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Effect of boundary treatments on quantum transport current in the Green's function and Wigner distribution methods for a nano-scale DG-MOSFET

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ABSTRACT

In this paper, we conduct a study of quantum transport models for a two-dimensional nano-size double gate (DG) MOSFET using two approaches: non-equilibrium Green's function (NEGF) and Wigner distribution. Both methods are implemented in the framework of the mode space methodology where the electron confinements below the gates are pre-calculated to produce subbands along the vertical direction of the device while the transport along the horizontal channel direction is described by either approach. Each approach handles the open quantum system along the transport direction in a different manner. The NEGF treats the open boundaries with boundary self-energy defined by a Dirichlet to Neumann mapping, which ensures non-reflection at the device boundaries for electron waves *leaving* the quantum device active region. On the other hand, the Wigner equation method imposes an inflow boundary treatment for the Wigner distribution, which in contrast ensures non-reflection at the boundaries for free electron waves *entering* the device active region. In both cases the space-charge effect is accounted for by a self-consistent coupling with a Poisson equation. Our goals are to study how the device boundaries are treated in both transport models affects the current calculations, and to investigate the performance of both approaches in modeling the DG-MOSFET. Numerical results show mostly consistent quantum transport characteristics of the DG-MOSFET using both methods, though with higher transport current for the Wigner equation method, and also provide the current–voltage (*I*–*V*) curve dependence on various physical parameters such as the gate voltage and the oxide thickness.

1. Introduction

With fast development of semiconductor technologies, MOSFET dimensions are scaled down continuously. Gate and channel lengths are considered as the characteristic size of a MOSFET. The classical Boltzmann equation can accurately describe the drift-diffusion transport of charge carriers when the characteristic size is much larger than the mean free path of the carriers. However, quantum transport models should be used to address quantum effects once the characteristic size becomes much smaller than the mean free path [1]. The quantum transport models from the Schrödinger wave function can be implemented with either the formulation of the Non-equilibrium Green's function (NEGF) [2] or that of the Wigner distribution function in a phase space [3]. Many simulations have been done on quantum devices such as the RTD (Resonant Tunneling Diode), bulk MOSFET, SOI MOSFET, and double gate (DG)-MOSFET [1,4–7]. Especially, the DG-MOSFET with symmetric oxide layers and gates is a promising new device for better and more effective control of short channel effects.

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A comprehensive description of quantum transport in nano-size MOSFETs is offered by the solution of NEGF, coupled with a Poisson equation self-consistently. However, the computational cost for solving the full NEGF is prohibitive; thus simplified models are usually employed to reduce the computational cost [6]. For thin body DG-MOSFETs, for which the confinement effect of the gates is strong, we could approximately decouple the solution of two- dimensional (2D) Schrödinger wave functions into two 1D problems [6,7]. Such an approximation is the basis of the mode space method where the electron confinements below the gates are pre-calculated to produce subbands along the vertical direction of the device while the channel transport is described by 1D Schrödinger equations with a subband energy profile along the transport direction. In many cases, one more approximation is done by assuming the eigenfunctions in the confinement direction do not change along the transport direction. Thus, those 1D Schrödinger equations for all subbands become decoupled, significantly reducing the total cost. Venugopal et al. analyzed the effectiveness of the mode space method by comparing it with the full real physical space discretization of the 2D Schrödinger equation for an ultra small DG-MOSFET [6]. It is concluded that the mode space method costs much less due to the fact that only a few subbands with lower energies need to be considered. The mode space method has also been used to compare the ballistic transport and the scattering transport of ultra thin body DG-MOSFETs [7].

In addition to the NEGF, a kinetic model can be derived using the Wigner distribution function [5,8] in the position-momentum phase space. The Wigner equation was first introduced by Wigner in 1932 by adding a correction term to the Boltzmann equation for a low temperature case [3]. Numerical methods for both NEGF and Wigner equations have attracted much attention recently due to the need of simulating quantum transport with computers [9,10]. The NEGF describes transport in a quantum open system using boundary self-energies to account for the effect of contacts to the device [20]. Within the NEGF formalism, a detailed treatment of the various scattering process is possible [11]. On the other hand, the Wigner formalism has found many advantages for theoretical analysis of quantum transport. The Wigner function is an electron quasi-distribution in the phase space, which can model ideal contacts by separating incoming and outgoing components of the distribution at the boundaries. This phase space description is similar to classical distributions and allows us to incorporate a Boltzmann type collision term to explicitly deal with the electron scattering from ionized impurities, acoustic phonons, and surface roughness at the Si/SiO_2 interface [5,12]. The Wigner equation can be solved by a probability method (Monte Carlo) [13,14] and deterministic methods (Finite Difference method, Spectral method, etc) [1,4,5,15,16]. Both steady-state and transient Wigner equations have been solved by the finite difference method to analyze the transport character of RTD [4]. The mode space method with 1D Wigner equations along the channel direction has been applied to determine the current through a nano-size SOI MOSFET and analyze the effect of the channel size to the current character. Scattering effects due to impurity, acoustic phonon, and surface roughness at the boundary between the silicon layer and the oxide layer are also considered in the Wigner-mode space combination [1,5].

In this paper, we will study both NEGF and Wigner function methods for quantum transport along the channel direction and investigate the different manners the device boundary conditions are treated and their effects on the transport current calculations for a nano-scale DG-MOSFET. As the Wigner equation is a reformulation of the Schrödinger equation by a Weyl transform and the Fourier transform, the NEGF and the Wigner equation descriptions are in principle equivalent. However, different treatments of boundaries and scatterings produce different levels of approximation accuracy and computational efficiency. In the case of NEGF, the contact boundaries are treated by self-energy terms which are basically Dirichlet to Neumann mappings for the Green's function on the boundaries [7,17,20]. The boundary conditions are so designed to observe the casuality of the system through an outgoing radiation condition; as a result, electron waves *leaving* the active device regions will not be reflected at the boundaries. On the other hand, inflow boundary conditions are posed for the Wigner distribution such that free electrons *entering* the device region will not be reflected at the boundaries, and the Wigner distribution effectively assumes Fermi–Dirac equilibrium distributions of the electrons in the contacts at the appropriate Fermi levels. The difference of imposing non-reflecting properties in the NEGF and the Wigner distribution methods will have effects on the transport current calculated by either method, as shown in our simulations of a nano-scale DG-MOSFET.

The paper is organized as follows. In Section 2, we first introduce the mode space method for 2D Schrödinger equations and the concept of subband, then the relevant formulas for density functions and Landauer formulation for the current using transmission probability coefficients. Section 3 describes the method of the NEGF and its treatment of quantum boundary using the self-energy to ensure the non-reflection at the device boundaries for electron waves *leaving* the quantum device active region, and most importantly, the relation between the transmission probability coefficient and the NEGF, and the subsequent current formula using the NEGF. In Section 4, the Wigner function method is introduced, and the inflow boundary condition for the Wigner distribution, which ensures the non-reflection at the boundaries for free electron waves *entering* the device active region, is elaborated. Section 5 contains the numerical simulations with both the NEGF and the Wigner equations in the channel direction in the framework of the mode space method for a nano-scale DG-MOSFET. Finally, a conclusion and a discussion are given in Section 6.

2. Current formula for transport in a DG-MOSFET in mode space methods

A DG-MOSFET has a structure shown in Fig. 1 with a silicon layer sandwiched by two symmetric oxide layers. The source and the drain are doped heavily, while the body (I) is made intrinsic to approximate the ballistic limit [7]. As the scale of the