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Quantum simulation of an ultrathin body field-effect transistor with channel imperfections

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ABSTRACT

An efficient program for the all-quantum simulation of nanometer field-effect transistors is elaborated. The model is based on the Landauer–Buttiker approach. Our calculation of transmission coefficients employs a transfer-matrix technique involving the arbitrary precision (multiprecision) arithmetic to cope with evanescent modes. Modified in such way, the transfer-matrix technique turns out to be much faster in practical simulations than that of scattering-matrix. Results of the simulation demonstrate the impact of realistic channel imperfections (random charged centers and wall roughness) on transistor characteristics. The Landauer–Buttiker approach is developed to incorporate calculation of the noise at an arbitrary temperature. We also validate the ballistic Landauer–Buttiker approach for the usual situation when heavily doped contacts are indispensably included into the simulation region.

1. Introduction

The continuing progress in silicon VLSI technology motivates a transition to silicon-on-insulator (SOI) wafers. Just these structures definitely suppress short channel effects which substantially impair the bulk MOSFET performance. This is the ultrathin body (UTB) (1–5 nm) fully depleted (FD) silicon on insulator (SOI) structure (Fig. 1) that will take an ultimate advantage of SOI wafers and provide an advancement of the silicon technology to extreme channel lengths. As a result, such structures will exhibit higher frequencies and a lower power consumption.

As a carrier wavelength becomes commensurable with the channel size, the all-quantum simulation of such small devices becomes challenging. One of the most intriguing issues is an impact of realistic channel imperfections (random charged centers and wall roughness) on transistor characteristics. It is crucial for the evaluation of the statistical variability of transistors in large integrated circuits. The most vital is a variability of threshold voltages [1,2] which encumber lowering of the drive voltage necessary for lower power applications.

Methods of quantum simulation were in a rapid progress for more than two preceding decades. The leading ones are the non-equilibrium Green's functions (NEGF) [3–12] and the Landauer–Büttiker (LB) approach [3,4,13–19]. In the ballistic regime they evidently coincide. To calculate the transmission coefficients one could exploit the transfer-matrix (T-matrix method) [20–23] or that of scattering-matrix (S-matrix) [3,4,24–29]. Previously, it was widely supposed that the conventional T-matrix method failed to cope with evanescent modes. However, recently an efficient method involving the arbitrary precession (multiprecision) arithmetic was put forward [30–32]. The advanced transfer-matrix technique is much faster in practical simulations than that of scattering-matrix. Moreover, the proposed means turned out to be powerful for simulations based on any wave equations, in particular, electromagnetic waves in non-uniform media, e.g., nanostructured solar cells [33,34].

Current noise is one of major transistor characteristics required for practical applications. We derive a general expression to calculate the current noise for an arbitrary temperature and voltage bias. This expression could be used in the same simulation of the field-effect transistor based on the Landauer–Buttiker approach.

We also address an issue of validity of the ballistic Landauer–Buttiker approach for the usual situation when heavily doped contacts with strong scattering are indispensably included into the simulation region. A question arises whether a transistor with a ballistic channel is really ballistic. Recently this 'perpetual' problem was also discussed in Ref. [35]. Here we ague that a fairly high and steep potential barrier at the contacts justifies the ballistic simulation.

2. Efficient T-matrix method for quantum simulation

We calculate transmission coefficients T_i from the Schrödinger equation and then evaluate dependence of the drain current I on

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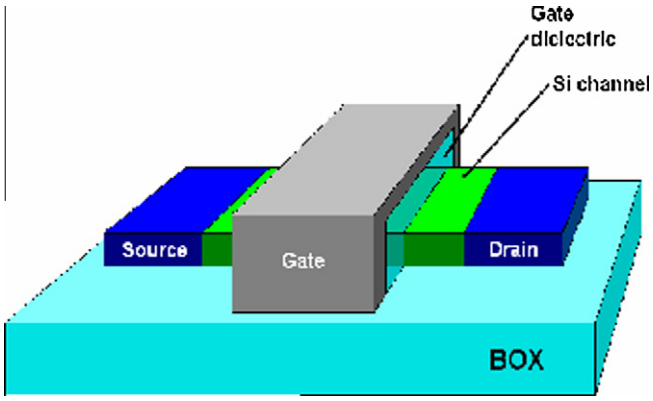

Fig. 1. Structure of FD ETSOI FET in simulation (spacers are removed for clarity).

the source-drain voltage V_D via the Landauer–Buttiker formula upgraded to the situation:

$$I = \frac{2e}{h}\sum_{\upsilon}\sum_{i}\int dE T_i(E)[f_S(E) - f_D(E)], \tag{1}$$

where f_S and f_D are the Fermi–Dirac distribution functions in the source and drain contacts, respectively, shifted by a drain bias eV_D, E is a total energy including the quantization energy and the longitudinal motion energy. Formula (1) implies the summation over all wave-guide modes i involved into the simulation and all conduction band valleys υ. The pre-summation factor originates in the conductance quantum for spin-unpolarized current $G_0 = 2e^2/h$, where h is the Planck constant, namely,

$$T_i = \frac{\sum_j |\mathbf{c}^+_{ij}|^2 k_j}{k_i} = 1 - R_i$$

is the total transmission coefficient of an incident wave belonging to the i-th mode with unity amplitude and the longitudinal wave vector k_i at the channel entrance, c^+_{ij} is an amplitude of the j-th outgoing mode at the channel exit with the wave vector k_j. The summation in the above formula for T_i conserves the current.

In spite of the fact that the Landauer–Buttiker approach is formulated explicitly, it is based on several suppositions which are not apparent. We discuss them in Appendix A.

The necessary transmission coefficients in Eq. (1) are determined via a self-consistent solution of the Schrödinger and Poisson equations (the Hartree mean field approach). To be more precise, the scattering problem for the three-dimensional stationary Schrödinger equation should be solved.

A brief description of the procedure is presented below. In fact, we follow a straightforward strategy which was widely used for a non-uniform electromagnetic wave-guide description long time ago. The stationary Schrödinger equation is:

$$\left[-\frac{\hbar^2\partial^2}{2m_x\partial x^2} - \frac{\hbar^2\partial^2}{2m_y\partial y^2} - \frac{\hbar^2\partial^2}{2m_z\partial z^2} + U(x,y,z)\right]\psi(x,y,z) = E\psi(x,y,z), \tag{2}$$

where $U(x, y, z) = -e\varphi(x, y, z)$ is a potential energy inside the channel, m_x, m_y, m_z are the electron effective masses along corresponding axes of the silicon conduction band structure (Fig. 2).

The exact wave function in any cross-section x is expanded over all transversal modes $\varphi_i(y, z)$ for the uniform wave-guide:

$$\psi(x,y,z) = \sum_{i=1}^{\infty} c_i(x)\cdot\varphi_i(y,z). \tag{3}$$

The complete set of functions $\varphi_i(y, z)$ obeys the two-dimensional Schrödinger equation.

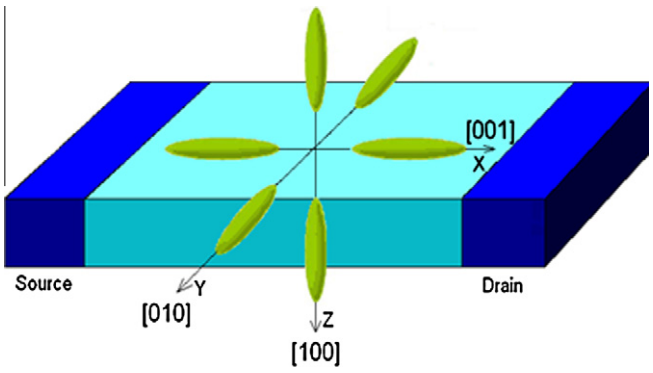

Fig. 2. Silicon conduction band structure matched with the channel.

$$\left[-\frac{\partial^2}{2m_y\partial y^2} - \frac{\partial^2}{2m_z\partial z^2}\right]\varphi_i(y,z) = \varepsilon_i\varphi_i(y,z) \tag{4}$$

with the following boundary conditions: the functions $\varphi_i(y, z)$ vanish on the wave-guide walls because of a high potential barrier at the contact of silicon with surrounding dielectrics. However, a microscopic description of those boundaries seems challenging [36,37]. Solutions of Eq. (4) give rise to the mode energies ε_i. For a uniform rectangular wave-guide the transversal functions are trivial

$$\varphi_i(y,z) = \frac{2}{\sqrt{Wd_{si}}}\sin\frac{\pi n y}{W}\sin\frac{\pi m z}{d_{si}}, \tag{5}$$

$$\varepsilon_i = \frac{\pi^2\hbar^2}{2}\left(\frac{n^2}{m_y W^2} + \frac{m^2}{m_z d_{si}^2}\right), \tag{6}$$

where W is the channel width (y-axis), d_{si} is the channel thickness (z-axis), $i = (n, m)$, n and m are non-negative integers. The functions $\varphi_i(y, z)$ are real, orthogonal, and normalized per unity so that

$$\int dy\int dz\varphi_i(y,z)\varphi_j(y,z) = \delta_{ij} \tag{7}$$

where δ_{ij} is the Kronecker delta symbol.

Substituting (3) for $\psi(x, y, z)$ into the Schrödinger Eq. (2), then multiplying it by $\varphi_j(y, z)$ and integrating over the transversal coordinates y and z, one obtains the following set of equations for amplitudes:

$$-\frac{\partial^2 c_i(x)}{2m_x\partial x^2} + \sum_j U_{ij}(x)c_j(x) = [E - \varepsilon_i]c_i(x), \tag{8}$$

where

$$U_{ij}(x) = \int dy\int dz\varphi_i(y,z)U(x,y,z)\varphi_j(y,z) \tag{9}$$

is nothing else but the matrix element of the potential.

We retain a finite number of modes in the expansion (3). Justification of such a reduction lies in the behavior of matrix elements of the bare Coulomb potential $U(r) \sim 1/r$ for upper modes $j = (n, m)$, $n \gg 1$, $m \gg 1$, namely,

$$U_{ij}(x) \sim \frac{1}{\sqrt{n^2 + m^2}}. \tag{10}$$

Therefore, under such circumstances, transformation of the incident mode i into upper modes j is negligible. The necessary number of modes involved into consideration could be determined immediately during the simulation.

Eq. (8) is to be solved on a uniform mesh with nodes in $x = x_k$, $k = -1, 0, 1, \ldots, N, N+1, N+2$ and step Δx. The finite difference approximation of Eq. (8) is