Quantum Mechanical Carrier Transport and Nano-scale MOS Modeling

Zhiping Yu, Xue Shao, Dawei Zhang, and Lilin Tian
Institute of Microelectronics, Tsinghua University, Beijing 100084, China
Email: yuzhip@tsinghua.edu.cn

Abstract— In the sub-100nm MOS regime, carrier transport exhibits the particle-wave dual nature. In this paper, the advance of quantum transport modeling at both the macroscopic and microscopic levels is reviewed. Starting from solving Schrödinger equation with open boundary condition, various methods including NEGF (non-equilibrium Green's function), QTBM (quantum transmitting boundary method), QDAME (quantum device analysis by modal evaluation), and QHD (quantum hydrodynamic) and DG (for density gradient) are introduced. The results of device simulation using NEGF are presented for a 3D FinFET and compact model based on 2D quantum mechanical effects and ballistic transport is described.

I. Introduction

Today's advanced MOS structure has its dimension fall well into the regime of so-called mesoscopic domain, where the free-flight path of carriers without scattering is comparable with the size of the device. It has long been realized that the quantum mechanical effects play ever important role in determining the device performance [1].

The modeling work of carrier quantum transport in MOSFETs can be categorized into two aspects: device simulation and compact circuit modeling. In the former, the quantum transport is further modeled at microscopic level, essentially solving the Schrödinger equation for wavefunctions, and macroscopic level which solves a set of continuity/conservation-based PDEs (partial differential equation) for such macro-quantities as carrier concentration and temperature. In the latter, efforts are mainly focused on the threshold voltage correction due to the QM effects and the impact of ballistic carrier transport on device I-V characteristics.

This paper discusses both the above modeling aspects with emphasis on modeling approach to quantum transport in MOS structures.

II. Wigner-Boltzmann Equation and Macroscopic QM Modeling Approaches

Wigner [2] proposed a distribution function in real and crystal momentum spaces, $\mathbf{r}, \mathbf{p}$, which is a Fourier transform of the density matrix for a quantum state governed by the Schrödinger equation. Wigner function can be obtained by solving the Wigner-Boltzmann equation,

$$\frac{\partial f_W}{\partial t} + \frac{\mathbf{p} \cdot \nabla f_W}{m^*} - \frac{2}{\hbar} \sin\left(\frac{\hbar}{2} \nabla^U \cdot \nabla_{\mathbf{p}}\right) U(\mathbf{r}) f_W(\mathbf{r}, \mathbf{p}) = 0 \tag{1}$$

where operator sin is understood as the power expansion of its argument and the gradient ∇^U operates only on the U part of its operands in the real space. Retaining the terms up to $\hbar^2$ in the series expansion and take the first three moments in $\mathbf{p}$-space $(1, \mathbf{p}, \mathbf{p} \cdot \mathbf{p}/2m^*)$ for the above equation, one obtains the set of quantum hydrodynamic (QHD) equations for carrier, momentum, and energy conservation [3]. The quantum corrections of order $\hbar^2$ are incorporated in the stress tensor, which is needed in QHD equations, and energy density as (for electrons)

$$\hat{P} = -nTI + \frac{\hbar^2 n}{12m^*} (\nabla\nabla) \ln n \tag{2}$$

$$W = \frac{3}{2} nT + \frac{1}{2} m^* n u^2 - \frac{\hbar^2 n}{24m^*} \nabla^2 \ln n \tag{3}$$

where I is the identity matrix and all QM correction terms are related to the gradient of the carrier density. A more specific density gradient (DG) approach is based on the modification of the drift-diffusion formulation [4]:

$$\mathbf{F}_n = -D_n \nabla n + \mu_n n \nabla (V + Q_n) \tag{4}$$

$$Q_n = 2b_n \frac{\nabla^2 \sqrt{n}}{\sqrt{n}}, \quad b_n = \frac{\hbar^2}{12 q m_n^*} \tag{5}$$

where $\mathbf{F}_n$ is the electron flux density, V is the potential solved from the Poisson's equation, and b_n for 3D case.

Another macroscopic QM modeling approach is the effective potential (EP) and it takes into consideration the finite size of the electron wavepacket [5]. The comparison of DG, EP, and a more complete Schrödinger/Poisson equation solver is shown in Fig. 1. The advantage of macroscopic QM modeling is the capability of analyzing non-planar, multi-dimensional device structures and for different modes of analysis: small signal ac, time transient, etc.

III. Solving Schrödinger Equation with Open Boundary Conditions

For sufficiently small scales, electrons are ballistic and coherent over the entire device region. Quantum states

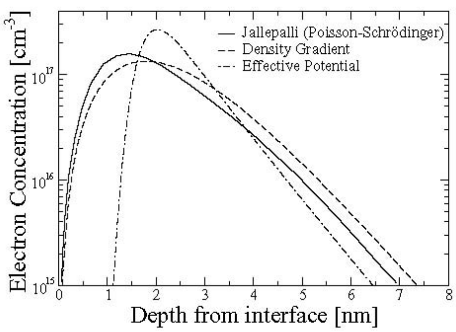

Fig. 1. Comparison between EP and DG against a complete Schrödinger-Poisson solver for the carrier distribution in an inversion layer.

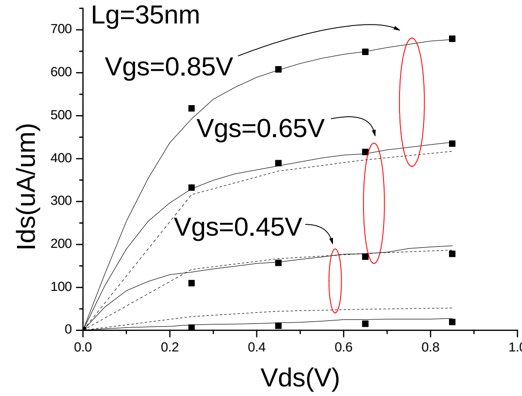

Fig. 2. Comparison between simulation (lines) and measurement (symbols) data for Toshiba 35 nm CMOS. Dashed line is without 2D QM correction to V_{th}.

which carry current, also called "scattering states", are more important in understanding current flow through small coherent regions. It is necessary to solve multi-dimensional Schrödinger equation directly with open boundary condition. There are basically two types of methods in this approach: using the transmitting boundary (QTBM [6] and QDAME [7]) for ballistic transport, and using Green's function [8] which can include the scattering inside the device. Once the wavefunction or Green's function is found, the relevant quantities to the device characteristics such as the carrier and current density can be calculated.

IV. Quasi-3D QM Simulation of FinFETs

Hybrid, two-dimensional (2D) approach which combines the charge distribution in the device region solved from Schrödinger and Poisson equations and semi-classical transport along the channel is useful in investigating the device performance during nano-scale MOS design. Recently, a quasi-3D model with complete QM theory but at limited dimensions (NEGF along the channel and Schrödinger in the cross-section of the channel) has been developed for the evaluation of FinFET performance as compared to double-gate SOI [9]. It is revealed that for the slab (or film in double-gate SOI) thickness of 3 nm and gate length of 10 nm, FinFET can provide better on/off current ratio than double-gate SOI.

V. Ballistic MOS Model (BMM) with 2D QM Effects

There have been tremendous efforts in building QM effects in the MOS compact modeling, mostly based on the 1D QM corrections to the threshold voltage and ballistic transport along the channel [10].

A new compact MOS model, which combines the ballistic transport and 2D QM effects, explores the WKB theory to model the subband lowering in the confined dimension (perpendicular to the channel) because of the open boundary along the channel [11]. An empirical formula for 2D-QM-corrected threshold voltage is proposed. The model has been applied to bulk CMOS with gate length ranging between 15 nm and 45 nm. In Fig. 2, the comparison of the output characteristics of the 35 nm device between experimental data and analytical results is presented. It is clear seen that without considering the QM effects along the channel, the analytical results grossly underestimate the real data.

References

[1] Z. Yu, R. W. Dutton, and R. A. Kiehl, *IEEE Trans. Electron Devices,* p. 1819, Oct. 2000.

[2] E. Wigner, *Phys. Rev.,* 40, 1932, pp. 749-759.

[3] C. L. Gardner, *SIAM J. Appl. Math.,* Vol. 54, pp. 409-427, April 1994.

[4] M. G. Ancona and H. F. Tiersten, *Phys. Rev.* **B**, 35 (1987), p. 7959.

[5] D. K. Ferry, R. Akis, and D. Vasileska, *Digest IEDM*, p. 287, 2000.

[6] C. Lent and D. Kirkner, *J. Appl. Phys.* 67, pp. 6353-6359, 1990.

[7] S. E. Laux, A. Kumar, and M. V. Fischetti, *IEEE Trans. Nanotechnol.,* Vol. 1, No. 4, pp. 255-259, Dec. 2002.

[8] S. Datta, *IEDM Tech. Digest,* pp. 703-706, 2002

[9] X. Shao and Z. Yu, "Nanosacale FinFET: A Quasi-3D Quantum Mechanical Model Using NEGF," submitted to *Solid-State Electronics*.

[10] K. Natori, *IEICE Trans. Electron.*, Vol. E84-C, 1029-1036, Aug. 2001.

[11] Z. Yu, D. Zhang, and L. Lin, "Ballistic MOS model (BMM) considering full 2D quantum effects," to be presented on the *3rd Workshop of Compact Modeling*, Boston, March 2004.