Atomistic simulation of quantum transport in nanoscale silicon transistors

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Introduction

Size-controlled silicon nanorods (SiNRs) have recently been developed using various growth techniques and used as a building block to form silicon nanodevices [1,2]. A thin film transistor has been fabricated with assembled SiNRs, and the carrier mobility has been shown as high as those for the conventional MOSFETs [3]. Since the assembly of the SiNRs can be performed on non-Si substrates such as glass and plastic, the bottom-up fabrication technique based on the SiNRs may contribute to high-performance nanoscale LSIs as well as economical large-area electronics. As the diameter of the SiNRs is reduced, the effects of Si surface atoms on the entire properties will be more important, and the quantum size effects are expected to be remarkable. Atomistic simulation is therefore inevitable to clarify the electronic and transport properties of the SiNRs.

Simulation of electronic properties of SiNRs

In the present work we first adopted a fully self-consistent DFT code SIESTA [4,5] with the double-ζ plus polarization (DZP) LCAO basis sets and studied the electronic properties of the SiNRs. Figure 1 shows the SiNR structure used in the present analysis. All the dangling bonds on the rod surface are terminated by hydrogen atoms. We calculated Total Density of States (TDOS) and evaluated the band gap E_g from the HOMO-LUMO separations for the SiNRs with the diameter d less than 2 nm and with the length L of 2nm and 3 nm. The resulting E_g shows a dramatic increase with decreasing d due to the quantum size effects (Fig. 2), which is a similar trend to the recent experimental results [1]. An underestimation seen for the calculated E_g is attributable to the use of LDA (local density approximation) in the DFT and is known for such *ab initio* calculations.

Simulation of transport properties of a SiNR transistor

Second, for investigating quantum transport properties of the SiNRs, we adopted TranSIESTA [6], which conducts a self-consistent calculation of the DFT and nonequilibrium Green's function (NEGF). We studied transport properties for the ultrasmall SiNR positioned between nanoscale electrodes. Length of the SiNR is varied from 4 Å to 12 Å while the diameter is fixed at 5 Å, and the source and drain electrodes are assumed to be Au(111). Figure 3 shows the L-dependence of transmission spectrum (a) and the associated LDOS isosurfaces ((b)-(d)) obtained at the Fermi energy. For the 4 Å-long SiNR the continuous transmission spectrum is observed without any gap, which implies metallic behaviors. With increasing L, the transmission spectra show a finite gap, namely semiconductor natures. Such transition from semiconductor to metallic behaviors with decreasing L is consistent with the previous report on the Si atomic wires by Landman *et al*.[7]. The spatial electron distribution is visualized in Fig. 4 for the 4 Å-long SiNR at three characteristic energies. It shows clearly that the electronic states in the band gap exhibit a hybrid nature of the Si and Au orbitals.

Source-drain voltage dependence of the current and transmission spectra are shown for the 4 Å- and 8 Å-long SiNRs in Figs. 5 and 6, respectively. The red regions in the spectra indicate the energy bands in which electrons can tunnel under the applied voltage. It should be noted that the I-V curve for the 8 Å SiNR is nonlinear while that for the 4 Å-long SiNR is virtually linear, which are consistent with the above discussion. We also calculated the gate bias dependence of the current for the 4 Å-long SiNR transistor under the source-drain voltage of 1 V (Fig. 6). The corresponding transmission spectra are shown in Fig. 7 for the gate bias from -5 V to 5 V. The transistors exhibit an interesting ambipolar behavior in the both gate bias polarities.

References

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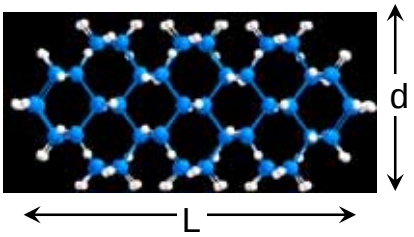

Fig.1: A SiNR structure used for simulation.

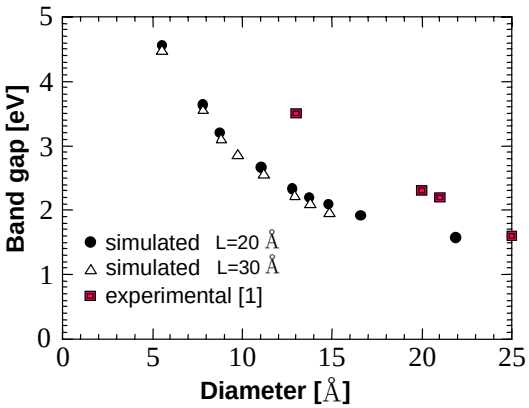

Fig.2: The bandgap as a function of the SiNR diameter.

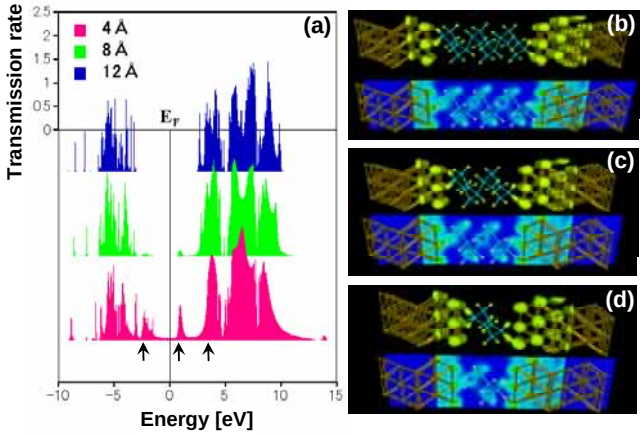

Fig.3: (a) Transmission spectra calculated for SiNRs with L = 4, 8 and 12 Å and (b) – (d) the associated LDOS isosurfaces at energy of E_F.

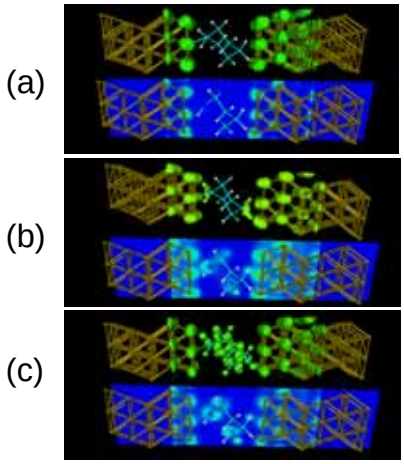

Fig.4: LDOS isosurfaces calculated for the 4 Å SiNR at three particular energies indicated by arrows in Fig. 3(a).

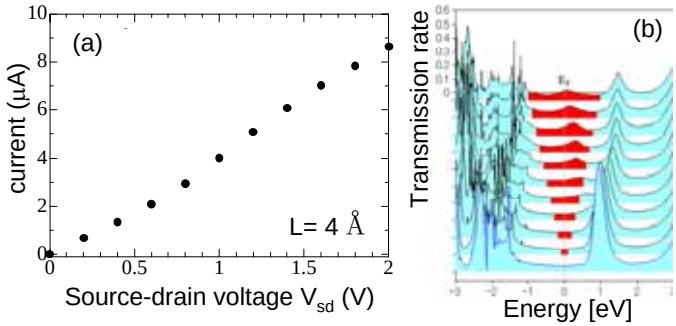

Fig.5: (a) Ids-Vds curve and (b) transmission spectra at Vds from 0 V to 2.0 V calculated for the 4 Å SiNR.

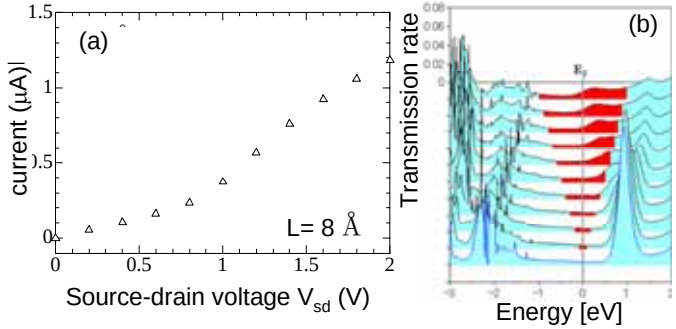

Fig.6: (a) Ids-Vds curve and (b) transmission spectra at Vds from 0 V to 2.0 V calculated for the 8 Å SiNR.

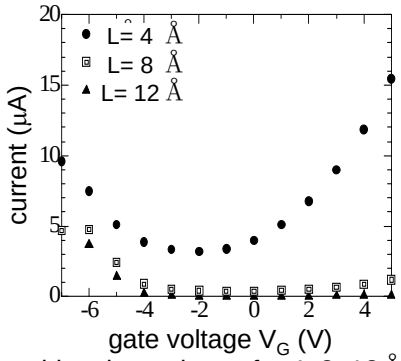

Fig.6: Gate bias dependence for 4, 8, 12 Å SiNRs.

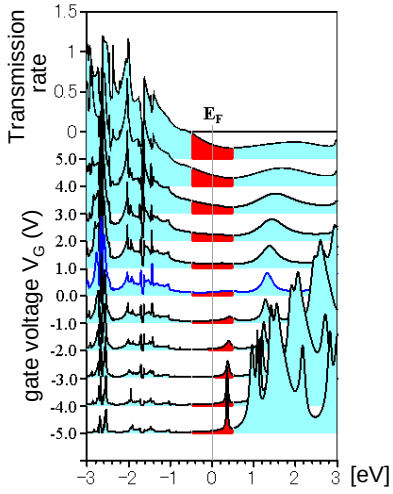

Fig.7:Transmission spectra for VG from -5.0 V to 5.0 V calculated for the 4 Å SiNR.