20a-D9-1

Impact of Surface Roughness on Thermoelectric Properties of Silicon Nanotubes

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Introduction

Nanostructured silicon (Si) has attracted considerable attention as an efficient thermoelectric (TE) material to obtain higher TE figure of merit: $ZT=(S^2G/\kappa)T$, where S is the Seebeck coefficient, G is the electrical conductance, κ is the thermal conductance, and T is the absolute temperature. Indeed, the ZT of Si nanowire (NW) has been shown to improve by two orders of magnitude with respect to bulk Si[1]. In order to further enhance the ZT, lower κ and larger power factor (S^2G) are required. Recently, it has been reported that a small hollow in SiNWs, i.e. Si nanotube (NT) structures, can show quite lower thermal conductivity than that of SiNWs due to the increased surface to volume ratio[2]. Therefore, the NT structure represents a promising candidate for emerging TE devices. However, much less has been learned for thermoelectric properties of SiNTs. In this work, we perform electron and phonon transport simulation based on the nonequilibrium Green's function (NEGF) formalism and compute the S, G, and κ for SiNWs and SiNTs. We predict the ZTs as a function of the amplitude of the surface roughness (SR).

Simulation Methods

As shown in Fig. 1, we consider square <100> NW and NT with channel width/thickness of 5.0 nm and length of 100.0 nm. The SR is included in the channel region and is assumed to be generated according to the exponential autocovariance function, which is characterized by the root mean square (RMS) and correlation length. The hole of NT is square in shape with an area of 1.0 nm^2.

Electron Transport: To estimate S and G, we address a quantum analysis based on the 3D self-consistent solution of the Poisson-Schödinger equation within the coupled mode-space NEGF formalism. Electron-phonon scattering is also considered and uniform donor doping of 1.0×10^{20}cm^{-3} is supposed in source and drain region. The channel region has doping concentration of 1.0×10^{19}cm^{-3}.

Phonon Transport: Phonon transport is solved by the NEGF technique to compute κ. The modified valence force field method[3] is chosen to describe the dynamical matrixes of NWs and NTs, and no phonon-phonon scattering is taken into account.

Results and Discussion

Figure 2 shows the ZT figure of merit of SiNWs and SiNTs as a function of the roughness RMS. In this work, we consider three surface roughness conditions with RMSs of 0.0, 0.2 and 0.4 nm. For the SiNWs, it is clearly observed that the ZT increases with RMS. This is because κ decreases as the surface disorder increases (12.0, 1.11, and 0.488 nW/K for models with RMS of 0.0, 0.2, 0.4 nm, respectively), while S^2G does not change significantly. The NTs with RMSs of 0.0 and 0.2 nm show higher values of the ZTs than those of SiNWs due to the reduction of κ caused by presence of hole. However, in the case of 0.4 nm RMS, a ZT lowering is observed. This is attributed to the deterioration of the electrical conductance, meaning S^2G rather than κ dominates over the ZT in NTs as the surface roughness increases. The present results indicate that it is essential to optimize the structure parameters, such as cross-sectional area, hole size, inner or outer surface roughness, and doping concentration, for NW and NT in order to extract the best TE performance.

References

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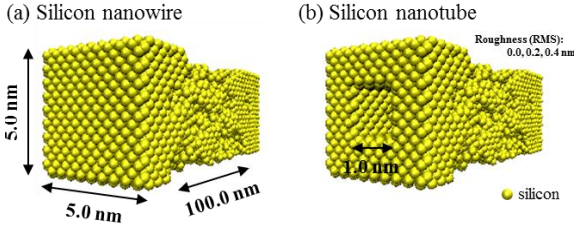

Fig. 1. Schematic view of the model of (a) SiNW and (b) SiNT with surface roughness.

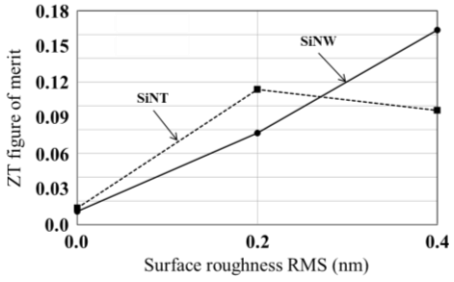

Fig. 2. ZTs of the SiNW and SiNT as a function of the surface roughness RMS.

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