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 (TDOS) and evaluated the band gap effects are expected to be remarkable. Atomistic simulation is therefore inevitable to clarify the electronic and transport properties of the SiNRs.

Transmission spectrum (a) and the associated LDOS (TDOS) and evaluated the band gap 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 nm to 12 nm while the diameter is fixed at 5 nm, 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 (TDOS) and evaluated the band gap is attributable to the use of LDA (local density approximation) in the DFT and is known for such ab initio calculations.

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 $\AA$ and (b) – (d) the associated LDOS isosurfaces at energy of $E_F$.

Fig. 4: LDOS isosurfaces calculated for the 4 $\AA$ 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 $\AA$ SiNR.

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

Fig. 6: Gate bias dependence for 4, 8, 12 $\AA$ SiNRs.

Fig. 7: Transmission spectra for $V_G$ from -5.0 V to 5.0 V calculated for the 4 $\AA$ SiNR.