Influence of Phonon Dispersion Relation on Thermal Resistance in Silicon Nanostructures

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INTRODUCTION

The accurate understanding of the thermal conduction properties in nanoscale regime becomes important because of the scaling of the electronic devices. In this study, we analyze the thermal resistance in Si nanostructures using a Monte Carlo (MC) method for solving the phonon Boltzmann transport equation, and discuss the quasi-ballistic transport properties depending on the phonon dispersion relation model.

SIMULATION METHOD AND RESULTS

Figure 1 shows a dispersion relation of phonons in bulk Si calculated with adiabatic bond charge model [1]. In many of the previous works, approximated dispersion curves were employed; e.g., as shown in Fig. 1, the dispersion relation were expressed by the analytical curve fitted only to [100] (Γ–X) direction [2]. In this study, we compare the [100] model to the more accurate approach, in which the phonon density of states and the group velocity averaged over constant-energy surfaces were calculated from the realistic dispersion relation and implemented as look-up tables (full-band model) in the phonon MC simulator [3,4].

Figure 2 shows the phonon average group velocity v as a function of temperature T. Note that the [100] model exhibits higher velocities, which is mainly due to the lack of TA2 branch having low group velocities. We have confirmed, however, that both two models can yield the correct thermal conductivity $\kappa(T)$ of bulk Si by adjusting the phonon scattering rates. Considering that κ is expressed as $\sim Cv\lambda/3$ (where C and λ are the heat capacity and phonon mean free path, respectively), lower λ value is needed for [100] model as shown in Fig. 3.

To investigate the difference between the two models, we have simulated the steady state temperature distribution in the simple one-dimensional structure of Si as shown in Fig. 4. Figure 5 shows the calculated thermal resistances $R_{\rm th}$ as a function of the device length L. In the large L limit, the two models exhibit the same $R_{\rm th}$, while the discrepancy was found in the small L region. As illustrated in Fig. 6, when $L \gg \lambda$, the phonon transport property is considered to be diffusive, and $R_{\rm th}$ is a function of κ. Since the scattering rate parameters for the both models were adjusted to yield the experimental κ, the both same $R_{\rm th}$ were obtained. On the other hand, when $L \ll \lambda$, the ballistic transport nature, which depends on v but not λ, becomes dominant, and thus [100] model shows lower $R_{\rm th}$.

SUMMARY

We have analyzed the thermal resistance in Si nanostructures using the MC method. It has been demonstrated that the correct implementation of the phonon dispersion relation is essential to accurately simulate the thermal conduction properties in the quasi-ballistic transport regime.

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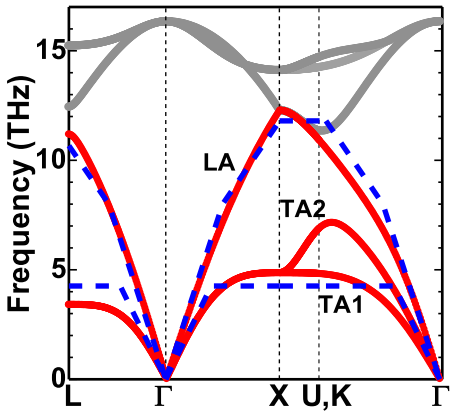

Fig. 1. Phonon dispersion curves for bulk Si obtained from adiabatic bond charge model [1]. Only acoustic phonons (TA1, TA2, and LA) were considered in this work. Lines are the approximated curves used in the previous work [2].

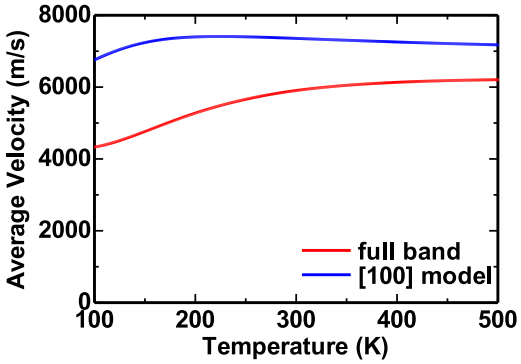

Fig. 2. Average group velocity of acoustic phonons as a function of temperature. The results calculated from a realistic dispersion relation (red line) and approximated model (blue line) are compared.

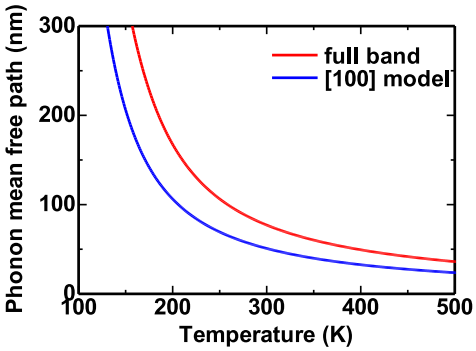

Fig. 3. Phonon mean free path as a function of temperature. Realistic dispersion relation (red line) and approximated model [2] (blue line) are compared.

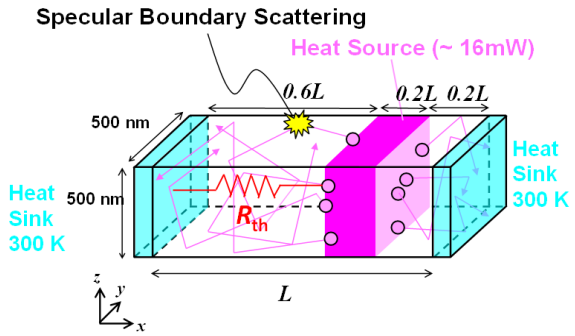

Fig. 4. Schematic view of the 1D structure to investigate the thermal resistance R_{th} in Si device with various L.

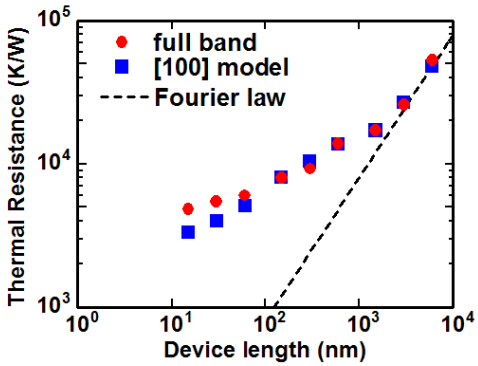

Fig. 5. Simulated $R_{\rm th}$ as a function of L. MC simulation results with the full band model and [100] phonon dispersion model are compared. The dashed line represent the theoretical dependence based on the Fourier law.

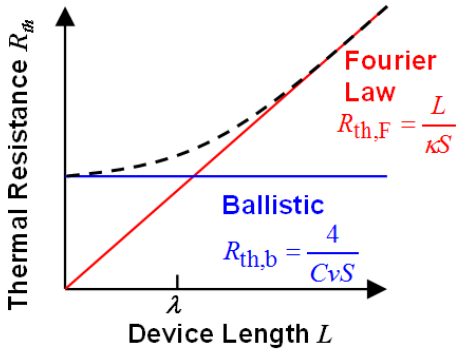

Fig. 6. Schematic view showing L-dependence of R_{th} described with the Fourier law and the ballistic transport model.