Evaluating Thermal Transport at The Axial Junction of Si-Ge Composite Nanowires

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Abstract

In this work, thermal transport is calculated for silicon-germanium (Si-Ge) composite nanowires that have curved interfaces at the axial junction between the two materials. This is done for regular straight and bent (floppy) wire categories. In real-life nanowire forests, there will be some bent wires present. We use the Müller-Plathe method, which is based on non-equilibrium molecular dynamics (NEMD), with the Tersoff potential to model thermal transport in nanowires with lengths ranging between 100 – 550 nm for two wire diameters in LAMMPS. We consider a range of curvatures at the junction between Si and Ge. The interfacial resistance at the axial junctions is also evaluated. The direction of heat flow, relevant to thermal rectification applications, is also taken into account, i.e., geometries are modeled for heat flowing from Ge(hot) to Si(cold) and vice-versa.

Introduction

To further the development of different materials for applications in thermal management and several industrial uses, we need to understand thermal transport across interfaces fully. The mechanical and thermal attributes of solid systems can be strongly dependent on these interfaces if present. Interfaces can act as a barrier to efficient thermal transport. Thermal transport in small-scale heterogeneous systems is controlled by interfacial resistance because of the large surface-to-volume ratio. This study will further our understanding of phonon thermal transport and the role of boundary scattering at the interfaces of low-dimensional materials. Our choice of nanowires, Si and Ge can be experimentally [1] synthesized in several ways. A stringent minimization criterion is used to enforce bending in the second group of systems such that the bent wires are also structurally relaxed.

Results

Thermal conductivity values calculated using the Müller-Plathe method, are plotted in Fig. **1** and Fig. **2** as a function of the wire length for all regular wire geometries. In addition to curved interfaces, the thermal conductivities of flat heterojunctions are also presented, labeled Si|hot| and Ge|hot|. In this set of data, we can easily observe that thermal conductivity (κ) increases with an increase in wire length, with some anomalies. Anomalies largely stem from the presence of resonating frequencies that lead to oscillations in the wires. For the bent counterparts (Fig. **4**), we observe an uncharacteristic decrease in thermal conductivity as length is increased with some outliers. This is likely the result of additional scattering due to the curvature of the nanowires.

In part due to limitations in the methodology employed, minimal changes are observed in the thermal conductivity of the wires due to interfacial curvature. Preliminary interfacial resistance calculations help shed light on the role of heterojunction curvature. We observe that notwithstanding the diameter being considered (5.43 or 10.86 nm), the resistance in Ge(hot) is lower than in Si(hot), as expected. It appears that, as a result, for thermal transport between Si(hot) and Ge(cold), larger curvatures (and thus interfacial surface areas) lead to slightly higher interfacial resistances, a trend that is not observed for transport between Ge(hot) and Si(cold), as shown in Fig. **5** and Fig. **6**. Further analysis is being conducted to fully understand these sets of results.

Acknowledgment

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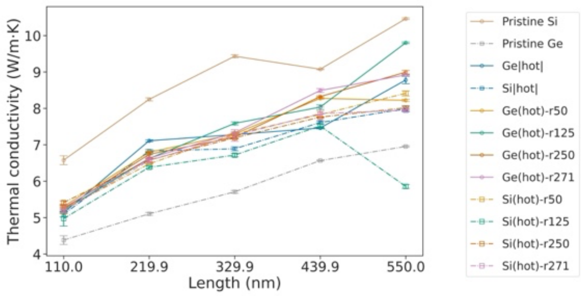

Fig. **1**. Size-dependent thermal conductivity of Ge(hot) and Si(hot) supercells with diameters of 5.43 nm for regular wires

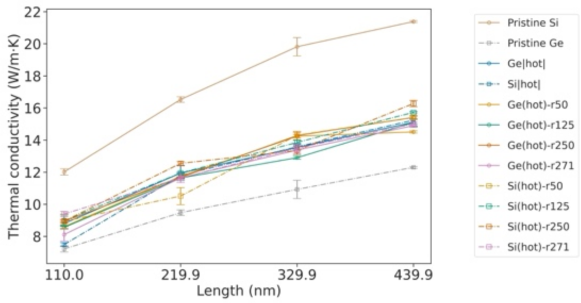

Fig. **2**. Size-dependent thermal conductivity of Ge(hot) and Si(hot) supercells with diameters of 10.8 nm for regular wires

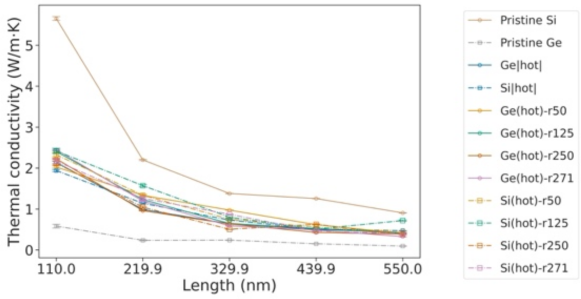

Fig. **3**. Size-dependent thermal conductivity of Ge(hot) and Si(hot) supercells with diameters of 5.43 nm for bent wires

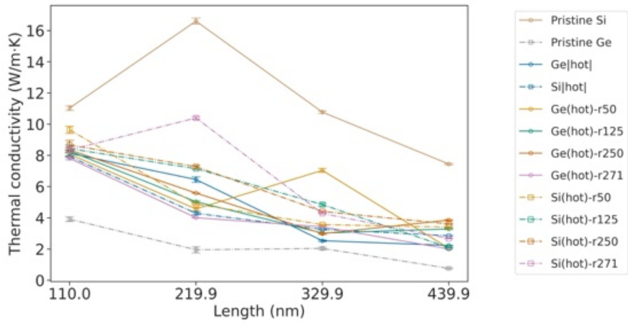

Fig. **4**. Size-dependent thermal conductivity of Ge(hot) and Si(hot) supercells with diameters of 10.86 nm for bent wires

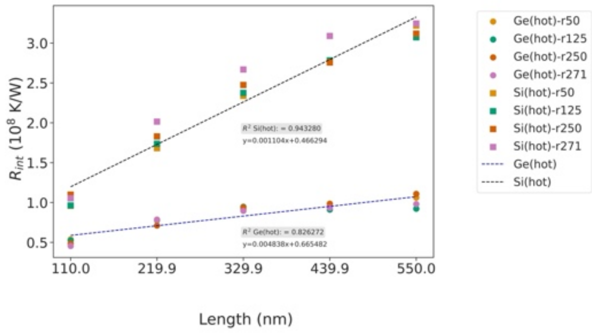

Fig. **5**. Interfacial resistance of Ge(hot) and Si(hot) across all sizes for 5.43 nm diameter wires for regular wires

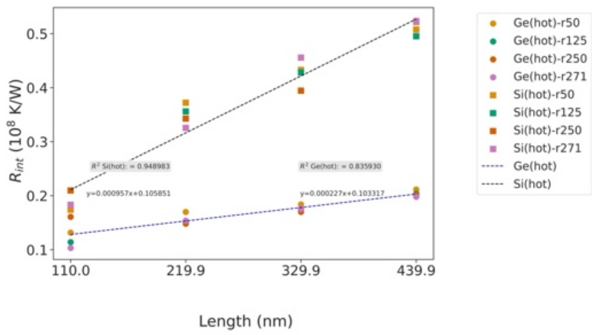

Fig. **6**. Interfacial resistance of Ge(hot) and Si(hot) across all sizes for 10.86 nm diameter wires for regular wires