SIMULATION SCHEMES IN 2D NANOSCALE MOSFET'S: WKB BASED METHOD

N. BEN ABDALLAH, C. NEGULESCU, M. MOUIS and E. POLIZZI

Mathématiques pour l'Industrie et la Physique, UMR CNRS 5640,
Université Paul Sabatier, 118, route de Narbonne,
F-31062 Toulouse Cedex, France

email: naoufel@mip.ups-tlse.fr, negulesc@mip.ups-tlse.fr, mouis@enserg.fr, epolizzi@ecn.purdue.edu

We present a numerical method to simulate quantum transport in Silicon ultrashort channel MOSFET (DGFET). The considered model is ballistic and consists in solving Schrödinger equations with quantum transmitting boundary conditions, coupled to the Poisson equation for the electrostatic potential.

There is an enormous amount of work (see References) dedicated to numerical solution of Schrödinger-Poisson systems (with open boundary conditions) either by finite element/difference methods or Greens function techniques. The aim of our work, which is based on finite element approximation, is to reduce the number of grid points in order to lower the computational cost, while keeping a good accuracy.

STEP I. Subband decomposition (SDM)

The resolution of the Schrödinger equation in the whole 2D domain

$$-\frac{\hbar^2}{2}\frac{1}{m_x(z)}\Delta_x\psi_\epsilon(x,z) - \frac{\hbar^2}{2}\frac{\partial}{\partial z}\left(\frac{1}{m_z(z)}\frac{\partial}{\partial z}\psi_\epsilon(x,z)\right) + V(x,z)\psi_\epsilon(x,z) = \epsilon\psi_\epsilon(x,z).$$

is replaced by the resolution of 1D eigenvalue problems in the confined direction

$$-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\left(\frac{1}{m_z(z)}\frac{\partial}{\partial z}\chi_i(z;x)\right) + V(x,z)\chi_i(z;x) = E_i(x)\chi_i(z;x), \quad \int_0^1 |\chi_i(z;x)|^2 dz = 1$$

and many 1D Schrödinger equations projected on the transport direction

$$-\frac{d^2}{dx^2}\varphi_\epsilon^i(x) - 2\sum_{j=1}^{\infty} a_{ij}(x)\frac{d}{dx}\varphi_\epsilon^j(x) - \sum_{j=1}^{\infty}\left(b_{ij}(x) + \frac{2}{\hbar^2}c_{ij}(x)(\epsilon - E_j(x))\right)\varphi_\epsilon^j(x) = 0$$

where we have the decomposition of the 2D wave function $\psi_\epsilon(x,z) = \sum_i \varphi_\epsilon^i(x)\chi_i(z;x)$. The number of unknowns is thus reduced from $N_x \times N_z$ for the standard method to $N_x \times M$ for the SDM method, where M is the number of modes, N_x resp. N_z the number of grid points in the transport resp. confined direction.

STEP II. WKB approximation (SDM/WKB)

Using oscillating interpolation functions instead of polynomial ones for the resolution of the 1D Schrödinger equation, enables us to reduce significantly the number of grid points in the x-direction. Starting from the Ansatz $\Phi(x) = exp(\mathbf{i}S(x)/\hbar)u(x)$, we express the wave function Φ by means of the so-called WKB basis functions. These functions oscillate with a frequency close to that of the wave function and in the limit $\Delta x \ll \lambda$ reduces to usual linear interpolation functions.

An extensive comparison between SDM and SDM/WKB has been performed. Accurate results have been obtained with much coarser grids and reduced computational time. [1]

[1] A full journal publication of this work will be published in the Journal of Computational Electronics

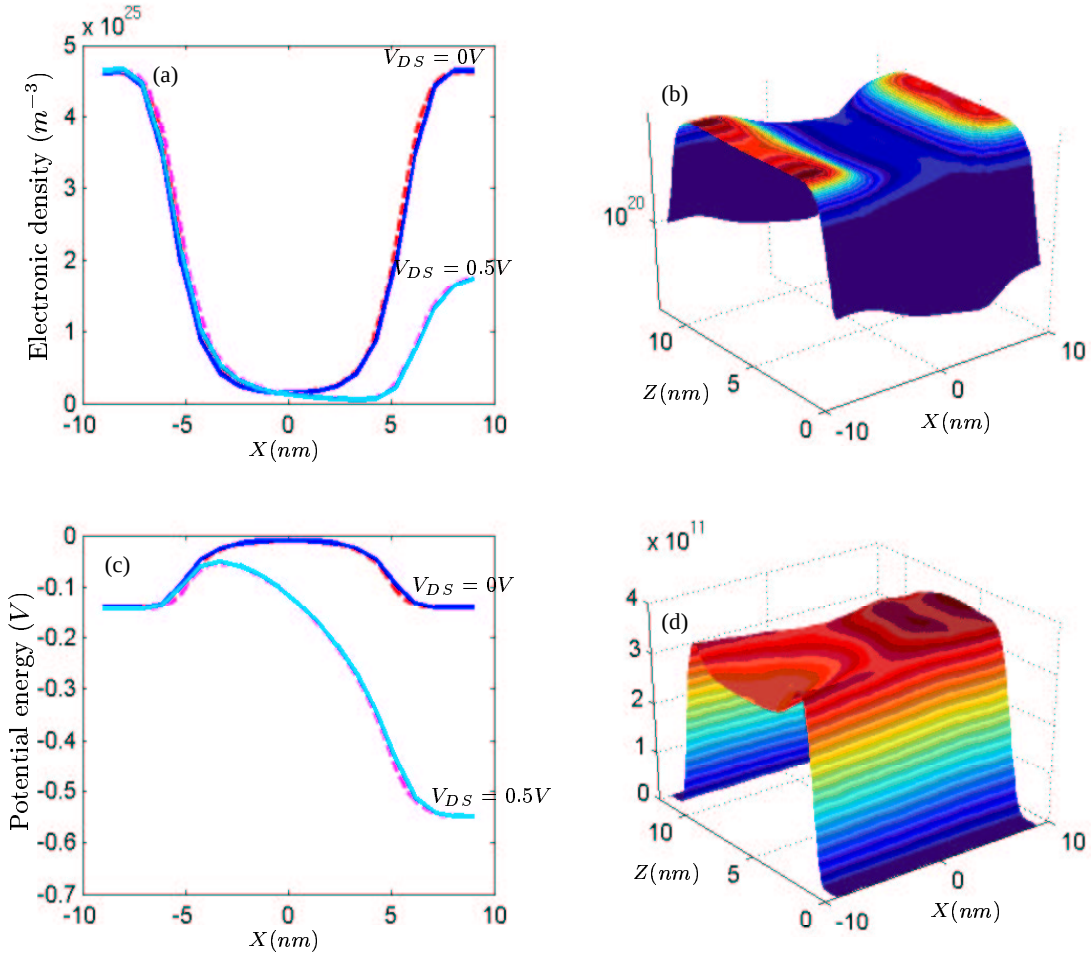

Figure 1: (a) Cross sections of the electron density at $1nm$ from the interface for $V_{GS} = 0.1V$. Full lines: SDM/WKB; Broken lines: SDM (b) 2D distribution of the electron density for $V_{GS} = 0.1V$ and $V_{DS} = 0.5V$ (SDM/WKB). (c) Cross sections of the potential energy at $1nm$ from the interface for$V_{GS} = 0.1V$. (d) 2D distribution of the current density for $V_{GS} = 0.1V$ and $V_{DS} = 0.5V$ (SDM/WKB).

References

[1] N. Ben Abdallah, O. Pinaud *Improved simulation of open quantum systems: resonances and WKB interpolation schemes*, submitted in J. Comp. Phys.

[2] N. Ben Abdallah, E. Polizzi *A general quantum subband decomposition method for the modeling of electron transport in the ultimate devices*, submitted in J. Comp. Phys.

[3] S. Datta *Nanoscale Device Modeling: the Green's Function Method*, Superlattices and Microstructures, **28**, 253-278, 2000.

[4] M.V. Fischetti, *Theory of electron transport in small semiconductor devices using the Pauli master equation* J.Appl.Phys. **83**, 270-291 (1998).

[5] M.V. Fischetti, Phys.Rev. B **59**, 4901 (1999).

[6] G. Klimeck, F. Oyafuso, T.B. Boykin, R.C. Bowen, P. von Allmen, Computer Modeling Eng. Sci. (CMES) **3**, 601 (2002).

[7] C.S. Lent, D.J. Kirkner, *The Quantum Transmitting Boundary Method*, J.Appl.Phys. **67**, 6353-6359 (1990).

[8] A. Svizhenko, M.P. Anatram, T.R. Govindan, B. Biegel, Device Research Conference 2001 (IEEE, Piscataway, NY 2001) 167-168 (2001).

2

[2]A full journal publication of this work will be published in the Journal of Computational Electronics