An Efficient Method for Atomistic-Level Non-Equilibrium Green's Function Simulations of Field-Effect Transistors involving Heterojunctions

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The device structure consisting of heteromaterials is being widely considered for the future field-effect transistors (FETs) such as tunneling FETs (TFETs) and Schottky barrier FETs. In order to properly describe the band gap and band offsets and to naturally capture the interface effects at heterojunctions, it is essential to model the heterostructure FETs in the atomistic level. Therefore, a density functional theory (DFT) based approach is called for. A recently developed framework where the DFT and non-equilibrium Green's function (NEGF) parts are performed sequentially provides a practical simulation platform [1], but when it comes to its application to heterostructure FETs, the large size of the junction Hamiltonians becomes the main obstacle to efficient NEGF simulations. This work presents a methodology to reduce the computational burden in the NEGF part. The main idea is to employ the recursive Green's function (RGF) method [2] for homogeneous unit cells and the R-matrix method [3] for the junction parts in a heterostructure FET, respectively (Fig. 1), to calculate the retarded Green's functions. For this purpose, we have extended the R-matrix algorithm to open boundary device. To assess the computational efficiency of the proposed RGF+R-matrix approach, we have measured the elapsed CPU time (Fig. 2) for calculating the retarded Green's functions of four two-dimensional heterostructures. The calculated transmission functions for the four heterostructures (Fig. 3) show the exactness of the computed retarded Green's functions. Our RGF+R-matrix method is numerically efficient for atomistic-level NEGF simulations of hetero-FETs. As an application, the self-consistent simulations of NEGF and Poisson equation have been performed for germanane/InSe vertical TFET (Fig. 4) using the RGF+R-matrix approach. It can be seen in Fig. 5 that the band-to-band tunneling occurs when the conduction band is lowered below the valence band, leading to the onset of the ON-state region. The approach of this work can be applied to the device having heterojunction of three-dimensional materials, surface roughness, and atomic vacancies or dopants.

[1] M. Shin et al., J. Appl. Phys., **119**, 154505 (2016).
[2] A. Svizhenko et al., J. Appl. Phys., **91**, 2343 (2002).
[3] G. Mil'nikov et al., Phys. Rev. B, **79**, 235337 (2009).

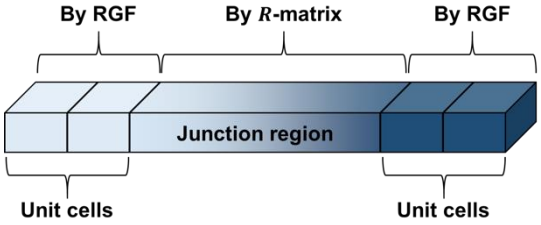

Fig.1: The concept of RGF+R-matrix method. RGF is used for the matrix calculations related to the homogeneous unit cells, while R-matrix is applied to those for the junction regions.

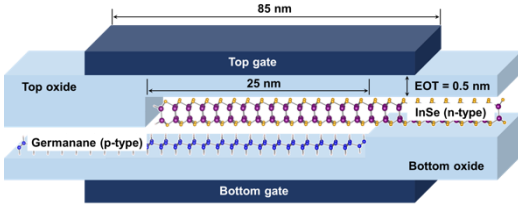

Fig.4: Schematic of the simulated germanane/InSe vertical TFET.

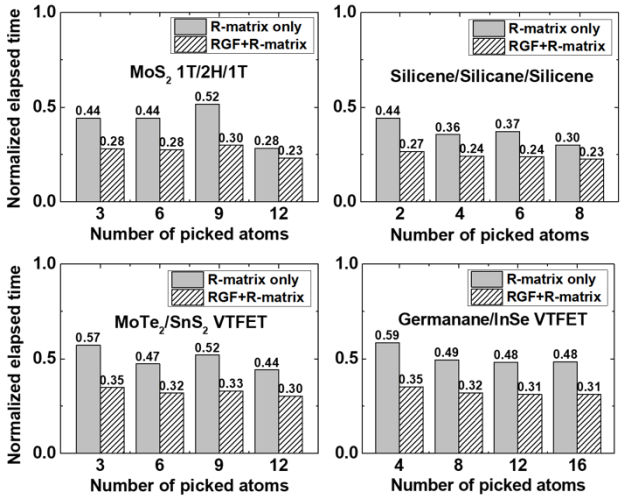

Fig.2: The elapsed CPU time per energy grid for calculating retarded Green's functions of four two-dimensional heterostructures. 1.0 is the reference elapsed time when the RGF method is used only.

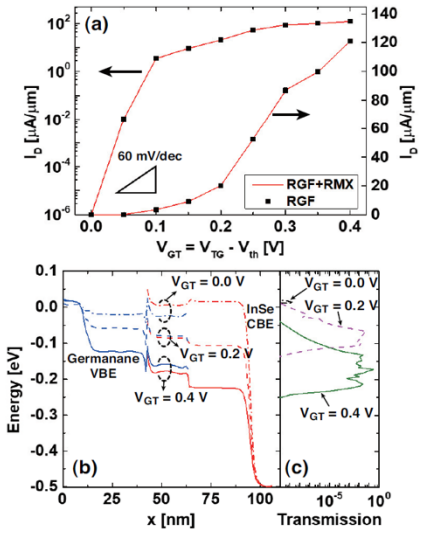

Fig.5 (a) Transfer characteristics of the simulated germanane/InSe vertical TFET at drain voltage of 0.4 V and top gate voltage (V_{TG}) of -0.8 V. Threshold voltage (V_{th}) is defined such that off-state current is 10^{-6} μA/μm. (b) Band edge profile and (c) transmission (log scale) of the simulated vertical TFET at various top gate voltages. V_{GT} denotes V_{TG}-V_{th}.

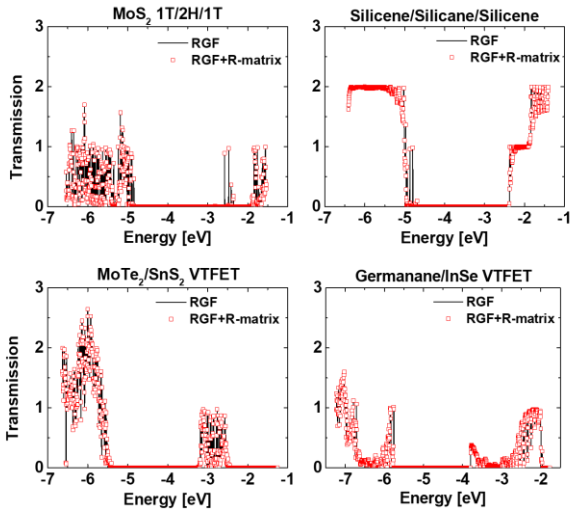

Fig.3: The transmission functions of the simulated heterostructures.