Full Quantum Mechanical Simulation of Ultra-Small Silicon Devices in Three-Dimensions: Physics and Issues*

M.J. Gilbert and D.K. Ferry
Department of Electrical Engineering and Center for Solid State Electronics Research
Arizona State University, Tempe, AZ 85287-5706
Tel: 1-480-965-3452, Fax: 1-480-965-8058
email: matthew.gilbert@asu.edu

The results of a full three-dimensional, ballistic quantum transport model for a quantum wire silicon MOSFET are presented. We use the recursive scattering matrix approach for simulation of the ballistic transport through the device [1]. While recent approaches have utilized the Green's function formalism to capture the proper physics present in certain types of ultra-small devices, such as DG-MOSFETs [2], the Green's function produces only the density of states and not the density itself. This requires a difficult integration over a fine energy grid in order to obtain the density. In the scattering matrix approach, we obtain the density directly, as we solve for the wave functions themselves in a site representation. As future devices will be quantized in all three directions, decomposing the solution space into uncoupled directions is no longer plausible and the interaction between subbands is necessary. The intermode interaction, and inter-subband interaction, are captured naturally in the site representation. We utilize an efficient, three-dimensional, self-consistent quantum simulation technique [1] with the inclusion of an adaptable non-uniform mesh to optimize the discretization of the solution space. One of the key issues surrounding the use of quantum simulations is the discretization of the solution space, as it is necessary that proper grid selection keep the corresponding energies within the artificially-created bandstructure, even when applying large bais across the device. Should the energies exceed the numerical bandstructure, then errors will result in the output. However, in addition to keeping the solutions physical, the grid must be optimized to reduce the number of grid points in order to hold the computational time, particularly at high bias (~ 0.5 V) to acceptable levels. These constraints stipulate the use of a non-uniform mesh with finer grid spacing in the high potential regions. We apply this methodology to the simulation of a quantum wire SOI MOSFET with a narrow channel (8 nm). As the channel barrier potential is lowered by the applied gate voltage, the channel populates and depopulates with electrons alternatively due to two competing effects: (1) the reflection from the oxide that defines the narrow channel and (2) the interaction with the dopant atoms in the system (in the channel and *in the source and drain*). As the electrons populate the available subbands in the channel, they can be trapped by reflections from the source-channel interface as well the channel-drain interface. Combined with the interaction with the channel dopants, we find a situation where a quasi-standing wave appears in the channel of the device and the density becomes trapped, as shown in fig.1. We find that the electrons entering the channel have an exaggerated interaction with the channel dopants causing the formation of resonant states within the channel. Incident electrons then tunnel through these states causing peaks in the device output characteristics, as shown in fig. 2.

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[1] M.J. Gilbert and D.K. Ferry, J. Appl. Phys., *In Press*.
[2] R. Venugopal, Z. Ren, S. Datta, M.S. Lundstrom, and D. Jovanovic, J. Appl. Phys. **92**, 3730 (2002).

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

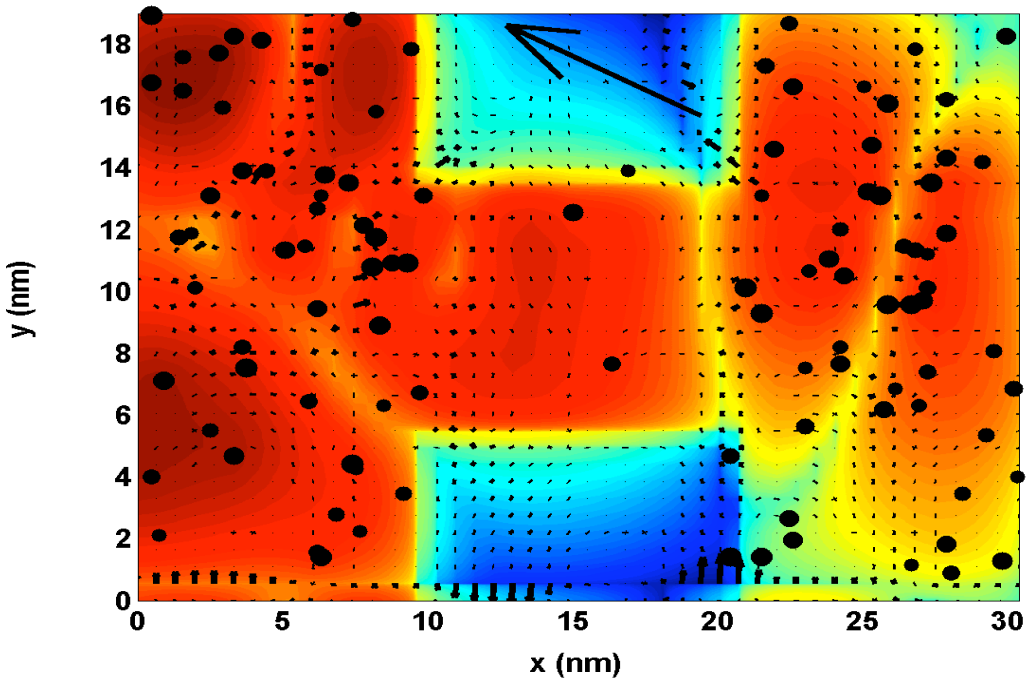

Figure 1: Electron density plotted at a depth of 7 nm into the device. The dots correspond to the locations of the dopants and the arrows correspond to the velocity field. The gate voltage is 2.4 V and the drain voltage is 10 mV. Here we see the density pooling near the locations of the dopants in the channel while being constricted by the channel dopants. Furthermore, we find the channel depopulating at this gate voltage as is evidenced by the rapid decrease in density towards the drain end of the device.

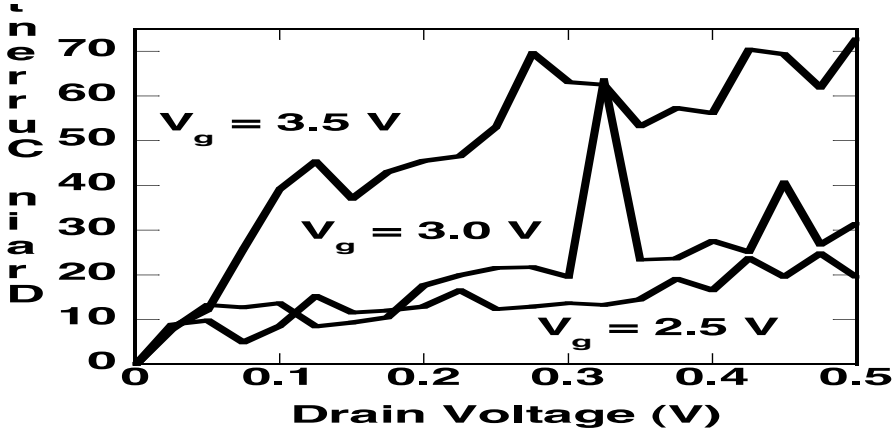

Figure 2: Typical Id-Vd curves for a narrow channel quantum wire SOI MOSFET. These curves detail the spikes formed by the interaction of the density with the channel dopants.

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