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A Finite Volume Method for the Multi Subband Boltzmann Equation with Realistic 2D Scattering in Double Gate MOSFETs

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Abstract. We propose a deterministic solver for the time-dependent multi-subband Boltzmann transport equation (MSBTE) for the two dimensional (2D) electron gas in double gate metal oxide semiconductor field effect transistors (MOSFETs) with flared out source/drain contacts. A realistic model with six-valleys of the conduction band of silicon and both intra-valley and inter-valley phonon-electron scattering is solved. We propose a second order finite volume method based on the positive and flux conservative (PFC) method to discretize the Boltzmann transport equations (BTEs). The transport part of the BTEs is split into two problems. One is a 1D transport problem in the position space, and the other is a 2D transport problem in the wavevector space. In order to reduce the splitting error, the 2D transport problem in the wavevector space is solved directly by using the PFC method instead of splitting into two 1D problems. The solver is applied to a nanoscale double gate MOSFET and the current-voltage characteristic is investigated. Comparison of the numerical results with ballistic solutions show that the scattering influence is not ignorable even when the size of a nanoscale semiconductor device goes to the scale of the electron mean free path.

AMS subject classifications: 35Q20, 35Q40, 65Z05

Key words: Double gate MOSFET, multi subband Boltzmann transport equation, 2D electron gas, deterministic solver, PFC method.

1 Introduction

The down-scaling is an important engine in the semiconductor industry. With the size of the semiconductor enters the deep sub-micro range, the conventional bulk MOSFET

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faces great challenge to be scaled down to 40 nm because of the short channel effects (SCEs) [3]. The SCEs modify the threshold voltage and the electron drift characteristics in the channel, so cause considerable distress for the device designers. The double gate (DG) MOSFET is a promising structure for next generation semiconductors because it provides an extra gate to suppress the SCEs. So its simulation has drawn the interest of many researchers, e.g., [1,6,15,19].

The double gate MOSFETs with a channel length greater than the mean free path of electrons can still use the semi-classical transport equation in the transport direction. But when the thickness of the Si body between the two gate stacks becomes thin, the quantum confinement results in energy quantization. The quantization's influence to the electron transport can not be disregarded. The quantum models like the nonequilibrium Green function (NEGF) method [7], the density matrix method and the Wigner transport equation are not mature enough for the devices with a channel length greater than the mean free path of electrons. These quantum-mechanical methods can be applied to the RTD and quantum dots, wires and wells and molecular devices where the electron scattering can be neglected [24]. The model under consideration in this paper solves the multi subband Boltzmann transport equation (BTE) self-consistently with the Schrödinger equation and the Poisson equation. So we can call it the Boltzmann-Schrödinger-Poisson (BSP) system.

Many deterministic solvers for the BTE have been proposed to solve the Boltzmann-Poisson system, such as the WENO solver [5], the spherical harmonic expansion (SHE) method [25], the deterministic particle method [8], the finite-difference scheme [10,18]. The positive and flux conservative (PFC) method using a splitting approach (which splits a multi-dimensional problem into many 1D problems) has been proposed in [12] to solve the transport part of the BTE (the Vlasov equation). The PFC method is not only conservative, but also preserves the positivity and the maximum value of the distribution function. Recently, Ben Abdallah et al. present a deterministic solver of the Boltzmann-Schrödinger-Poisson system with an effective valley and a very simple scattering term (relaxation time approximation) [1]. The quantum confinement in the z-direction forms 2D electron gas (2DEG), so the scattering should be considered as 2Dk scattering. However, the deterministic methods for the Boltzmann-Schrödinger-Poisson system with 2Dk scattering has not been well investigated.

The relaxation time approximation is questionable when the size of the devices is comparable with the mean free path of electrons and the system is far away from the equilibrium (the high source-drain voltage V_{DS} often drives the system far away from the equilibrium). High doping density requires the consideration of the Pauli exclusion principle. In this paper, we present a deterministic solver for a more complete time-dependent Boltzmann-Schrödinger-Poisson system. Here "more complete" means in two aspects: (1) the six valleys of Δ-band instead of an effective valley of silicon are considered; and (2) the intra-valley and inter-valley phonon-electron 2Dk scattering including the Pauli exclusion principle is considered, instead of only a relaxation time approximation of scattering. We include an acoustic phonon and an optical phonon for the intra-