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# Effects of Polytypism on the Thermoelectric Properties of Si Nanowires : a Combination of Density Functional Theory and Boltzmann Transport Equation Calculations

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**Abstract**

**The effects of polytypism on the thermoelectric properties of Si nanowires (NWs) are investigated on the basis of Boltzmann transport equation within constant relaxation time approximation combined with density functional calculations. We find that the value of *ZT* for *n*-type Si NWs with 2H structure is about twice larger than that of 3C structure due to the enhancement of electrical conductivity and Seebeck coefficient in 2H structure. Our calculated results imply that thermoelectric properties of Si NWs can be tuned by controlling polytypes of NWs.**

## 1. Introduction

Semiconductor nanomaterials such as NWs are attractive candidates for wide range of future devices. Furthermore, interest in thermoelectric materials using semiconductor NWs have been pained much attentions. Many theoretical and experimental studies have been demonstrated [1-3] to improve the dimensionless figure of merit $ZT=\sigma S^2T/(\kappa_e+\kappa_l)$, where $\sigma$ is electrical conductivity, $S$ is Seebeck coefficient, $T$ is temperature, $\kappa_e$ is electrical thermal conductivity, and $\kappa_l$ is lattice thermal conductivity. It has also been theoretically reported that the growth direction and core-shell structure influence on the thermoelectric properties of Si NWs [4-5].

Recently, Si NW with hexagonal diamond (2H) structure and cubic/hexagonal heterostructure have been successfully fabricated [6-7] by chemical vapor deposition. These experimental findings inspire us to investigate effects of polytypes on the thermoelectric properties of Si NWs from theoretical viewpoint. In this study, we investigate thermoelectric properties of Si NWs with 3C, 6H, 4H and 2H structures on the basis of a combination of density functional theory (DFT) and Boltzmann transport equation calculations.

## 2. Computational methods

The electronic structure calculations are performed within the DFT using the generalized gradient approximation [8]. We use norm-conserving pseudo potential [9] to simulate nuclei and core electrons. The conjugate gradient technique is employed both for the electronic structure calculations and for geometry optimization. The valence wave functions are expanded by the plane-wave basis set with cutoff energy of 16 Ry. These calculations have been performed using Tokyo Ab initio program package (TAPP) [10]. Figure 1 shows the calculation models used in this study. The diameter of Si NWs are ~1.1 nm and dangling bonds of nanowires side facets are terminated by H atoms.

The calculations based on Boltzmann transport theory are performed to calculate thermoelectric properties. Thermoelectric properties are obtained by using BoltzTraP program [11] in the constant relaxation time approximation. The value of relaxation time in this study is obtained by fitting the variation between the measured mobility and carrier concentration for both *n*- and *p*-type bulk Si with 3C structure.

## 3. Results and discussions

Figures 2 and 3 show calculated electrical conductivity $\sigma$, Seebeck coefficient $S$, electronic thermal conductivity $\kappa^e$, and $ZT$ at 300 K of *n*-type and *p*-type Si NWs with 3C, 6H, 4H and 2H structure as a function of carrier concentration $n$,

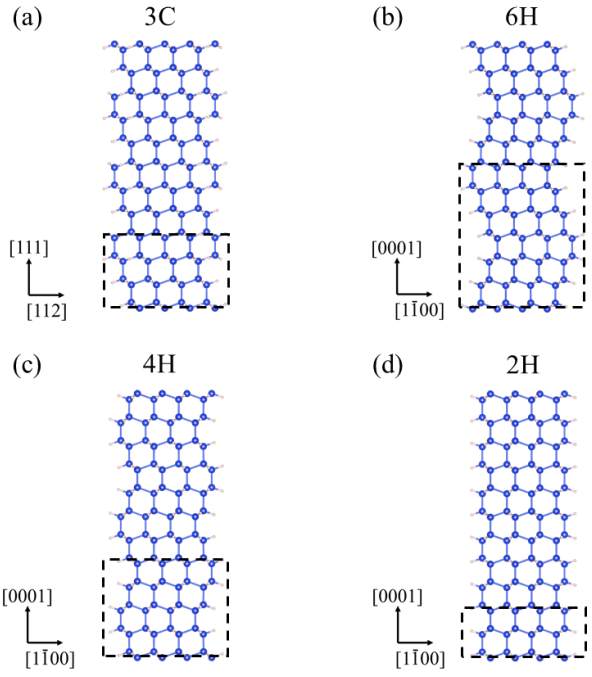


Fig. 1: Calculation models of Si NWs with (a) 3C, (b) 6H, (c) 4H and (d) 2H structure. Areas surrounded by dashed line denote unit cells used in this study. Large and small circles represent Si and H atoms, respectively.

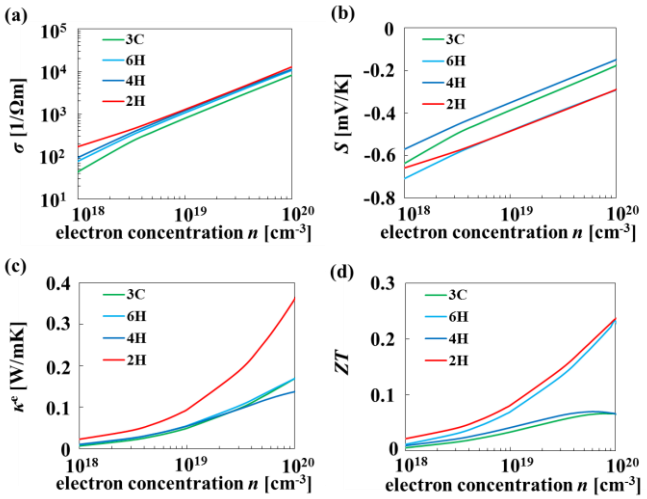


Fig. 2: Calculated (a) electrical conductivity, (b) Seebeck coefficient, (c) electronic thermal conductivity and (d) *ZT* at 300 K for *n*-type Si NWs with various polytypes as a function of carrier concentration. In the calculations of *ZT*, the value of lattice thermal conductivity $\kappa^l$ is assumed as $\kappa^l$=1 W/mK.

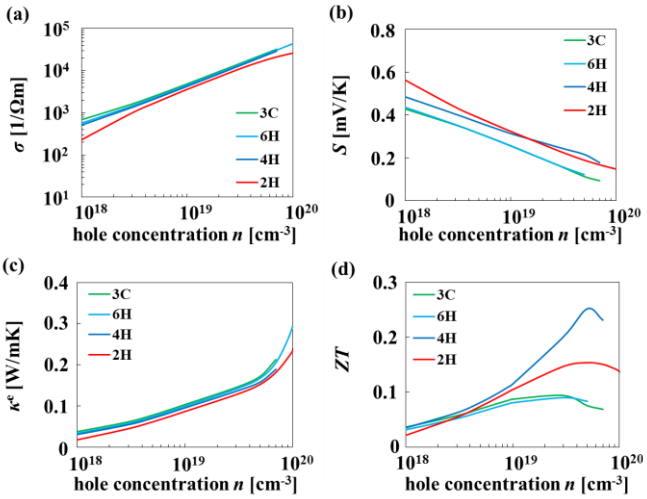


Fig. 3: Calculated (a) electrical conductivity, (b) Seebeck coefficient, (c) electronic thermal conductivity and (d) *ZT* at 300 K for *p*-type Si NWs with various polytypes as a function of carrier concentration. In the calculations of *ZT*, the value of lattice thermal conductivity $\kappa^l$ is assumed as $\kappa^l$=1 W/mK.

respectively. Here, the carrier concentration $n$ is defined as $n = \int d\varepsilon\, N(\varepsilon) f_\mu(\varepsilon)$, where $N(\varepsilon)$ is the electronic density of states and $f_\mu(\varepsilon)$ is the Fermi distribution function. Our calculated results indicate that electrical conductivity of n-type Si NWs shown in Fig. 2(a) has proportional relation to hexagonality, and electrical conductivity of Si NWs with 2H structure is 61% larger than that of 3C structure. On the other hand, electrical conductivity of *p*-type Si NWs shown in Fig. 3(a) has inverse relationship to hexagonality, and 2H structure is 26% smaller than that of 3C structure. As shown in Figs. 2(b) and 3(b), for both *n*-type and *p*-type Si NWs Seebeck coefficients with 2H structure are 23~25% larger than those with 3C structure. Consequently, the value of *ZT* of Si NWs with 2H structure shown in Figs. 2(d) and 3(d) is larger than that of 3C structure. In particular, the value of *ZT* for *n*-type Si NW with 2H structure is 152% larger than that of 3C structure. This is because that the electronic structure of Si NW with 2H structure is different from that with 3C structure. The calculated band gap of Si NWs with 2H structure is 0.25 eV larger than that with 3C structure, and Si NWs with 2H, 4H and 6H structure possess direct band gap different from 3C structure.

## 4. Conclusions

We have investigated thermoelectric properties of Si NWs with different polytypes on the basis of a combination of DFT and Boltzmann transport equation calculations. We have found that thermoelectric properties of Si NWs depend on the crystal structure of NWs. Our calculations also predict that the value of *ZT* of *n*-type Si NW with 2H structure is 152% larger than that of 3C structure. It is thus expected that thermoelectric properties can be tuned by controlling the polytypes of Si NWs.


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