Improved Convergence Behavior of Real-Space NEGF Solvers Using Linear Responses of Green Functions

Phil-Hun Ahn and Sung-Min Hong
School of Electrical Engineering and Computer Science, Gwangju Institute of Science and Technology,
123 Cheomdan-gwagiro (Oryong-dong), Buk-gu, Gwangju, 61005, Republic of Korea
E-mail: smhong@gist.ac.kr

Abstract

In this work, a coupled scheme for solving the Non-equilibrium Green function (NEGF) equations and the Poisson equation is presented. The linear response of the electron density to a potential perturbation is rigorously calculated with the first order correction of Green functions. As an example, the real-space NEGF simulation is conducted for a double-gate MOSFET. Compared to the conventional Gummel type method, the coupled scheme exhibits better convergence behavior.

Introduction

The NEGF method [1],[2] is a standard approach to consider the quantum transport in the nanoscale devices. However, it is well known that its convergence behavior is much worse than that of the conventional device simulation. In the case of solvers for the Boltzmann transport equation (BTE), which is the governing equation of the semi-classical transport, there have been reports to obtain the quadratic convergence behavior [3],[4]. Unfortunately, in the case of the NEGF, it is difficult to find such an attempt.

In this work, it is presented that we can improve the convergence behavior by employing a coupled scheme for the NEGF and Poisson equations. An example of a two-dimensional double-gate MOSFET is shown. The well-established AC NEGF theory [5],[6] is used in order to evaluate the linear response of Green functions with respect to a potential perturbation.

Methodology

In the proposed method, the AC Green functions are used to consider the linear response with respect to a potential perturbation. The AC Green functions can be obtained from the DC Green functions and the DC self-energy functions [5],[6]. The DC Green function is calculated by solving the equations in [2],[7]. The two-dimensional real-space NEGF is used in this work.

For the coupled implementation, with the discretized form, a set of the linear equations can be written as:

$$\phi(\boldsymbol{r}) + \delta\phi(\boldsymbol{r}) - \phi_{fixed}(\boldsymbol{r}) = \sum_{\boldsymbol{r}' \in \beta} \frac{\partial \phi(\boldsymbol{r})}{\partial n(\boldsymbol{r}')} [\, n(\boldsymbol{r}') + \delta n(\boldsymbol{r}') \,] \qquad (\boldsymbol{r} \in \alpha) \quad (1)$$

$$\delta n(\boldsymbol{r}'') = \sum_{\boldsymbol{r}''' \in \beta} \frac{\partial n(\boldsymbol{r}'')}{\partial \phi(\boldsymbol{r}''')} \phi(\boldsymbol{r}''') \qquad (\boldsymbol{r}'' \in \beta) \quad (2)$$

where α index represents the entire device region, while β index indicates only the silicon region. $\phi(\boldsymbol{r})$ and $n(\boldsymbol{r})$ indicate the electronstatic potential and electron density, respectively. $\delta\phi(\boldsymbol{r})$ and $\delta n(\boldsymbol{r})$ represent the update of unknown variables. They are obtained by solving (1) and (2) together. ϕ_{fixed} is calculated from the Poisson equation only with the boundary conditions and dopant profile. In (1), $\frac{\partial \phi(\boldsymbol{r})}{\partial n(\boldsymbol{r}')}$ can be obtained from the potential response due to the electron perturbation at nodes in the silicon region, by solving the Poisson equation. Similarly, $\frac{\partial n(\boldsymbol{r}'')}{\partial \phi(\boldsymbol{r}''')}$ in (2) can be obtained from the electron response due to the potential perturbation at the nodes. It can be easily calculated from the AC Green functions. For the next Newton iteration, the potential is updated with $\delta\phi(\boldsymbol{r})$:

$$\phi^{(k+1)}(\boldsymbol{r}) = \phi^{(k)}(\boldsymbol{r}) + \delta\phi^{(k)}(\boldsymbol{r}) \,, \qquad (\boldsymbol{r} \in \alpha) \quad (3)$$

while the electron density is recalculated under the updated potential profile. In order to prevent the divergence, a few iterations using the conventional Gummel type method are performed before the proposed coupled scheme is applied, as in [3].

Numerical Result : Coupled-Method

For the demonstration, a two-dimensional double-gate MOSFET (as illustrated in Fig. 1) is simulated. It is stressed that the proposed method can be applied to the three-dimensional devices without any modification. Thickness of the silicon substrate is 5 nm. The length of the channel, drain, and source regions is equal to 5 nm. The source and drain regions are heavily doped with donors, while the channel region is intrinsic. Semi-infinite leads are assumed [7]. The simulation code has been implemented under the ballistic transport and effective mass approximations. The oxide penetration is neglected. The DC IV result from the real-space NEGF code is shown in Fig. 2. For the verification, the result from a tool in nanoHUB (NanoMOS) is compared [8].

In Fig. 3, the physical quantities from the proposed method and the conventional Gummel type method are shown. The drain bias is fixed to 0.2 V. In Fig. 4, the potential update at each Newton iteration is shown. Rapid reduction of the update vector can be clearly observed. The convergence behaviors of the two methods are shown in Fig. 5. The conventional Gummel type method exhibits poor convergence behavior. On the other hand, the proposed method shows a faster decrease in errors. Fig .6 shows a case where the proposed method is directly applied without a few stabilizing Gummel iterations. Even in this case, the convergence has been obtained without difficulty.

Conclusions

In summary, the improvement of convergence by the coupled method when implementing NEGF has been demonstrated for a two-dimensional double-gate MOSFET. The result shows that the better convergence can be achieved by considering the linear response of Green functions. Moreover, it is expected that the quadratic convergence can be achieved when the AC contact self-energy functions are also fully considered in the calculation. When the scattering is concerned for the calculation, the simulation time is expected to be reduced remarkably.

References

[1] S. Datta, *Superlattices and Microstructures*, vol. 28, pp. 253-278, 2000.

[2] S. Datta, *Quantum Transport: Atom to Transistor*. Cambridge University Press, 2005

[3] D. Ruic and C. Jungemann, *SISPAD*, p. 356-359, 2013

[4] M. Noei and C. Jungemann, *SISPAD*, p. 15-18, 2016

[5] Y. Wei and J. Wang, *PRB*, vol. 79, p. 195315, 2009.

[6] O. Shevtsov and X. Waintal, *PRB*, vol. 87, p. 085304, 2013

[7] R. Venugopal, et al, *Journal or Applied physics*, vol. 92, no. 7, pp. 3730-3739, 2002

[8] Z. Ren, et al, "NanoMOS", 2016, Available: https://nanohub.org/resources/nanomos

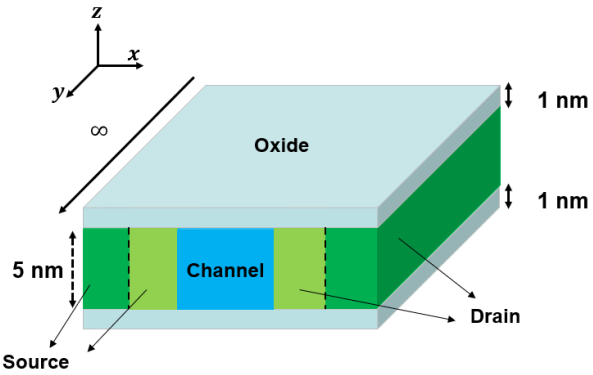

Figure 1. Double-gate MOSFET under simulation. The drain/source regions have a step-like doping profile ($2 \times 10^{20}\text{cm}^{-3}$ and $2 \times 10^{19}\text{cm}^{-3}$).

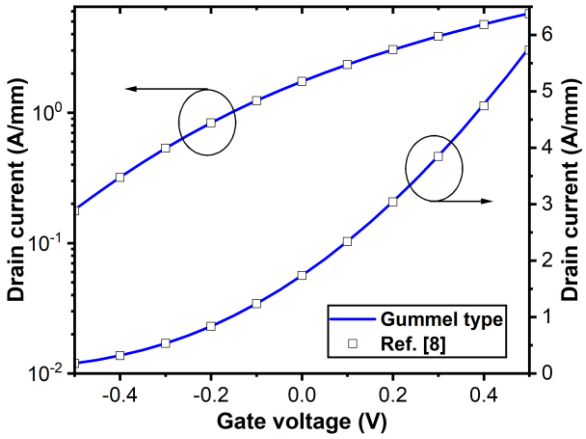

Figure 2. I_D-V_G graph when the drain voltage is 0.2 V. The result from a tool in nanoHUB (NanoMOS) is compared for verification.

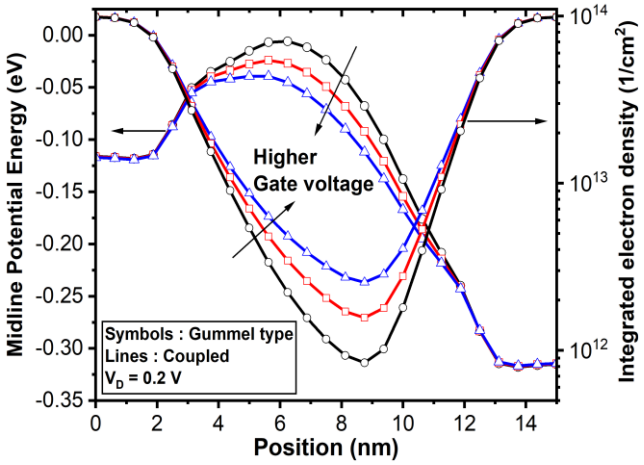

Figure 3. Intergrated electron density and potential along the channel. The black, red, and blue lines represent gate biases of 0.1V, 0.2V and 0.3V, respectively. $V_D = 0.2$ V.

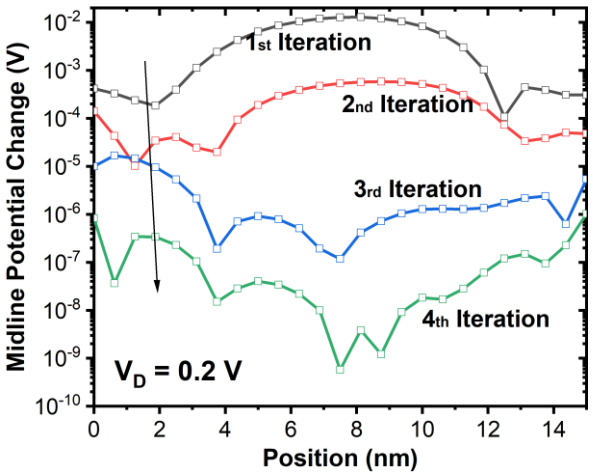

Figure 4. Potential update at each Newton iteration. $V_G = 0.2$ V and $V_D = 0.2$ V. The coupled method is directly used without any stabilizing Gummel iteration.

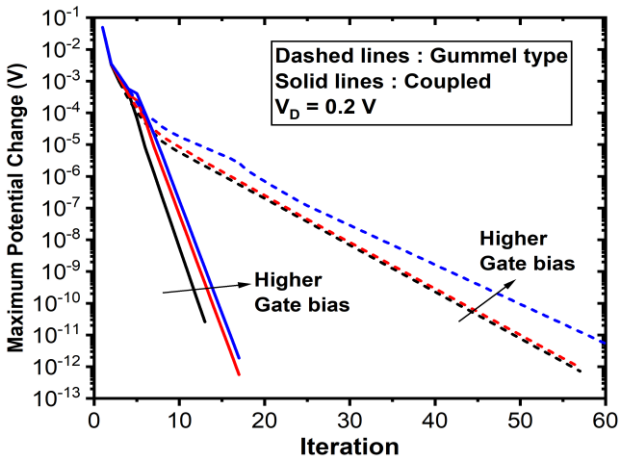

Figure 5. Maximum absolute change of the electrostatic potential. The black, red, and blue lines represent gate biases of 0.1V, 0.2V and 0.3V, respectively. $V_D = 0.2$ V.

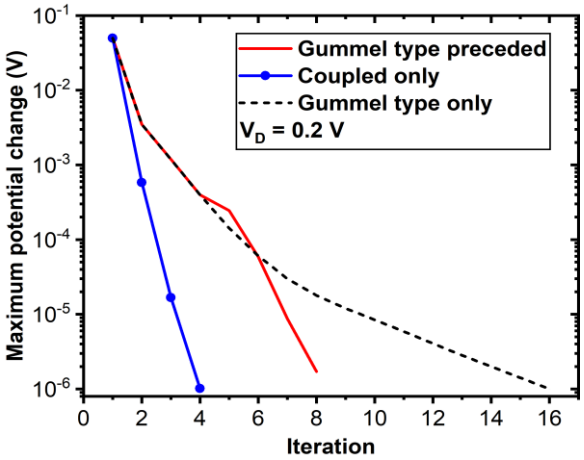

Figure 6. Maximum absolute change of potential. The solid red line is for a case where the coupled method is used after a few Gummel type iterations. In the blue line, the coupled mthod is used directly. The black dashed line is for the conventional Gummel type method. $V_G = 0.2$ V and $V_D = 0.2$ V.