Thermal Boundary Resistance Predictions with Non-Equilibrium Green's Function and Molecular Dynamics Simulations

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Semiconductor heterostructures are widely used in the design of devices such as quantum cascade laser, transistors and thermoelectric devices. Scattering of thermal energy carriers at the interface between two solids results in thermal boundary resistance. Thermal boundary resistance was previously reported to be comparable to that of pure material with length of few to tens of nanometers [1] so that it cannot be neglected in systems of nanoscale. The non-equilibrium molecular dynamics (NEMD) method is often used to atomically model the thermal boundary resistance at interfaces since it has a good agreement with experiments [2]. The non-equilibrium Green's function (NEGF) method allows for atomic resolution and is widely accepted as one of the most consistent methods for transport properties in nanodevices in the presence of quantum phenomena including quantum confinement, tunneling, interferences, etc. However, the NEGF method has been used predominantly in the coherent (harmonic) phonon transport regime due to the fact that the inclusion of incoherent mechanisms usually requires solution of Green's functions and polarization graphs in the self-consistent Born approximation which entails a large numerical load [3]. In this work, a numerically highly efficient method to solve phonon transport in the NEGF framework including incoherent scattering phenomenologically (with Büttiker probes) is benchmarked against NEMD. For simplicity, the benchmark system is chosen to be an atomically resolved interface of Si/"heavy-Si". Nonzero interface resistance results in homogeneous structures that plague Landauer approaches [4] are absent in the presented NEGF approach. The thermal boundary resistance calculated by NEGF is compared with NEMD and shows good agreement. Subtle discrepancies of the methods are explained. Additional spectral transport information is extracted from NEGF, which shows that the different phonon modal contributions play an important role in thermal transport across the interface. This work confirms the reliability of scattered phonon NEGF and promotes its unique numerical and physical benefits for phonon transport nanodevice applications (full quantum mechanics, spectral approach compatible with periodicity, scalable method, etc.).

[1] E. S. Landry et al, *Phys. Rev. B*, vol. 80, no. 16, 2009. [2] P. K. Schelling et al, *Phys. Rev. B*, vol. 65, no. 14, 2002. [3] M. Luisier, *Phys. Rev. B*, vol. 86, no. 24, 2012. [4] G. Chen, *Appl. Phys. Lett.*, vol. 82, no. 6, 2003.

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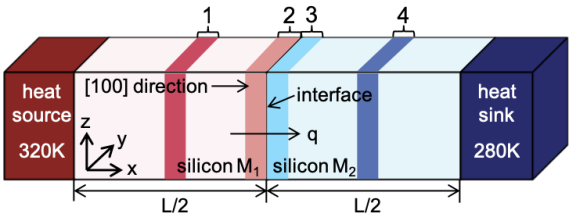

Figure.1: Simulation domain considered in this work. Left side is Si with mass M_1=28.085, right side is heavy Si with mass M2. Temperature in the heat source and hear sink are 320K and 280K, respectively. NEGF has semi-infinite leads while as NEMD has finite length reservoirs. Regions 1~4 marked by numbers are three atomic layers at middle of Si, left to the interface, right to the interface and middle of heavy Si, respectively.

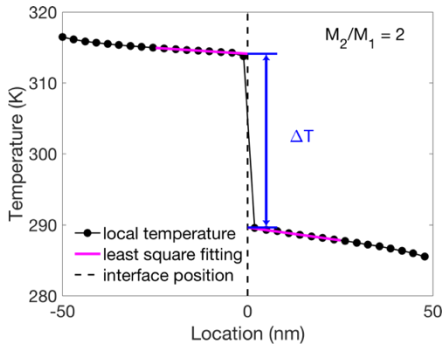

Figure.2: Schematic of extraction of the boundary thermal resistance. Linear fitting of local temperature inside Si and heavy Si, ΔT is obtained at the interface location. The thermal boundary resistance is equal to ΔT/q with q being the heat flux.

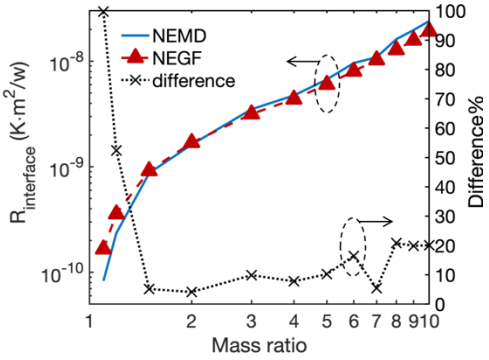

Figure.3: Thermal boundary resistance vs mass ratio calculated by two methods. Dashed line is percentage difference between the two methods defined as (NEGF-NEMD)/NEMD x 100%.

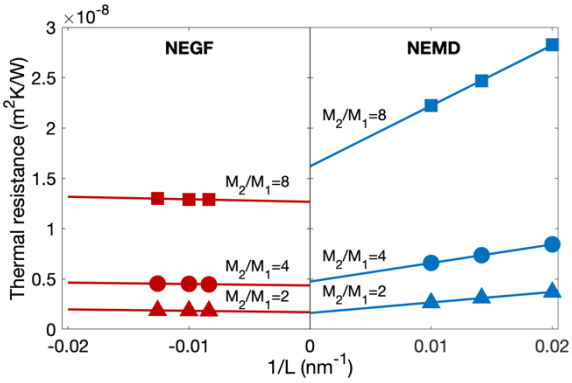

Figure.4: Linear extrapolation for NEGF and NEMD for three mass ratio values. NEMD results show a stronger dependence on the length of the device. True open boundary conditions of NEGF give virtually size independent results.

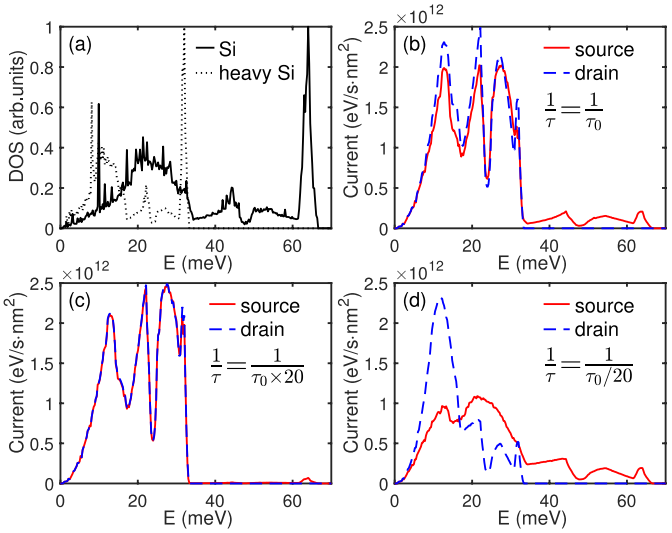

Figure.5: (a) Energy resolved (k integrated) DOS in Si and heavy Si leads. (b)~(d) Energy resolved (k integrated) net current of NEGF calculated with normal, artificially weak and artificially strong scattering strengths, respectively. The results reveal that stronger scattering increases inelastic processes and put the system in more pronounced local thermodynamic equilibrium.

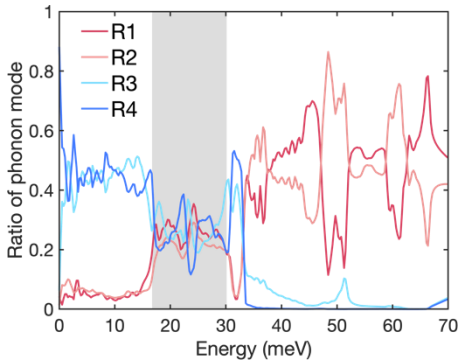

Figure.6: The ratio of the phonon mode in regions 1~4 is defined as $R_i = \|\phi_i(\omega)\|/\|\phi_{tot}(\omega)\|$, where i is the region index and $\|\phi_{tot}(\omega)\| = \sum_{i=1}^{4}\|\phi_i(\omega)\|$. The evenly distributed phonon modes around 20 meV (marked by the gray area) results in the highest current peak at 22 meV (see Fig. 5(b)) although having a low DOS and group velocity. This result shows that the different phonon modal contributions play an important role in determining the energy current flow across the interface.