Fast Uncoupled Mode Space Approach for Nano-Scale Device Simulation Based on Bridge-Function Pseudo-Spectral Method

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1 Introduction

Miniaturization of metal-oxide field-effect-transistors (MOSFETs) has been aggressively accelerated and they have become as small as a few tens nm regime. It has been very difficult to fabricate such ultra small devices in small turn-around time within reasonable fabrication cost. Therefore, it is essential to develop a device simulator which predicts the device performances with possible quantum mechanical effects for the new era of nano-scale devices, which allows us to develop the LSI technology with conventional pace.

A non-equilibrium Green's function (NEGF) is one of the attracting methods for such quantum device simulations, since it can take into account both quantum mechanical effects and open boundary conditions. It is solved with Poisson's equation self-consistently. A real-space method (RSM) for solving the NEGF is considered to be suitable for accurate simulations. However, the RSM requires quite expensive computational costs and is difficult to apply for large-scale calculation physical model. On the other hand, in a mode space method (MSM), the transverse spatial coordinate system is replaced by the corresponding eigenmode energies and only 2D Schrödinger equation has to be solved in each cross-section of the device along the channel direction. The MSM for solving the NEGF transport equations can greatly save the computational resources. Although the MSM could reduce the computational time, in the actual numerical simulations, conventional discretized schemes, *i.e.*, a finite difference method (FDM) or a finite element method (FEM) are still inappropriate for large-scale calculation without loss of accuracy.

In this paper, we have adopted a perturbative treatment, namely, a fast uncoupled mode space approach (FUMS)[1] into our previous *Bridge-Function Pseudospectral Method* (BPSM) [2] to reduce further the computational time. This method (FUMS-BPSM) enables us to calculate much faster than our previous method, retaining high accuracy. We have affirmed that we can calculate more accurately and faster than FDM or FEM by using BPSM, CPU time for calculation by the BPSM is 60 times faster than that of FDM.

2 Theory

2.1 Bridge-Function-PseudoSpectral-Method (BPSM)

The BPSM is composed of the bridge-functions, connections of two Lagrange polynomials (Fig.1) and the Gauss-Lobatto quandrature [3]. The continuity of electrical flux density and probability current density, which appear in Poisson's equation and NEGF, respectively, are naturally guaranteed by the bridge-function (solid line) at any boundaries. The fact enables us to take the boundary conditions into account in much easier manner than the conventional PSMs. In addition, the FUMS is easily implemented in the BPSM formalism.

2.2 Fast-Uncoupled-Mode-Space-approach (FUMS)

An uncoupled mode space approach (UMS) [1] requires to solve the 2D Schrödinger equation-1D NEGF calculation repeatedly on each cross-section of the device under consideration. Because of that, it is found that the computational costs and time rapidly increase as the number of longitudinal mesh points increase. On the other hand, in the FUMS approach, the subband profile is approximated up to the first order by considering the change from the average of potential profile as the perturbation. Here, we have only to solve the non-perturbative Schrödinger equation once in the coupled 2D Schrödinger equation-1D NEGF calculation, even when the number of longitudinal mesh points increase.

3 Results and discussions

In order to show the superiority of the present method (FUMS-BPSM) over our previous BPSM (UMS-BPSM: BPSM without perturbational treatment), we have applied the FUMS-BPSM to the analysis of I-V characteristics of a gate-all-around Si nano-wire MOSFET (SiNW FET) as shown in Fig. 2 [4]. In the analysis, Schrödinger-Poisson equations and NEGF are solved simultaneously and self-consistently. The orientation dependent effective masses in the conduction band of Si are also taken into account.

Figure 3 and 4 show the local density of states and the first five subband profiles along the channel calculated by the UMS-BPSM (Fig.3) and FUMS-BPSM (Fig.4), respectively. In both figures, quantum interferences and tunneling effects can be observed. It should be noteworthy that the results of the FUMS-BPSM coincide quite well with those of the UMS-BPSM, in spite of the fact that Schrödinger equation is solved only once in the latter method.

In Fig. 5, the comparison of the computational time is shown to obtain the subband profiles with increasing longitudinal nodal number N_x. The result of the UMS-BPSM (blue line) increases linearly as N_x increases, whereas the FUMS-BPSM (green line) keeps constant, practically. The

present FUMS-BPSM remarkably shows that it is 20 times faster than the previous UMS-BPSM on the same computational platform. This is mainly because, as mentioned above, Schrödinger equation needs to be solved only one time in the present method even when N_x increases.

4 Conclusion

We have developed a fast-uncoupled mode-space bridge-function pseudo-spectral method (FUMS-BPSM) for nano-scaled device simulation where quantum effects are fully taken into account.

As a result, it is found that the FUMS-BPSM reduces the simulation time while keeping computational accuracy. Therefore, the present FUMS-BPSM can be an efficient simulation method for the nano-scale devices.

References

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[4] S. Bangsaruntip, A. Majumdar, and J.W. Sleight, "Gate-all-around silicon nanowire," 2010 Symposium on VLSI Technology Digest, p.21, 2010.

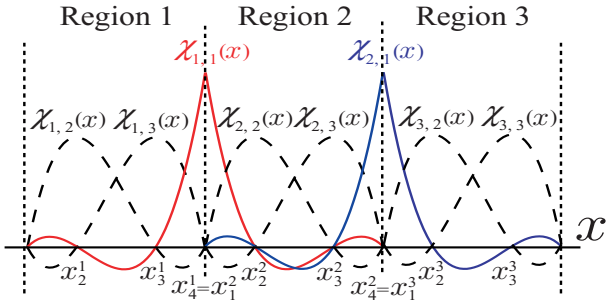

Fig. 1. 1D basis functions $\chi_{i,m}(x)$ ($i = 3$ and $m = 3$), where i indicates the region, and m the basis. The solid lines are the *bridge functions*, which ensure the continuity of any physical quantities between the adjacent regions.

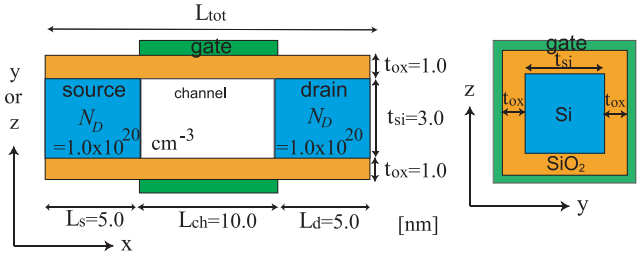

Fig. 2. Model structure of a SiNW MOSFET[4] under investigation. The channel orientation is along ⟨100⟩.

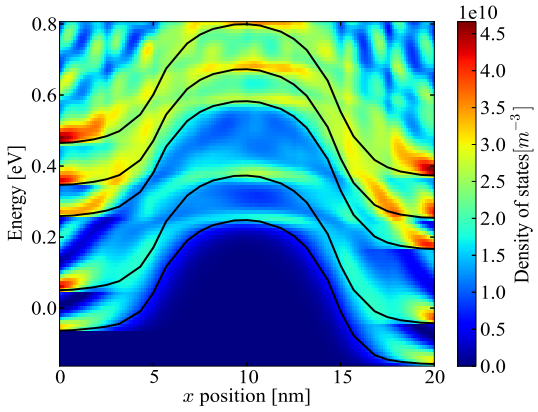

Fig. 3. The computed local density of states and electron subbands (solid lines) of SiNW FET (source region is located from $x = 0$ to 5 nm, channel is $x = 5$ to 15 nm, drain is $x = 15$ to 20 nm) by FUMS-BPSM($V_g = 0.1$ and $V_d = 0.1$ V).

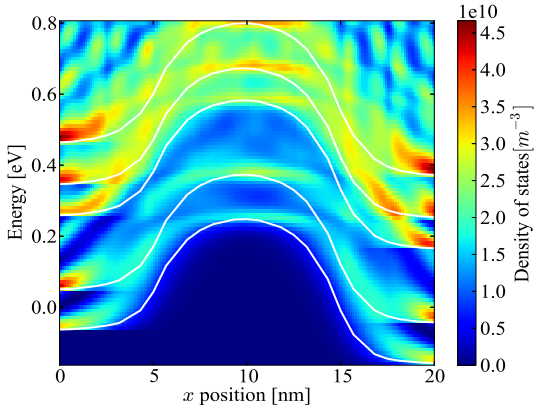

Fig. 4. The computed local density of states and electron subbands (solid lines) of SiNW FET (source region is located from $x = 0$ to 5 nm, channel is $x = 5$ to 15 nm, drain is $x = 15$ to 20 nm) by FUMS-BPSM($V_g = 0.1$ and $V_d = 0.1$ V).

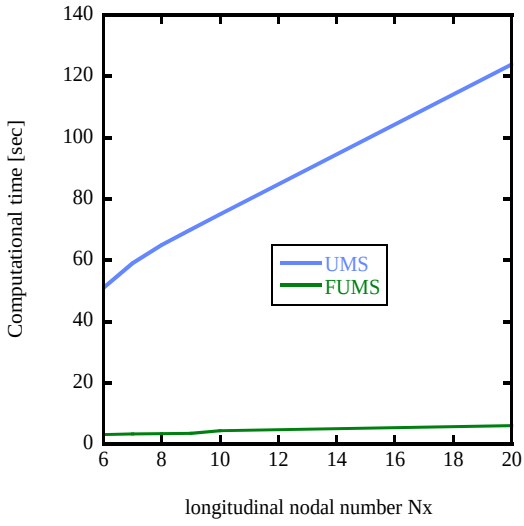

Fig. 5. The computational time for solving Schrödinger equation at $V_g = 0.1$ V $V_d = 0.1$ V, increasing the longitudinal nodal number N_x.