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Coarse-Grain 3D Quantum Simulations of Nanoscale MOSFET

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1. Introduction

The nonequilibrium Green's function (NEGF) formalism provides a suitable framework for quantum simulations in nanoscale devices. However, commonly used finite difference grid representation schemes involve large number of the mesh points which makes computations very challenging for 3D nanostructures with complex geometry [1]. Realistic random charge distribution in MOS devices also presents crucial obstacle to reliable application of the grid methods. In this work we formulate a conceptually new method which gives a way around these problems. The method is applied to quantum ballistic transport in 3D Double Gate and Gate-all-Around MOSFETs [2].

2. Theory

Quantum simulations in nanoscale device require accurate and efficient calculation of the Green's function. In the effective mass approximation it satisfies the equation

$$\left[-\frac{\hbar^2}{2m^*}\Delta_{\mathbf{R}} - e\varphi(\mathbf{R}) - E\right] G(\mathbf{R},\mathbf{R}',E) = \delta(\mathbf{R}-\mathbf{R}'). \qquad (1)$$

Eq.(1) must be solved self consistently along with the Poisson equation for the electrostatic potential φ(**R**) which includes the response to the carriers charge $-en_e(\mathbf{R})$. Instead of using the real space grid we construct all physical quantities ($G(\mathbf{R},\mathbf{R}',E)$, $n_e(\mathbf{R})$, φ(**R**)) in the form of basis expansion.

We show that in arbitrary open area of the device the effect of its boundaries can be analytically extracted from Eq.(1) so that the remaining part is equivalent to a closed system where the basis functions $\Phi_n(\mathbf{R})$ can be defined. As a result, we can derive the basis representation for the Green's function in the open area

$$G(\mathbf{R},\mathbf{R}',E) = \sum_n \frac{\Phi_n(\mathbf{R})}{E-E_n}\left[\Phi_n(\mathbf{R}') + \sum_i \Phi_n(\mathbf{R}_i) I_i\right], \quad (2)$$

where E_n are the corresponding eigen energies, $\mathbf{R}_i$ are the quadrature points at the area boundary and the numerical parameters I_i are related with the electric current at these points. In all physically interesting cases these parameters can be found analytically. In particular, by imposing the outgoing boundary conditions we construct the retarded Green's function, calculate the corresponding self energies and the carrier density $n_e(\mathbf{R})$. Similar solution is derived for the electrostatic potential φ(**R**) [3].

3. Numerical Method and Simulation Results

Eq.(2) and similar representations for $n_e(\mathbf{R})$ and φ(**R**) provide building blocks of effective quantum simulator. The basis in arbitrary open area is found in terms of DVR (Discrete Variable Representation) functions [4] consistent with the area geometry. This significantly reduces the volume of computations. Figure 1 shows typical behaviour of numerical error for 1D version of Eq.(1). The grid in the DVR representation is just the corresponding Gaussian quadrature.

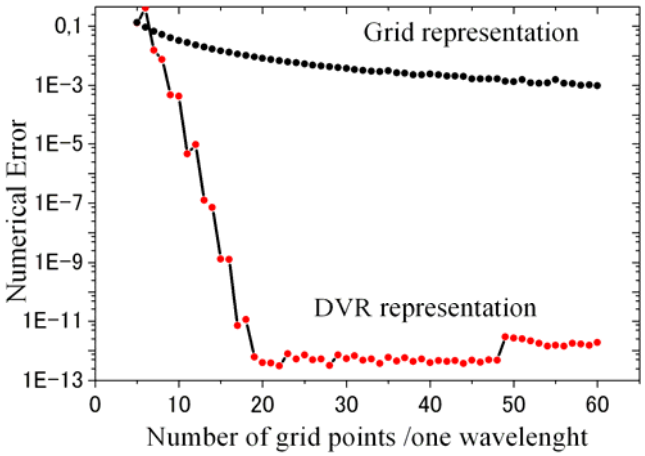

Fig.1 Accuracy of one-dimensional DVR basis representation in comparison with the grid method.

The whole computational domain can be split into a set of small separate open areas where the basis is easy to compute. Adjacent areas are coupled by the continuity conditions for the Green's function and the electric current at the corresponding boundaries. The numerical coefficients I_i in Eq.(2) become boundary parameters which couple the adjacent areas. In the case of the Poisson equation, the normal components of the displacement filed at the boundary $D_n(\mathbf{R}_i)$ act in similar way. The number of the quadrature points $\mathbf{R}_i$ at the internal boundaries between the areas becomes the size of the problem to be solved numerically.

We formulate the coarse grain method which is based on idea of successive propagation through the device. In scope of this method the computational domain is allowed to grow by adding small open areas one by one. In the course of propagation the current I_i and displacement field

$D_n(\mathbf{R}_i)$ at the internal boundaries can be computed successively and the computational time scales linearly with the device volume.

As a test, we calculate ballistic quantum transport in 3D Double Gate and Gate-All-Around MOSFETs shown on Figures 2a and 3a. Their I-V characteristics are compared on Figure 4. In the case of Gate-All-Around geometry better control of the potential in the gate area (see Figs. 2b and 3b) improves the device performance. In particular, we have obtained the subthreshold swing close to the ideal value 60 mV/d.

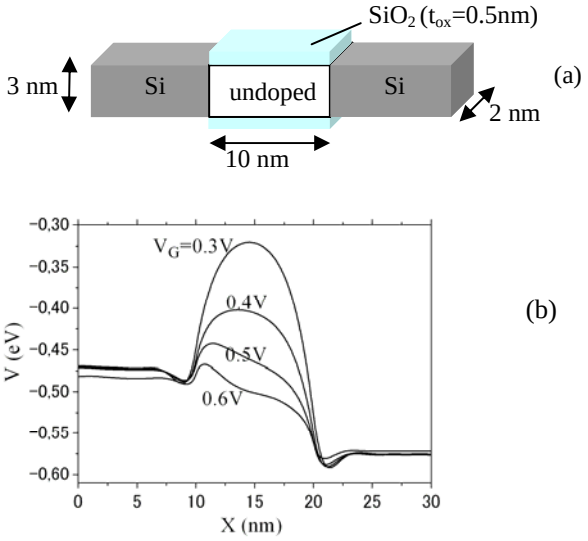

Fig. 2 (a)3D Double Gate MOSFET; (b) The potential profile along the current direction for V_{SD}=0.1 V and V_G=0.3-0.6 V.

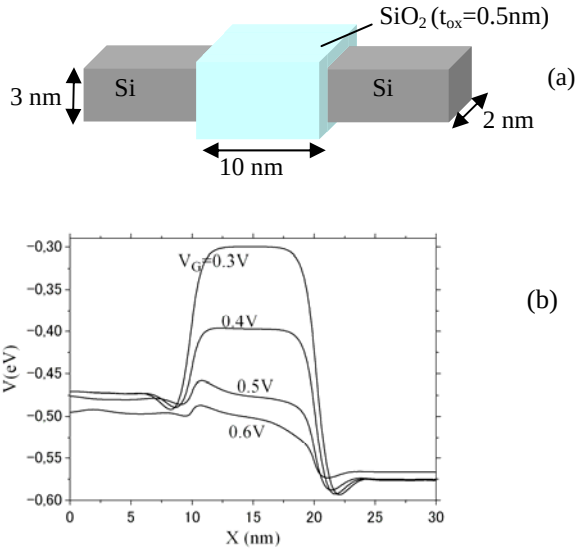

Fig. 3 (a)3D Gate-All-Around MOSFET; (b) The potential profile along the current direction for V_{SD}=0.1 V and V_G=0.3-0.6 V.

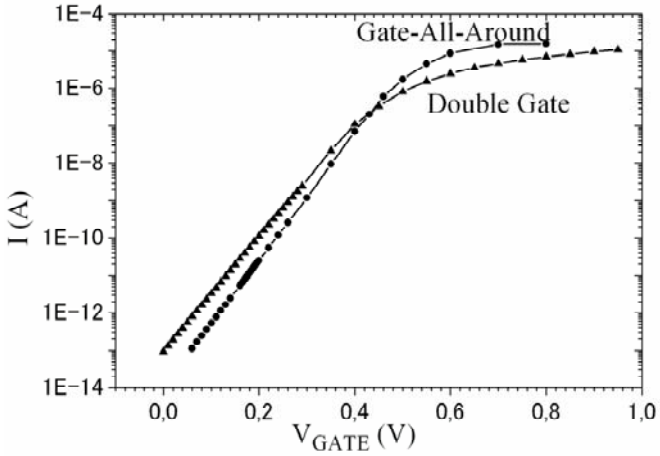

Fig. 4 Drain current in 3D Double Gate and Gate-all-Around MOSFETs as a function of the gate voltage. The applied bias is 0.1 V.

The present method greatly facilitates quantum simulations. Thus, one loop of iteration includes solving the Poisson equation followed by calculation of the Green's function, corresponding self-energies and carrier density. Computing the current on Fig.4 with 4 significant digits of accuracy takes only 4-5 sec/one loop on a workstation (Opteron 254 2.8GHz).

Conclusion

We have derived continuous basis representation of the Green's function in open system and formulated the numerical method which: 1) greatly reduces the computational size compared to the grid method, 2) splits the device into a set of simple elements which are treated independently, 3) propagate physical solutions through the device in any desired way. As a result, the major portion of the computations does not depend on the device size. This also enables one to treat realistic random charge distribution exactly by using appropriate shape of the elements and their internal coordinate representation. With the present method, 3D Quantum NEGF simulations are easily carried out on personal computer.

Acknowledgements

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