

Monte Carlo Simulation of Phonon Transport in Silicon Nanowires Including Realistic Dispersion Relation

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Abstract

Monte Carlo simulations are performed to solve the phonon Boltzmann transport equation in silicon nanowires, and the thermal conductivity is analyzed. By taking account of the realistic phonon dispersion relation, it is revealed that the experimental characteristics are well reproduced by simply assuming the completely diffusive scattering at the wire surface without introducing any fitting parameters regarding specularity.

1. Introduction

Correct understanding of the thermal properties in silicon nanowires (SiNWs) is very important for engineering applications such as ultrascaled silicon MOSFETs [1], biological and chemical sensors [2], and thermoelectric devices [3]. In comparison with the bulk value, the heat conduction property in SiNWs is known to become significantly worse because of the frequent phonon scatterings at the wire surface. The impact of the phonon boundary scattering on the thermal conductivity κ is strongly correlated to the phonon mean free path, which depends not only on the relaxation time, but also on the phonon group velocity, i.e., the phonon dispersion relation.

In this work, the thermal conduction in SiNWs is analyzed by using a Monte Carlo (MC) method for solving the phonon Boltzmann transport equation taking account of the realistic dispersion relation of acoustic phonons in bulk Si. We then discuss the validity or limitations of the conventional approach considering the approximated dispersion curves.

2. Simulation Method

Figure 1 shows a realistic dispersion relation of phonons in bulk Si calculated from the adiabatic bond charge model [4]. In many of the previous works, approximated dispersion curves were employed; e.g., as shown in Fig. 1, the dispersion relation was expressed by the curves fitted only to [100] (Γ -X) direction [5]. In this study, we compare the [100] model to the more accurate approach, in which the phonon density of states (DOS) and the group velocity averaged over constant-energy surfaces were numerically calculated from the realistic dispersion relation and implemented as look-up tables in the phonon MC simulator [6]. Figure 2 shows the specific heat per volume and phonon averaged group velocity as a function of temperature. Note that the [100] model exhibits lower specific heat and higher velocity, which is mainly due to inaccurate modeling of the transverse acoustic (TA) branch around W, U, and K points. In MC simulation, as shown in Fig. 3, the random walks of phonons were tracked considering the phonon-phonon and phonon-defect collisions, whose rates were carefully

calibrated to reproduce the experimental data of κ for bulk Si [6]. Furthermore, we assumed phonon boundary scattering at the wire surface as a completely diffusive scattering process which obeys Lambert's law [7].

3. Results and Discussion

Figures 4 and 5 shows κ in SiNWs simulated with the approximated and realistic dispersion curves, respectively. Compared to the experimental data, the simulation with [100] model underestimates κ in thick diameter ($d = 37$ – 115 nm) SiNWs, and the partially specular reflection mechanism had to be introduced for the boundary scattering to obtain the agreement [5]. On the other hand, this work revealed that the experimental κ are well reproduced by simply assuming the completely diffusive boundary scattering, which is consistent with the recent theoretical prediction [8].

Figure 6 compares the distribution of the phonon mean free path between the successive collisions obtained with the MC simulation in bulk Si. Note that the approximated model generates the phonons with longer free paths, which is mainly due to the higher group velocity observed in Fig. 2 (b). This results in more sensitive reduction of κ when additional collisions are introduced at the boundary. In the case of thinnest SiNW of $d = 22$ nm, however, this work's approach significantly overestimates κ . Although the phonon confinement effect may modulate the dispersion relation, its effect has been suggested to be weak in SiNWs with $d \sim 20$ nm [9]. We may have to consider the additional mechanisms, such as the strain at the Si/SiO₂ interface [10], and further investigations are required to understand the thermal conduction in the thinner NWs.

4. Conclusions

We have analyzed the thermal conduction in SiNWs using a MC method. By taking account of the realistic phonon dispersion relation and completely diffusive boundary scattering, good agreements have been obtained with the experimental data of κ in SiNWs with $d = 37$ – 115 nm.

References

- [1] N. Singh *et al.*: IEEE Electron Device Lett. **27** (2006) 383.
- [2] Y. Cui *et al.*: Science **293** (2001) 1289.
- [3] A. I. Boukai *et al.*: Nature **451** (2008) 168.
- [4] W. Weber *et al.*: Phys. Rev. B. **15** (1977) 4789.
- [5] P. Chantrenne *et al.*: J. Appl. Phys. **97** (2005) 104318.
- [6] K. Kukita *et al.*: Tech. Digh. IEDM (2012) 17.5.
- [7] D. Marx *et al.*: Z. Phys. B Condens. Mat. **48** (1982) 277.
- [8] J. C. Duda *et al.*: J. Appl. Phys. **108** (2010) 073515.
- [9] K. W. Adu *et al.*: Appl. Phys. A **85** (2006) 287.
- [10] H. Minari *et al.*: VLSI Tech. (2011) 122.
- [11] P. Flubacher *et al.*: Philos. Mag. **4** (1959) 273.
- [12] D. Li *et al.*: Appl. Phys. Lett. **83** (2003) 2934.

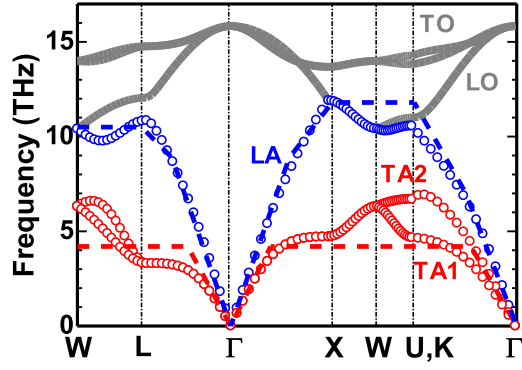


Fig. 1 Phonon dispersion relationship for bulk Si obtained with the adiabatic bond charge model [4]. Only acoustic phonons (TA1, TA2, and LA) were considered in this work (open dots), and the contribution of optical modes (thick curves) to the thermal transport was assumed to be negligible due to their small group velocities. Dashed lines are the approximated curves fitted to [100] direction used in the previous work [5].

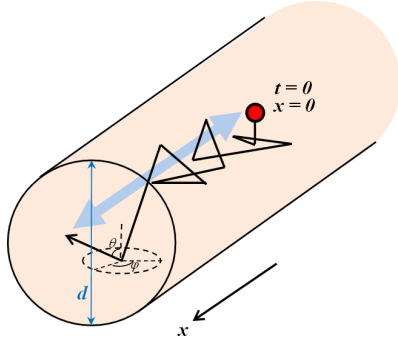


Fig. 3 Schematic illustration of the MC method for simulating the thermal conduction in SiNWs. Phonons were modeled as particles, and their random walks were tracked. By calculating the diffusion length along the longitudinal direction, thermal diffusivities were obtained. In this study, completely diffusive boundary scattering was assumed and the scattering angle θ , ϕ is randomly selected using the Lambert's cosine law [7].

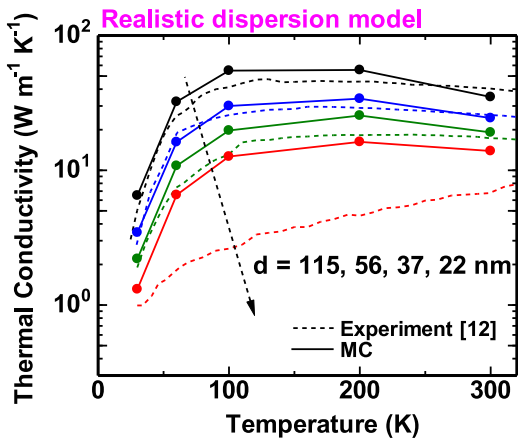


Fig. 5 Comparison of the simulated (solid lines) and experimental (dashed lines) thermal conductivities of SiNWs with various diameters plotted as a function of temperature. In MC simulator, the *realistic* dispersion model was included.

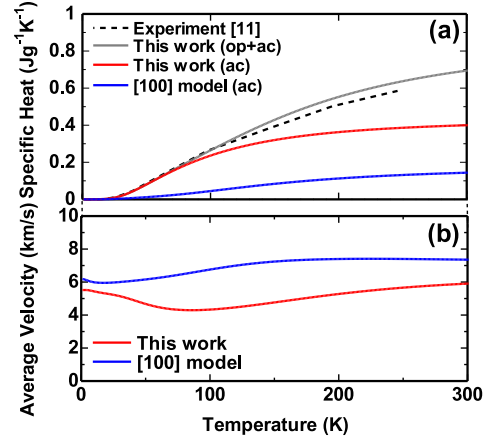


Fig. 2 Specific heat capacity per volume for bulk Si (a) and the average group velocity (b) plotted as a function of temperature. The results calculated with the various dispersion models are compared.

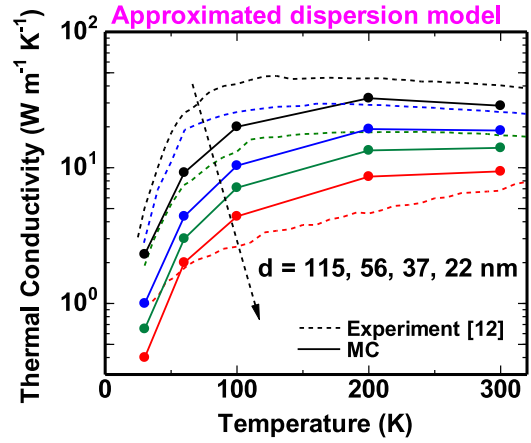


Fig. 4 Comparison of the simulated (solid lines) and experimental (dashed lines) thermal conductivities of SiNWs with various diameters plotted as a function of temperature. In MC simulator, the *approximated* dispersion model was included.

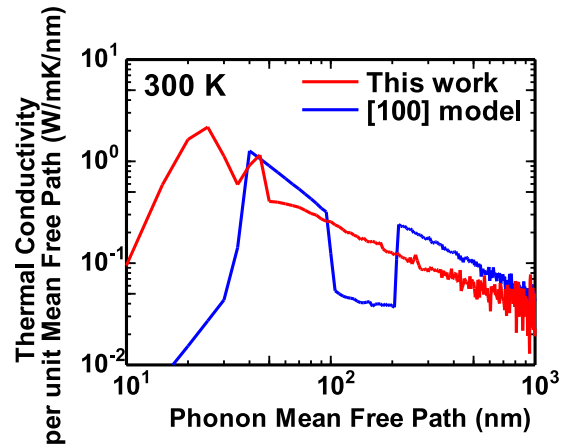


Fig. 6 Distribution of the phonon mean free path obtained with the MC simulation in bulk Si at 300 K.