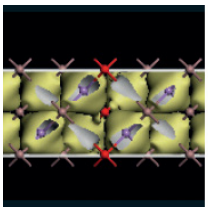

Equivalent model representation in first-principle transport simulations of nanowire MOSFETs

G Mil'nikov[1], N Mori[1], J Iwata[2] and A Oshiyama[2]

[1]Osaka University, Japan, [2]The University of Tokyo, Japan

With continuing advances in semiconductor fabrication technology, it is predicted that the physical channel length in electronic devices will scales down to sub- 10 nm regime. Semiconductor nanowires (NWs) have been recently considered as promising novel devices to realize the scaling merit in the ultra-small scale. However, it is also anticipated that their practical implementation will face technical issues such as characteristics fluctuations. Theoretical study of the device performance of NW transistors requires detailed atomistic transport simulations based of first-principles modeling of semi- conductor nanostructures.

In this presentation, we report on our recent progress in developing a first-principle quantum transport simulator based on the real-space density functional theory (RSDFT) [1] and the Troullier-Martins pseudopotentials [2]. The RSDFT method has been shown to be applicable to large atomic clusters and nanowire structures which enables one to obtain an optimized nanostructure geometry and the Kohn-Sham Hamiltonian in the real-space representation. In this work, we utilize the *R*-matrix method [3] and perform RSDFT-based non-equilibrium Green's function (NEGF) transport simulations in ballis- tic regime

In scope of the *R*-matrix method, the computational domain is split into a set of fragments (i.e. small clusters of mesh points) and the *R*-matrix propagation algorithm is used for constructing the Green's function in the close device with no leads attached. The contact self-energies are computed independently at the end of calculation. This would generally involve a difficult numerical task of computing all the outgoing/decaying Bloch states in the leads. However, since the current is actually formed by mobile carriers in a few scattering states, one can make use of an appropriate low-dimension equivalent transport model (EM) to obtain the relevant physical solutions within a transport energy interval (Fig. 1). Small size of the EM representation greatly simplifies atomistic transport simulations [4].

We have developed a parallel computer code for con- structing the EM representation within an arbitrary finite energy interval. The primary low-dimensional atomistic basis is extracted from a set of Bloch states computed at equidistant set of *k*-points in the Brillouin zone by the FEAST method [5]. Extra basis states are further constructed by minimizing the number of branches in the electronic band structure. Effective algorithms have been developed for optimizing parameters in the variational functional [4] and choice of the initial variational state.

The numerical tests in a thin SiNW with diameter of 1 nm have confirmed applicability of the method within a wide energy range in both conduction and valence bands. Figure 2 shows an example of the EM band structure within $\sim$4 eV energy window in the SiNW. For an ideal nanostructure, the EM provides an effective quantum chain model with equivalent transport characteristics. In general case, one can still make use of the EM in the lead area in order to compute the equilibrium states in the leads and obtain the contact self-energies in the NEGF formalism. The numerical tests confirm that such mixed EM-RSDFT representation causes no unphysical reflection at the contact interfaces (Fig. 3) and describes correctly the electron transport through the device channel.

Figure 4 presents an example of calculated IV char- acteristics in a [100] NW MOSFET with 10 nm gate length and 1 nm channel diameter. In these simulations, we have assumed a continuous dielectric layer in the insulator region and used the bulk parameters to account for polarization effects in the device electrostatics. More accurate analysis would require self-consistent calculation of the polarization charge distribution in the nanostructure which can also be greatly accelerated by implementing the EM representation.

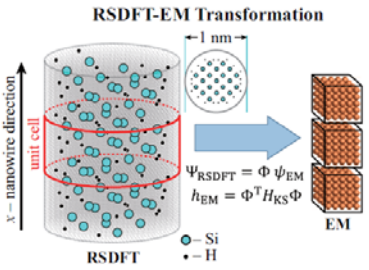

Fig. 1. EM transformation of the RSDFT Hamiltonian. The left panel shows mesh points (small gray dots) in three unit cells of a [100] Si nanowire with diameter of 1 nm. The rectangular $N_{\mathrm{RSDFT}} \times N_{\mathrm{EM}}$ real-valued basis matrix Φ is constructed in order to obtain a computationally inexpensive N_{EM}-dimensional model of a quantum chain with Hamiltonian h_{EM} which reproduces the scattering states Ψ_{RSDFT} within the transport energy interval.

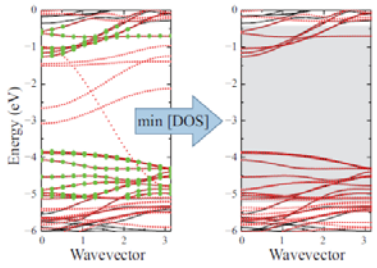

Fig. 2. Constructing the EM basis for RSDFT Hamiltonian in Fig. 1. The solid lines and small red points correspond to the exact RSDFT band structure and the EM approximation, respectively. The large green marks in the left panel represent the original set of atomistic Bloch states in the EM model with extra unphysical branches. The right panel shows the final EM band structure obtained by minimizing the number of branches (number of red points) within the shaded area.

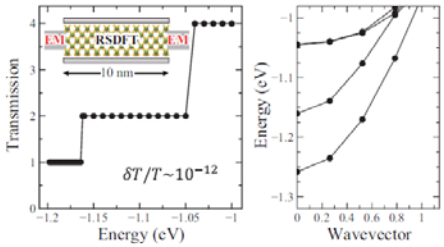

Fig. 3. Transmission function and the band structure in the SiNW in Fig. 1. The exact R-matrix is propagated through a central "device" area of 10 nm length. The EM representation is only used to compute the outgoing/decaying scattering states in the two leads and construct the contact self-energy. The computed transmission coefficient reproduces the exact (integer) values up to 12 significant digits, indicating the accuracy of the R-matrix propagation in the first-principle transport calculations.

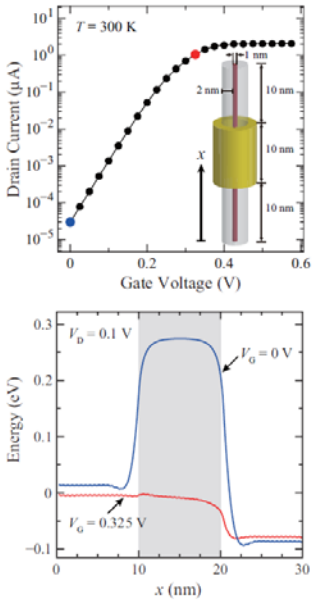

Fig. 4. Current-voltage characteristics and potential profiles in a n-SiNW MOSFET. The first-principle RSDFT method is only used in the silicon core region. The oxide layer in the gate region is treated as a continuous dielectric media, and the device electrostatics is calculated using the bulk parameters $\epsilon_{\mathrm{Si}} = 11.9$ and $\epsilon_{\mathrm{SiO_2}} = 3.8$.

[1] J.-I. Iwata, D. Takahashi, A. Oshiyama, B. Boku, K. Shiraishi, S. Okada, and K. Yabana, A massively-parallel electronicstructureccalculations based on real-space density functional theory, Journal of Computational Physics 229, 2339 (2010).

[2] N. Troullier and J. L. Martins, Efficient pseudopotentials for plane-wave calculations, Physical Review B 43, 1993 (1991).

[3] G. Mil'nikov, N. Mori, and Y. Kamakura, R-matrix method for quantum transport simulations in discrete systems, Physical Review B 79, 235337 (2009).

[4] G. Mil'nikov, N. Mori, and Y. Kamakura, Equivalent transport models in atomistic quantum wires, Physical Review B 85, 035327 (2012).

[5] E. Polizzi, Density-matrix-based algorithm for solving eigenvalue problems, Physical Review B 79, 115112 (2009).