# Monte Carlo Simulation of Phonon Transport in Silicon Thin films Including Realistic Dispersion Relation

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## INTRODUCTION

Growing heat dissipation has become one of the main issues in today's IC chips limiting the reliability and performance. To correctly understand the heating properties in nanoscale devices, it is considered that the conventional approach based on the Fourier's law is no longer appropriate. In this study, we analyze the thermal conduction in ultrathin Si films using a Monte Carlo (MC) method taking account of a realistic dispersion relation of acoustic phonons.

## SIMULATION METHOD AND RESULTS

Figure 1 shows a realistic dispersion relation of phonons in bulk Si calculated from adiabatic bond charge model [1]. In many of the previous works, approximated dispersion curves were employed, e.g., as dashed lines in Fig. 1, which were fitted to the realistic curves along [100] direction [2]. Considering that our aim is to simulate the phonon transport at temperatures larger than 300 K, where phonons are distributed in the wide frequency range, the inclusion of the more accurate dispersion relation is preferable. So in this work, the phonon density of states (DOS) and group velocity were calculated from the realistic dispersion relation, and the data as a function of the phonon energy $E$ were included into the MC simulator as look-up tables.

The phonon DOS is shown in Fig. 2, while the phonon group velocity (Fig. 3) was obtained by taking the average over constant-energy surfaces in the 1st Brillouin zone (BZ):

$$\bar{v}_p(E) = \frac{1}{8\pi^3 \rho_p(E)} \int_{\mathrm{BZ}} d^3q \, |\nabla_q \omega_p| \, \delta(\hbar\omega_p(\mathbf{q}) - E),$$

where $\hbar$ is the Planck constant, $\omega_p(\mathbf{q})$ is the frequency of phonons with the wave vector $\mathbf{q}$ and polarization $p$, and $\rho_p(E)$ is the phonon DOS. Compared with the isotropic [100] linear dispersion model [2], the phonon velocity is larger in the region of $E >\sim 20$ meV, where a large number of phonons exist at room temperature (see Fig. 4). Fig. 5 shows the specific heat capacity of bulk Si calculated from the phonon DOS, showing the validity of the phonon dispersion model used in this study.

To simulate the thermal diffusivity and the conductivity, the random walks of phonons were simulated with a MC method considering the phonon-phonon and phonon-defect collisions. In this study, the formulas given in [2] were employed for the scattering rate model, but the parameters were adjusted to reproduce the measured bulk thermal conductivity at 300 K [5] (the magnitude of scattering rates had to be enlarged by x2.5 due to higher phonon velocities in the present model). Fig. 6 shows the simulated thermal conductivities of Si films with various thicknesses. By assuming the fully diffusive phonon scattering at the boundary based on Lambert's cosine law, good agreement was obtained with the measurements [2,6] without introducing any fitting parameters for the boundary scattering. This is consistent with the recent theoretical prediction [7].

## SUMMARY

We have analyzed the thermal conduction in Si thin films using a MC method. By taking account of the realistic phonon dispersion relation and the pure diffusive boundary scattering, good agreement with the experimental data has been obtained.

## REFERENCES

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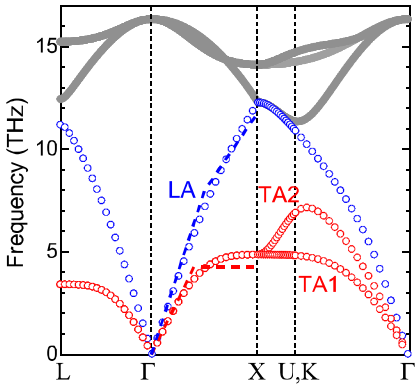


Fig. 1. Phonon dispersion curves for bulk Si obtained from adiabatic bond charge model [1]. The dashed lines are the approximated model used in [2]. Only acoustic phonons (TA1, TA2, and LA) were considered in this work.

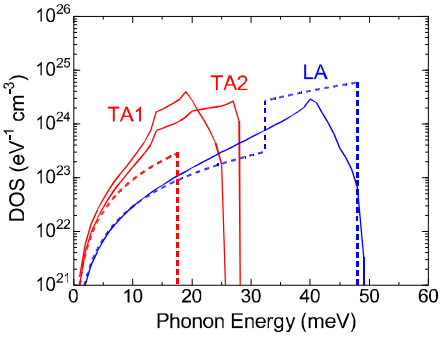


Fig. 2. Density of states (DOS) of acoustic phonons as a function of energy. The results calculated from a realistic dispersion relation (solid lines) and approximated model [2] (dashed lines) are compared.

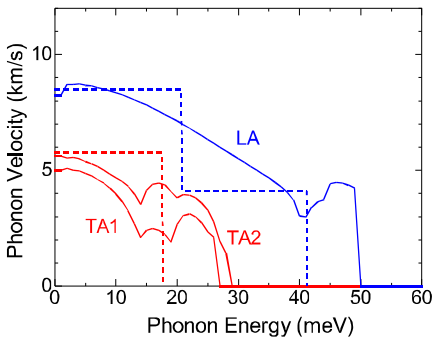


Fig. 3. Phonon group velocity averaged over surfaces of constant energy in the realistic phonon dispersion relation (solid lines). The results calculated from the approximated model [2] are also plotted (dashed lines).

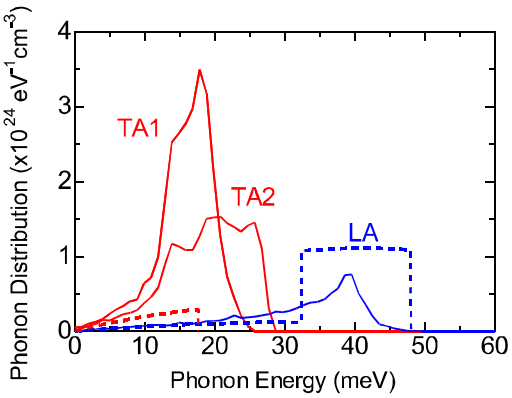


Fig. 4. Phonon distribution at 300 K calculated with the phonon DOS assuming Bose-Einstein statistics. The results calculated from a realistic dispersion relation (solid lines) and approximated model [2] (dashed lines) are compared.

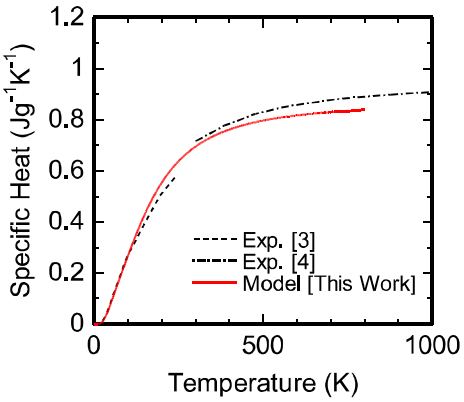


Fig. 5. Specific heat capacity per volume for bulk Si plotted as function of temperature. The results calculated from the realistic phonon DOS (see Fig. 2) is compared to the experimental data [3,4].

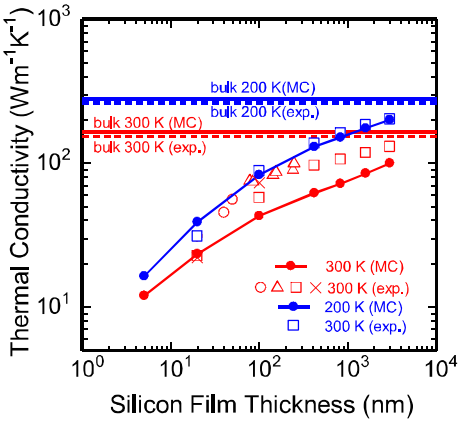


Fig. 6. Comparison of the simulated (lines) and experimental (dots) thermal conductivities at 300 (red) and 200 K (blue) plotted as a function of Si film thickness. The sources of the experimental data are presented in [2,6].