# Efficient TB-NEGF Simulations of Ultra-Thin Body Tunnel FETs

Woo Jin Jeong, Junbeom Seo, and Mincheol Shin School of Electrical Engineering Korea Advanced Institute of Science and Technology Daejeon, Republic of Korea wjjeong@kaist.ac.kr, jbseo@kaist.ac.kr, mshin@kaist.ac.kr

Abstract—InAs ultra-thin-body (UTB) tunnel FETs (TFETs) are investigated by the  $sp^3d^5s^*$  spin-on tight-binding (TB) method. We have successively implemented the reduced transformation for the TB Hamiltonian and thus highly efficient quantum-mechanical calculations based on the non-equilibrium Green's function method are made possible. Simulations of the UTB devices with body thickness up to 10nm are performed. Full quantum transport calculations by using the full TB Hamiltonian and reduced-sized mode-space Hamiltonian agree very well, while the agreement between the two depends on both the energy range for extracting the basis set and the band-to-band tunneling energy range of TFETs.

Keywords— Empirical tight-binding, Ultra-thin body, Tunnel FET, Quantum transport, Non-equilibrium Green's function, Modespace transformation

#### I. INTRODUCTION

Device performances of tunnel FETs (TFETs), which are considered as one of the most promising candidates for low power electronics, sensitively depend on the band gap and the tunneling effective mass of the material [1]. The atomistic quantum transport simulation is therefore essential for accurate prediction of the TFET performance [2] and the empirical tight-binding (TB) method is regarded most suitable for the purpose [3-5]. However, there are large constraints in dealing with realistically-sized devices by the TB method due to huge computational burden [5].

A solution to the problem is to extract only the transport modes that contribute to the current within a pre-specified energy range and thereby construct a reduced-sized, modespace Hamiltonian. The basic idea of the mode-space approach is to reduce the basis set of a Hamiltonian of rank N to that of rank n ( $n \ll N$ ) by a unitary transformation. For the TB Hamiltonian, unphysical states inevitably appear in the basis reduction process. Recently, a novel scheme to remove the unphysical states, called the equivalent transport model (EM) [6], has been introduced and successfully applied to simulations of Si nanowire transistors.

In this work, we have successfully implemented the EM method for ultra-thin body (UTB) TFETs. Using the  $sp^3d^5s^*$  TB method with spin orbit coupling, devices from 1 nm up to 10 nm thickness were simulated, which is unprecedented



Fig. 1. The process of the mode-space Hamiltonians construction from the full TB Hamiltonians in the UTB device.

considering the size of the device Hamiltonian. The ballistic transport are then calculated by self-consistently solving non-equilibrium Green's function (NEGF) and Poisson's equation. Our main contribution of this work is to have developed an efficient scheme to systematically construct the mode-space Hamiltonian for each  $k_y$ , where  $k_y$  is the wave vector in the periodic direction, and applied to UTB TFETs of large size.

### II. APPROACH

The EM method is applied for the UTB device simulations as follows. See Fig. 1 shows for the flow chart. 1) The electronic band structure by using the full TB Hamiltonian, H, is first calculated. 2) The unitary transformation matrix,  $U(k_y)$ , is constructed by selecting the appropriate Bloch states from the full electronic band [6]. The Bloch states are selected within the energy range (ER) by using the scheme in Ref. [7]. (3) If the spurious states appear in the band structures calculated by using



Fig. 2. Schematic diagram of the double-gate InAs UTB TFET. The channel length  $L_{ch} = 15$  nm and equivalent oxide thickness 0.5nm. The source and drain region are p-doped and n-doped with  $5 \times 10^{19}$  cm<sup>-3</sup>, respectively.



Fig. 3. The band structures calculated by using the full TB Hamiltonian (black solid lines) and mode-space Hamiltonian (red circle symbols) for  $T_{ch} = 4$  nm. ER = (a) 0.5, (b) 1.0, and (c) 1.5 eV for  $k_y = 0$ . (d) ER = 1.5 eV for  $k_y = 2.305 (1/nm)$ .

the mode-space Hamiltonian,  $H_m(k_y)$ , they are removed by the scheme proposed in Ref. [6]. Steps (1) – (3) are performed independently for each  $k_y$  where  $-\frac{\pi}{u_y} < k_y < \frac{\pi}{u_y}$  ( $u_y$  is the length of the unit cell in the periodic direction). (4) Each of the reduced-sized, mode-space Hamiltonian,  $H_m(k_y)$ , is then imported into the Schrodinger-Poisson solver where the NEGF approach for the current and charge densities are employed.

#### III. RESULTS

The ballistic transport characteristics of (100)/<100> InAs UTB-TFET shown in Fig. 2 are studied in this work. The channel thickness is varied from  $T_{ch} = 0.91$  nm to 10 nm. The channel length  $L_{ch}$  is 15 nm and the equivalent oxide thickness 0.5nm (the oxide thickness  $T_{ox}$  is set to 1.6 nm with the relative dielectric constant of 12.7). The source and drain regions are heavily doped with the concentrations of  $N_s = 5 \times 10^{19}$  cm<sup>-3</sup> (p-type) and  $N_d = 5 \times 10^{19}$  cm<sup>-3</sup> (n-type), respectively, and the channel is intrinsic. The drain bias  $V_{DS}$  of 0.5 V is applied.

Figs. 3 (a) - (c) show the band structures by using the reducedsized, mode-space Hamiltonian for  $T_{ch} = 4$  nm, as ER is



Fig. 4. (a) The reduced mode-space Hamiltonian size as a function of  $k_y$  and (b) the transfer characteristics at  $V_{DS} = 0.5$  V for  $T_{ch} = 0.91$  nm for selected values of ER.

gradually expanded from 0.5 to 1.5 eV. In each figure, it can be seen that the band structure by using the mode-space Hamiltonian excellently match with that by using the full Hamiltonian within the energy window specified by ER. Fig. 3 (d) demonstrates the band structures at an off gamma point  $(k_y = 2.305 nm^{-1})$  calculated by the mode-space Hamiltonian.

Fig. 4 (a) shows the size of the mode-space Hamiltonian matrix for each  $k_y$  of a UTB TFET of  $T_{ch} = 0.91$  nm. As the ER is widened, the mode-space Hamiltonian size tends to increase since the number of the extracted basis is increased (See Figs. 3 (a)-(c)). Occasionally, it does not follow this trend at some  $k_y$  values in Fig. 4 (a) because the variational functional method is applied in the process of obtaining the mode-space Hamiltonian [6]. For the same reason, the size of the mode-space Hamiltonians of the same device structure may slightly vary depending on the detailed conditions for selecting



Fig. 5. The relative error of (a)  $|I_{Full} - I_{ER=0.3 \text{ eV}(0.5 \text{ eV},0.7 \text{ eV})}|$   $/I_{Full}$  for  $T_{ch} = 0.91$  nm and (b)  $|I_{ER=1.5 \text{ eV}} - I_{ER=0.5 \text{ eV}(1.0 \text{ eV})}|$   $/I_{ER=1.5 \text{ eV}}$  for  $T_{ch} = 4$  nm.



Fig. 6. (a, c) Band edge profiles and energy current spectrum for selected values of ER (a, b) at  $V_{DS} = 0.5$  V and  $V_G = 0.6$  V for  $T_{ch} = 0.91$  nm and (c, d) at on-state (solid-lines) and ambipolar state (dashed lines) for  $T_{ch} = 4$  nm, respectively. The relative error in energy-current density compared to that of (b) full TB and (d) ER = 1.5 eV.

the initial Bloch states.

The calculated transfer characteristics are shown in Fig. 4 (b). Although the Hamiltonian sizes are greatly reduced to less than 40, it can be seen in the figure that if  $ER \ge BTR$  (=0.64 eV), where BTR is the band-to-band-tunneling energy range, the mode-space calculation results almost overlap with that of the full TB calculation. See Fig. 5 for the relative errors in the total



Fig. 7. (a) The Hamiltonian size reduction ratio as a function of  $T_{ch}$ . ER is set to 1.0eV. (b) The BTBT range with respect to  $T_{ch}$  and  $V_{DS} = 0.5$  V. (c) The  $I_{OFF}$  and  $I_{ON}/I_{OFF}$  as a function of  $T_{ch}$  for  $V_{DS} = 0.5$  V.

current by the ER values. In Figs. 5 (a) and (b), the transfer characteristics are compared to the full Hamiltonian for  $T_{ch} = 0.91$  nm and the mode-space Hamiltonian with ER > BTR for  $T_{ch} = 4.0$  nm, respectively. We conclude that, if the condition of ER > BTR is satisfied, the transport calculations by the mode-space Hamiltonian is accurate within less than 5 %.

The energy-current spectra are shown in Figs. 6 (a) for  $T_{ch} = 0.91$  nm and (c) for  $T_{ch} = 4.0$  nm, respectively. Fig. 6 (b) and (d) show the relative errors for the current levels (> 1 × 10<sup>-6</sup> A/eV and > 0.1 A/eV, respectively) and the peaky features explain the source of errors for the case of ER < BTR. We therefore find that the error in the current density occurs near the BTR boundary if insufficient ER is taken.

Fig. 7 (a) shows the Hamiltonian size reduction ratio as a function of  $T_{ch}$ . The ER is set to 1.0 eV that is close to or greater than BTR at  $V_{DS} = 0.5$  V as shown in Fig. 7 (b). The Hamiltonian size is reduced to ~ 10% of the original size: for instance, the matrix size for  $T_{ch} = 10$  nm is reduced from 2680 x 2680 to 267 x 267, greatly alleviating the computational burden. Fig. 7 (c) shows OFF currents ( $I_{OFF}$ ) and ON/OFF current ratio ( $I_{ON} / I_{OFF}$ ) as a function of channel thickness. The  $I_{ON} / I_{OFF}$  improves with decreasing  $T_{ch}$  thanks to the widened band gap by the quantization effect.

## IV. CONCLUSION

We have developed a highly efficient method for atomistic simulations of UTB TFETs, based on the equivalent transport model or the reduced basis transformation method. For the TFET simulations, it is found that the energy range in the band structure for the Hamiltonian size reduction should cover the entire range of the band-to-band-tunneling. This makes the present method less efficient compared to the cases where only the conduction band (n-type devices) or valence band (p-type devices) is considered. Nevertheless, the Hamiltonian size is reduced to about 10 % of its original size, which makes it possible to simulate UTB TFETs of up to 10 nm in thickness with 20 TB orbitals per atom.

#### ACKNOWLEDGEMENT

This research was supported by the Pioneer Research Center Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (Grant No.NRF-2011-0027906).

#### REFERENCES

- A. C. Seabaugh and Z. Qin, "Low-Voltage Tunnel Transistors for Beyond CMOS Logic," Proc. IEEE, vol. 98, pp. 2095-2110, 2010.
- [2] D. Basu, R. Kotlyar, C. E. Weber, and M. A. Stettler, "Ballistic Band-to-Band Tunneling in the OFF State in InGaAs MOSFETs," *IEEE Trans. Electron Devices*, vol. 61, pp. 3417-3422, 2014.
- [3] M. Luisier, "Performance Comparison of GaSb, Strained-Si, and InGaAs Double-Gate Ultrathin-Body n-FETs," *IEEE Electron Device Lett.*, vol. 32, pp. 1686-1688, 2011.
- [4] Y. Liu, N. Neophytou, T. Low, G. Klimeck, and M. S. Lundstrom, "A Tight-Binding Study of the Ballistic Injection Velocity for Ultrathin-Body SOI MOSFETs," *IEEE Trans. Electron Devices*, vol. 55, pp. 866-871, 2008.
- [5] M. Luisier and A. Schenk, "Atomistic Simulation of Nanowire Transistors," J. Comput. Theor. Nanosci., vol. 5, pp. 1031-1045, 2008.
- [6] G. Mil'nikov, N. Mori, and Y. Kamakura, "Equivalent transport models in atomistic quantum wires," *Phys. Rev. B*, vol. 85, p. 035317, Jan, 2012.
- [7] M. Shin, W. J. Jeong, and J. Lee, "Density functional theory based simulations of silicon nanowire field effect transistors," *J. Appl. Phys.*, vol. 119, p. 154505, 2016.