Surface Roughness and Electron Transport Statistics in Si Nanowires

G. Mil'nikov*‡, T. Zushi†, M. Tomita†, T. Watanabe†‡, Y. Kamakura*‡, and N. Mori*‡
*Graduate School of Engineering, Osaka University, 2-1 Yamada-oka, Suita, Osaka 565-0871, Japan
†Faculty of Science and Engineering, Waseda University, Shinjiku, Tokyo 169-8555, Japan-0075, Japan
‡CREST, JST, 7 Gobancho, Chiyoda-ku, Tokyo 102-0075, Japan
gena@si.eei.eng.osaka-u.ac.jp

Semiconductor nanowires (NW) has been recently considered as promising building blocks for future nanoelectronic devices and integrated circuits. One of the key issues for their practical applications is sample-to-sample variability caused by structural disorder at the wire interface. Application of the first-principle calculations to statistical modeling in realistic NW devices is prohibitively time-consuming. In this work we analyze statistics of electron transport in Si wires with surface disorder and propose a numerically cheap approximate model for statistical transport studies.

The model under consideration has been extracted from a realistic oxidized SiNW with interface atomic disorder obtained by the MD simulations [1]. Si atoms in the core part of the wire with moderate local strain $< 3\%$ have been used to construct NW samples for our statistical analysis (Fig. 1). We use the $sp^3d^5s^*$ tight-binding (TB) Hamiltonian of a strain Si crystal [2] with H termination model for the dangling bonds and employ the NEGF formalism for transport calculations. The obtained transport data are compared with the results calculated by using the equivalent model (EM) representation [3] which is an analog of the basis expansion approach for discrete systems with arbitrary band structure. The EM method enables a small atomistic basis of most relevant modes to be extracted from the original set of atomic orbitals. In the present case, the 24D EM representation has been constructed based on a periodic reference Si wire with the averaged local strain distribution (Fig.2). The EM was found to give similar fluctuations in the band structure and well reproduce the behavior of the transmission coefficient $T(\varepsilon, L)$ along the SiNW samples (Fig. 3).

Qualitative statistical analysis has been performed by fitting the computed averaged transmission $\langle T \rangle$ and its variance $var(T)$ by the "universal" L-dependent statistics calculated from the DMPK equation (β=1) [4] or its multidimensional generalization [5] (Fig. 4). We have confirmed the quasi-one-dimensional universal statistical behavior (Fig.5) which can be characterized by a single length parameter (Fig.6). The larger fluctuations in short samples cannot be explained by the dimensionality effects and are likely to be caused by the enhanced reflection at the contacts with leads.

Our results show that the localization of the electronic states due to the surface roughness scattering is an important factor effecting the NW device performance. The universal one-parameter transport statistics also suggests that one can predict their statistical properties without time consuming transport simulations at atomistic level and the EM may provide an effective tool for statistical device modeling. This study is currently in progress.

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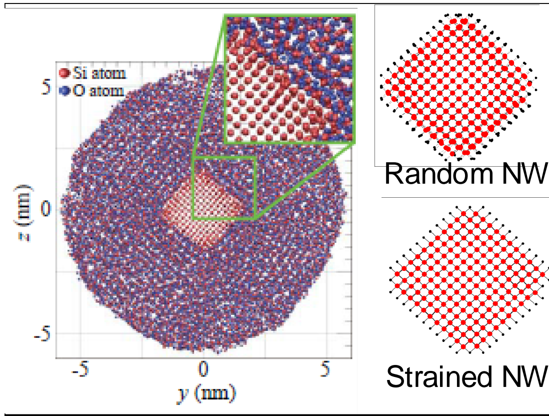

Fig. 1. Realistic nanostructure obtained in the MD simulations. The right panels show the core part of the wire used in the present simulations and the corresponding periodic NW with averaged strain.

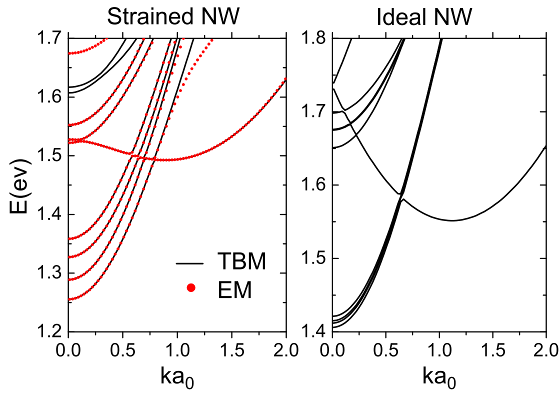

Fig. 2. The band structure in the strained NW in Fig. 1. The dots correspond to the 24D EM for the bottom part of the conduction band within $\sim$ 0.3 eV energy interval. The band structure in the corresponding ideal [100] SiNW is shown for comparison.

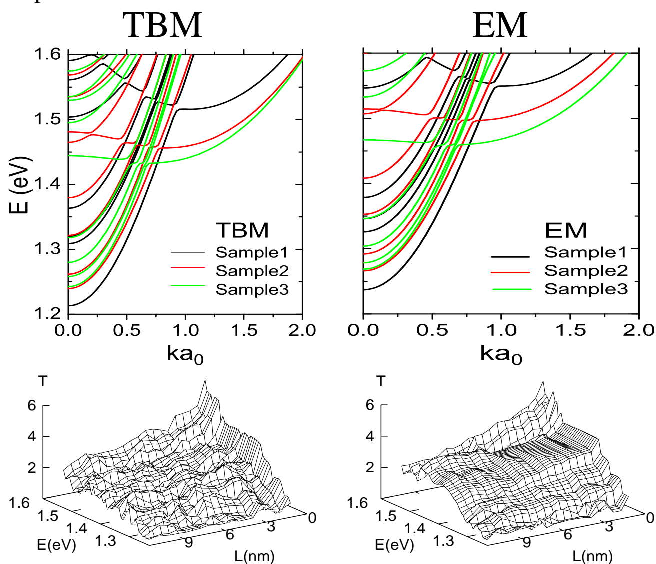

Fig. 3. Fluctuation of the band structure calculated by taking various blocks of the random wire (upper panels) and transmission function in a sample composed from such blocks (lower panels) in the TBM and EM representation.

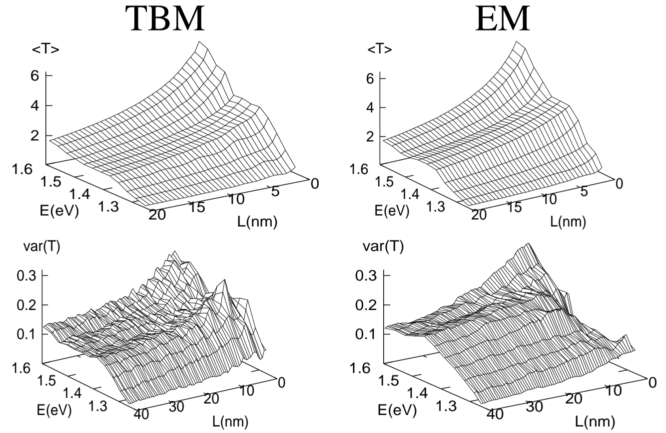

Fig. 4. The averaged transmission coefficient and its variance in the TBM and EM representation.

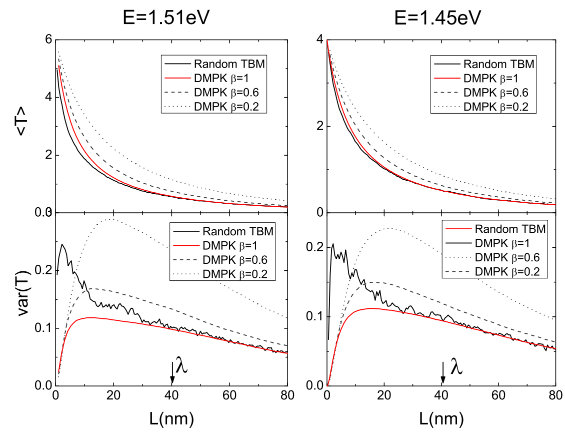

Fig. 5. Fitting $\langle T \rangle$ and $var(T)$ in Fig.(4) at two energy values by the universal functions of L/λ calculated from the DMPK equation (red line). The corresponding solutions of the DMPK equation with fractional βs are shown for comparison.

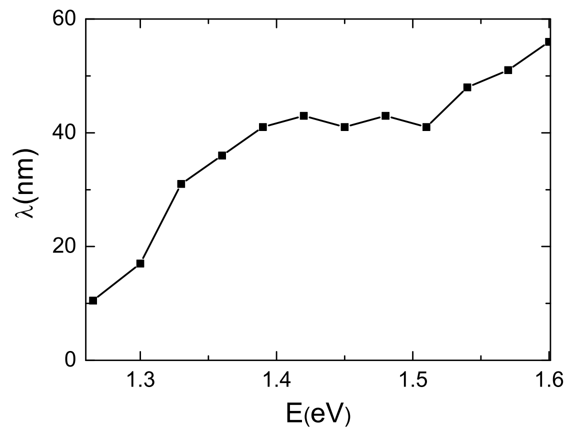

Fig. 6. The localization length as a function of energy.