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Phononic thermal transport in nanostructured ultra-thin silicon membranes

The investigation of the role of phononic thermal transport in nanostructured materials has received considerable attention in recent years due to the interest in thermal management in nanostructures and energy harvesting using thermolectric devices. Phonon engineering in nanostructured semiconductors has been shown to improve the efficiency of thermoelectric systems, by reducing the thermal conductivity of the crystalline materials while preserving their electronic properties. Reduction of the phonon group velocities leading to a strong reduction in the thermal conductivity, is recently being shown by experiments in sub-10 nm free-standing Si membranes[1]. However, a microscopic understanding of thermal transport in ultra-thin membranes especially the correlation between phonon surface scattering and thermal transport, is still lacking. The theoretical studies reported, mostly rely on bulk phonon properties and use of specularity parameters to model surface scattering of phonons[2]. A detailed understanding of the role and behavior of phonons in confined structures is necessary in the design of nanostructured materials with tailored thermal transport properties.

We use the combination of harmonic lattice dynamics (HLD) and classical molecular dynamics (MD) to investigate the nature of phononic thermal transport in nanostructured silicon membranes with thicknesses of the order of 20 nm and below. We find that dimensionality reduction has a significant effect on the phonon dispersion, in converting one of the TA modes of the bulk to an out-of-plane ZA mode in the membranes. Dimensional reduction has the direct consequence of suppression of group velocities of phonons and leads to a 3-fold reduction in the thermal conductivity of the membranes with respect to bulk silicon. The reduction alone is not sufficient to bring down the thermal conductivity in the membranes but with the presence of surface nanostructures, by means of pattern formation and surface oxidation, it leads to a 25-fold reduction in the in-plane thermal conductivity of the membranes for membranes with high surface to volume ratio. This implies a 25-fold enhancement of the thermoelectric figure of merit at room temperature. Such figures make nanostructured silicon membranes viable materials for thermoelectric units.

Acknowledgment: This project is funded by the program FP7-ENERGY-2012-1-2STAGE under contract number 309150

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