Thermal Conductivity of Si Nanowires Using Atomistic Phonon Dispersions

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INTRODUCTION

The thermal properties of Si nanowires (NWs) are of high interest for a variety of applications such as thermal management and thermoelectricity. Most simulation studies to date use the Si bulk dispersion within a confined geometry. The phonon dispersion in ultra-narrow 1D NWs, however, is different from the bulk dispersion, and can lead to different thermal properties. In this work, we study the thermal conductivity (κ_l) of ultra-narrow silicon NWs using the full-band confined phonon dispersion and Boltzmann transport theory.

COMPUTATIONAL METHOD

We calculate the phonon dispersion using the modified valence force field method which captures the phonon details in the entire Si Brillouin Zone [1]. The lattice thermal conductivity is calculated using the BTE for phonons as [2]:

$$\kappa_l = \sum_{\alpha,q} \frac{\hbar^2 \omega_\alpha(q)^2}{k_{\mathrm{B}}^2 T} \frac{e^{(\hbar\omega_\alpha(q)/k_{\mathrm{B}}T)}}{\left[e^{(\hbar\omega_\alpha(q)/k_{\mathrm{B}}T)}-1\right]^2} \tau_\alpha(q) v_\alpha(q)^2$$

where $v_\alpha(q)$ is the group velocity of a phonon with wavevector q in subband α. For the calculation of the relaxation times, we follow the bulk formalism for Umklapp scattering, $\tau_{\mathrm{U}}^{-1} = \mathrm{B}\omega_\alpha(q)^2 T \exp(-\mathrm{C}/T)$ [3]. For boundary scattering we use $\tau_{\mathrm{B}}^{-1} = (1-p)/(1+p)v_\alpha(q)/D$, where D is NW diameter and p is specularity parameter given by $p(q) = \exp(-4q^2\Delta_{\mathrm{rms}}^2)$ [3] where $\Delta_{\mathrm{rms}} = 0.3\ \mathrm{nm}$. NWs have a finite phonon density of states (*DOS*) at low frequencies, in contrast to bulk. Therefore, the bulk scattering model for Umklapp scattering causes divergence in κ_l. To remove the singularity, as proposed by Mingo [4], an additional second order 3-phonon scattering rate can be introduced as $\tau_{\mathrm{U2}}^{-1} = \mathrm{A}T^2$. Finally, the overall relaxation rate is computed using Mathiensens rule.

RESULTS AND DISCUSSION

Figure 1 shows the Umklapp scattering-limited κ_l for NWs in the $<100>$, $<110>$, and $<111>$ orientations, vs. D. To obtain this, we use $\mathrm{A} = 15000\ 1/\mathrm{sK}^2$, which provides good agreement with molecular dynamics (MD) results [5]. Our results also show good agreement with results from MD [5] and NEGF simulations [6] in a large temperature range (especially above $200\ \mathrm{K}$), as shown in Fig. 2 and 3. In ultra-narrow NWs, however, the most important scattering mechanism is boundary scattering [5]. Its effect as a function of p at $T = 200$ and $300\ \mathrm{K}$ is shown in Fig. 4. Here, we use a constant p for all q-points. The conductivity increases as p increases (specular boundaries) as expected. The solid symbols show κ_l when we consider a q-dependent p. The empty symbols with errorbars are MD results from [5]. Interestingly, the effective p is ~ 0.8, indicating that the overall scattering is almost specular, even for such narrow NWs ($D = 2\ \mathrm{nm}$), in contrast to what normally assumed for nanostructures. The low-q phonons have high p and undergo mostly specular scattering on the surfaces. This low scattering rate at low frequencies, the high group velocity of acoustic branches, as well as the non-zero *DOS* at low frequency, result in a major κ_l contribution of the low frequency phonons (inset of Fig. 5). The cumulative κ_l vs. mean-free-path (MFP) is shown in Fig. 5. For Umklapp-limited scattering (blue), the heat is carried by phonons with MFPs from a few nanometers to a few microns. In the presence of boundary scattering, however, almost 50% of the heat is carried by phonons with MFPs of a few nanometers. The contribution of phonons with $\lambda > 3\ \mu\mathrm{m}$ is not affected by boundary scattering because these are low frequency phonons, that undergo mostly specular boundary scattering.

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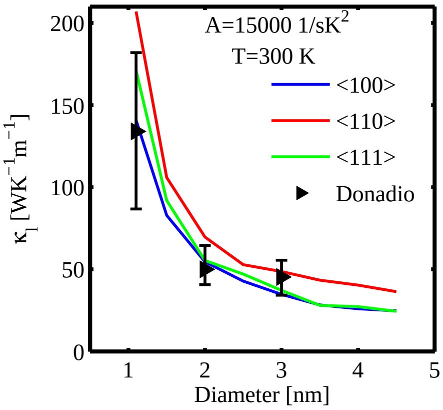

Fig. 1. Thermal conductivity of NWs vs. diameter at $T = 300$ K. The parameter for second order 3-phonon scattering processes is A $= 15000\ 1/\text{sK}^2$. Symbols are MD results from [5].

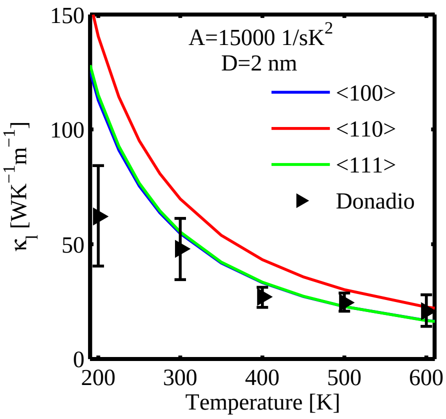

Fig. 2. Thermal conductivity of the $D = 2$ nm NWs vs. temperature. The parameter for second order 3-phonon scattering processes is A $= 15000\ 1/\text{sK}^2$. Symbols are MD results from [5].

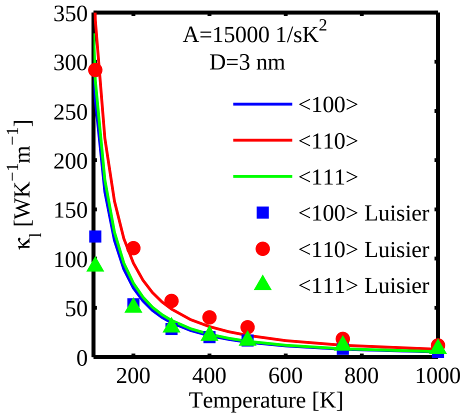

Fig. 3. Thermal conductivity of the $D = 3$ nm NWs vs. temperature. Symbols are NEGF results from [6].

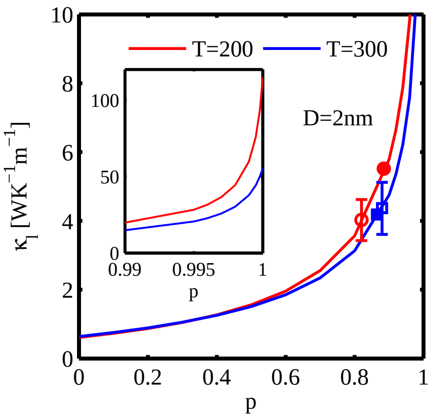

Fig. 4. The thermal conductivity of the $D = 2$ nm <111> NW vs. the boundary scattering specularity parameters p. Solid symbols show the results using a q-dependent p. Empty symbols with errorbars show MD results from [5]. Inset: zoom-in around $p \sim 1$.

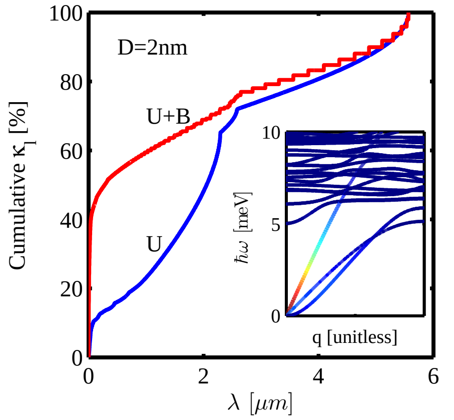

Fig. 5. The cumulative thermal conductivity of the $D = 2$ nm <111> NW vs. the phonon mean-free-path. Results for Umklapp-limited κ_l (U), and Umklapp plus boundary scattering-limited κ_l (U+B) are shown. Inset: The contribution of each mode in κ_l in the Umklapp scattering-limited case.