Self-consistent contact block reduction method for ballistic nanodevices

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We have extended our previously developed contact block reduction (CBR) method [1] for ballistic currents through arbitrarily shaped, multi-terminal two- or three-dimensional open devices to include charge self-consistency. We show that the calculation of the charge density of the open system throughout the device can be performed with an effort comparable to a single calculation of the eigenstates of a properly defined closed system. It is also shown that it is crucial to properly take into account both bound states and current carrying states.

The efficiency of the CBR method for the fully quantum mechanical calculation of the transmission function, the density of states, and the carrier density rests on 3 key points: (i) the evaluation of all of theses observables requires only that part of the retarded Green's function G^R that connects the contacts to the interior device; (ii) G^R can be evaluated efficiently by calculating only a few percent of the eigenstates of a suitably defined Hermitian Hamiltonian of the size of the device; (iii) the size of the contact part of the G^R matrix can be grossly reduced by transforming into the basis of all propagating lead modes which amount to a few percent of all modes.

In effect, the solution of the ballistic quantum transport problem is reduced to the calculation of few eigenstates of the decoupled device, and the subsequent inversion of small matrices of dimension proportional to the number of propagating lead modes for each energy step. The self-consistency is achieved by the implementation of a predictor-corrector scheme for the Schrodinger-Poisson equation [2], which leads to a well converged electrostatic potential within a few iteration steps.

We exemplify the method by a ballistic double-gate field effect transistor (DGFET). The characteristic dimensions of the DGFET modeled in this work have been taken from [3], but the gates and oxide tunneling barriers are fully included in the self-consistent scheme. The band-structure is modeled by a single parabolic band with anisotropic effective mass for silicon and a spherical mass for the oxide. Figure 1 depicts the charge density in the entire device region. The resulting I-V characteristic, including the gate leakage, is shown in Fig. 2. The quantum mechanical charge depletion near the interface between the highly doped gate and the oxide barrier leads to a non-current-carrying bound state below the Fermi surface that has a dramatic influence on the I-V characteristics, as shown in Fig. 3.

The calculation of a single bias point for the entire 2D device with more than 7000 grid points requires 2 to 3 hours on a 3 GHz Pentium 4 PC.

[1] D. Mamaluy, M. Sabathil, P. Vogl, J. Appl. Phys. 93, 4628 (2003)
[2] A. Trellakis, A.T. Galick, U. Ravaioli, J.H. Arends, Y. Saad, J. Appl. Phys. **81**, 3461 (1997)
[3] http://falcon.ecn.purdue.edu:8080/mosfet/10nmstructure.pdf

A full journal publication of this work will be published in the Journal of Computational Electronics.

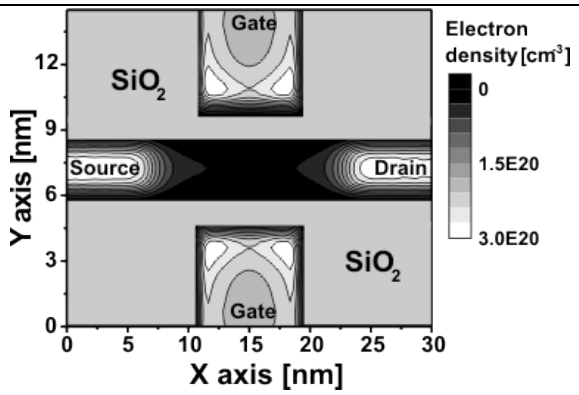

Figure 1: 2-D Geometry of the ballistic DGFET showing the self-consistently calculated charge density in the channel and in the gate regions. All contact regions are taken to have a doping density of 2×10^{20} cm^{-3}. The symmetrically located density peaks at the gate-oxide interface originate from bound states that form near the charge depletion at the interface.

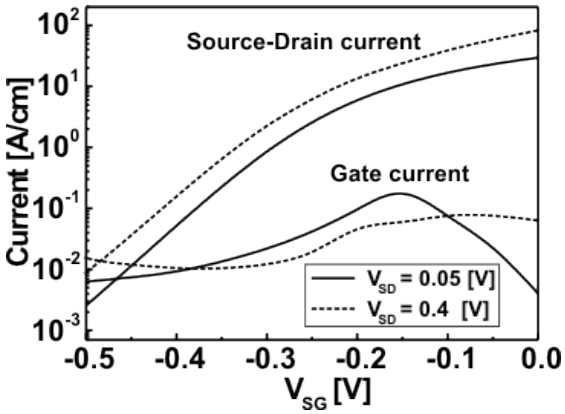

Figure 2: Calculated transfer characteristics of ballistic DGFET, showing the drain and (tunneling-induced) gate current for two values of the source-drain voltage.

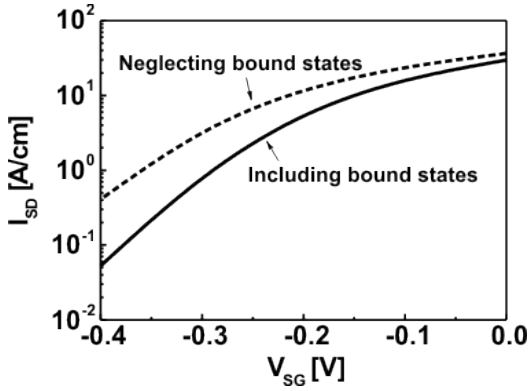

Figure 3: Comparison of transfer characteristics with (solid curve) or without (dashed curve) taking into account the non-current-carrying bound states near the gate-oxide interface depicted in Fig. 1. In a strictly ballistic calculation, these bound states would not get occupied, in spite of lying below the local Fermi energy, because they do not overlap with the propagating modes.

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