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Calculation of Confined Phonon Spectrum in Narrow Silicon Nanowires Using the Valence Force Field Method

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We study the effect of confinement on the phonon properties of ultra-narrow silicon nanowires of side sizes of 1 nm to 10 nm. We use the modified valence force field (MVFF) method to compute the phononic dispersion and extract the density of states, the transmission function, the sound velocity, the ballistic thermal conductance, and boundary-scattering-limited diffusive thermal conductivity. We find that the phononic dispersion and the ballistic thermal conductance are functions of the geometrical features of the structures, i.e., the transport orientation and confinement dimension. The phonon group velocity and thermal conductance can vary by a factor of two depending on the geometrical features of the channel. The $\langle 110\rangle$ nanowire has the highest group velocity and thermal conductance, whereas the $\langle 111\rangle$ has the lowest. The $\langle 111\rangle$ channel is thus the most suitable orientation for thermoelectric devices based on Si nanowires since it also has a large power factor. Our findings could be useful in the thermal transport design of silicon-based devices for thermoelectric and thermal management applications.

Key words: Confined phonons, silicon nanowires, lattice thermal conductance, modified valence force field method, Landauer formula

INTRODUCTION

Low-dimensional silicon nanowires (NWs) and silicon-based ultra-thin layers have attracted significant attention as efficient thermoelectric (TE) materials after it was demonstrated that the thermal conductivity in such materials can be drastically reduced compared with bulk Si. Values as low as $\kappa = 2$ W/mK (compared with $\kappa = 140$ W/mK for bulk Si) were achieved.[1,2] This resulted in ZT values close to $ZT \approx 0.5$, a large improvement compared with the ZT of bulk Si, $ZT_{\text{bulk}} \approx 0.01$.[1,2] This large reduction in thermal conductivity was attributed to enhanced scattering of phonons on the surfaces of the nanochannels.

Numerous studies can be found in the literature regarding the thermal conductivity of Si NWs.[3–7] The effects of different scattering mechanisms, i.e., surface roughness scattering, mass doping, phonon–phonon scattering, and phonon–electron scattering, have been investigated by several authors.[8–11] In these works, it is demonstrated that the thermal conductivity in ultra-narrow Si NWs drastically degrades once the diameter of the NW is reduced below 50 nm, or when scattering centers are incorporated. For even smaller NW diameters, i.e., below 10 nm, the effect of confinement could further change the phonon spectrum significantly, and provide an additional mechanism for the reduction of the thermal conductivity.[12] This could provide additional benefits to the thermoelectric figure of merit ZT. In this work, we employ the modified valence force field (MVFF) method[13] to address the

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