W. Electron-phonon and ionized impurity scattering are included. As expected, for a thick barrier the classical and quantum calculations yield the same result (W = 20 nm). For W = 2.5 nm, the additional space charge of electrons tunneling through the barrier results in an increase of the barrier height. Despite the increased barrier, the current I_{WTE} is nearly 20% higher than the classical value I_{BTE} (Fig.3, W = 2.5 nm). The relative difference between I_{WTE} and I_{BALL} for a "ballistic" device with scattering inside the intrinsic and transition regions turned off is shown in Fig.3. For W = 2.5 nm the relative differences due to quantum effects and scattering in the barrier area still in the order of 25% and cannot be neglected.

Self-consistent carrier concentration profiles for a double-barrier GaAs RTD are shown in Fig.4. Before the barrier, an accumulation layer forms, depending on the applied voltage. The result is an additional voltage shift of the resonance peak of the I/V characteristics as demonstrated in Fig.5.

In conclusion, the importance of both scattering and quantum interference effects for simulations of decananometer devices at room temperature is demonstrated. Space charge effects cannot be neglected, as tunneling currents would be overestimated otherwise.

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REFERENCES

[1] P. Palestri *et al.*, "Understanding Quasi-Ballistic Transport in Nano-MOSFETs: Part1-Scattering in the Channel and in the Drain", *IEEE T-ED* **52**, 2727 (2005).

[2] H. Kosina *et al.*, "A Monte Carlo Method Seamlessly Linking Quantum and Classical Transport Calculations", *J. Computational Electronics* **2**, 147 (2003).

[3] W.R Frensley, "Boundary Conditions for Open Quantum Systems Driven far from Equilibrium", *Rev.Mod.Phys.*, **62**, 745 (1990).

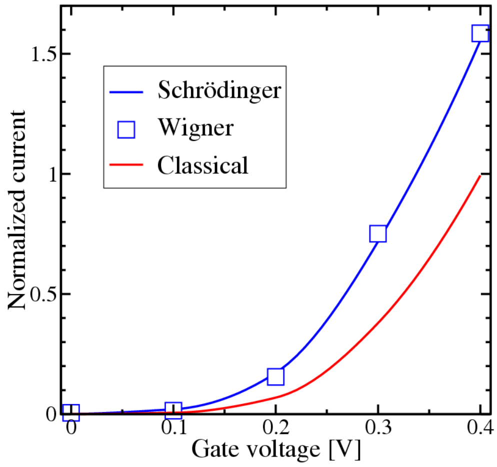

Fig. 1. Relative ballistic currents calculated classically (red) and quantum mechanically (blue). Wigner MC results are shown with open squres.

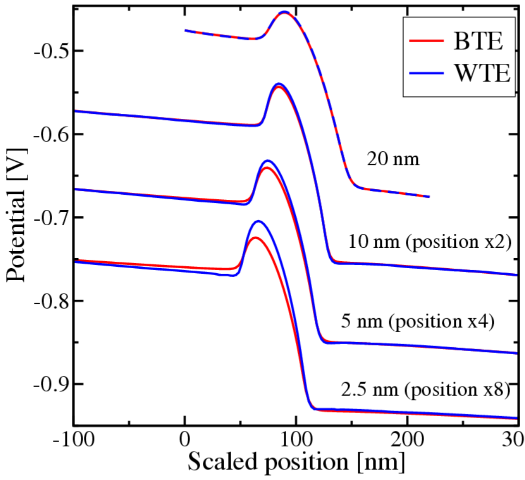

Fig. 2. Initial and self-consistent potential profiles calculated with Wigner (blue) and Boltzmann (red) MC.

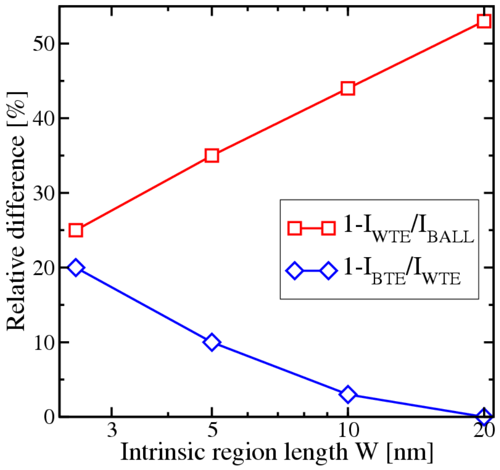

Fig. 3. Relative difference between currents calculated with Wigner and Boltzmann Monte Carlo methods (blue) and with and without scattering in the intrinsic region of *n-i-n* structure.

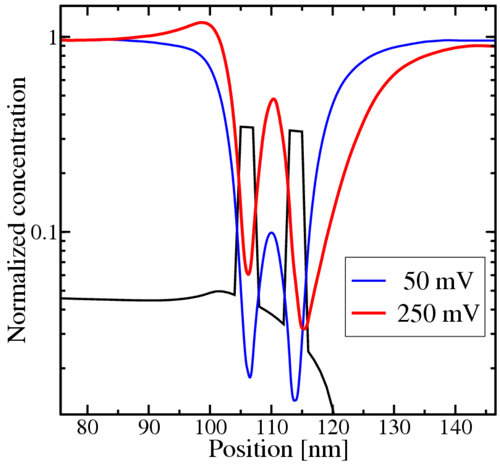

Fig. 4. Normalized electron concentration off-resonance (blue) and at resonance (red) in double-barrier structure. Space charge accumulation is seen at the cathode side of resonant tunneling diode.

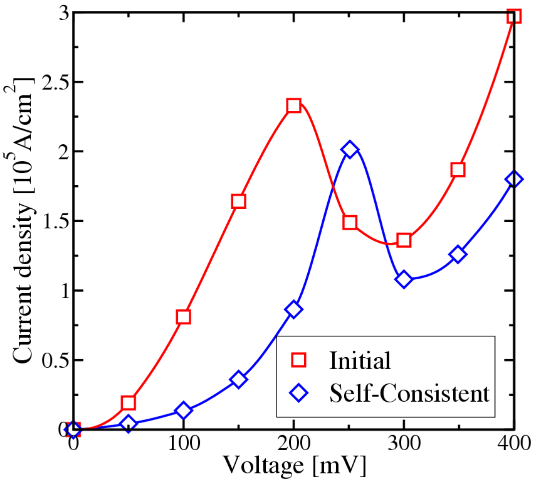

Fig. 5. Space charge accumulation at the cathode leads to significant shift of the resonance peak.