Thermal boundary conductance of Si/Ge interface by anharmonic phonon non-equilibrium Green function formalism

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Understanding heat transport at solid-solid interface is crucial for both the fundamentals of thermal science and the engineering applications such as thermal management in semiconductor devices. The role of anharmonic phonon-phonon scattering at interface has been investigated by the classical molecular dynamics (MD) simulation and also by quantum modeling via the non-equilibrium Green's function (NEGF) formalism recently. However, the investigations on the role of lattice anharmonicity on heat transport at interface remain inconclusive.

In this report, we study the heat transport at an ideal smooth Si/Ge interface shown in Figure 1(a) by a validated anharmonic phonon NEGF formalism developed in our recent work [1]. As shown in Figure 1(b) and Figure 1(c), the thermal boundary conductance predicted by the anharmonic NEGF is higher than that by the harmonic one, because of the new inelastic channels opened by the anharmonic phonon scattering beyond the cut-off frequency of Ge demonstrated in Figure 1(d). The increase of thermal boundary conductance due to anharmonic phonon scattering is around 10% at room temperature and reaches about 15% at 500K. Those figures are much smaller than the ones of a recent study [2] based on an unverified anharmonic NEGF. Our result is qualitatively consistent with some previous MD works which show that the anharmonicity near the interface is more important than that at the interface. Our work will promote a clarification of the role of lattice anharmonicity in heat transport at interface.

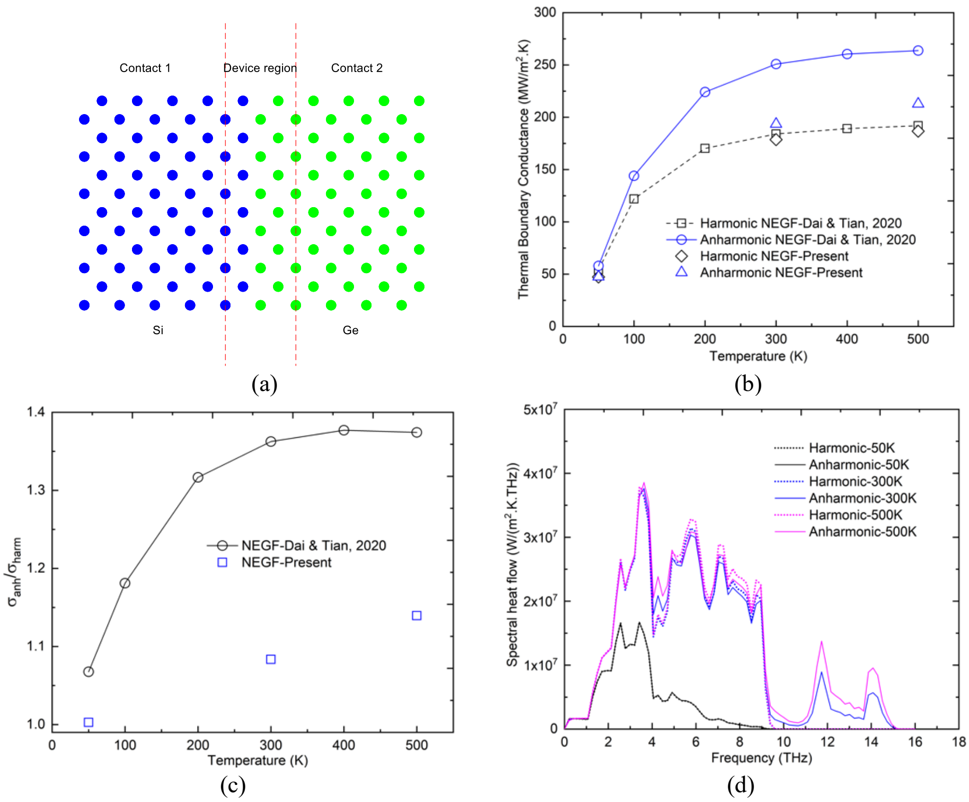

Figure 1. Heat transport at smooth Si/Ge interface by anharmonic phonon non-equilibrium Green's function (NEGF) formalism: (a) schematic of physical model, with the anharmonic phonon scattering only considered in the interface device region; (b) temperature-dependent thermal boundary conductance; (c) thermal boundary conductance ratio from anharmonic NEGF (σ_{anh}) and harmonic NEGF (σ_{harm}); (d) spectral heat flow from Si (contact 1) to the interface (device region).

[1] Y. Guo, M. Bescond, Z. Zhang, M. Luisier, M. Nomura and S. Volz, Phys. Rev. B 102, 195412(2020).
[2] J. Dai and Z. Tian, Phys. Rev. B 101, 041301(R) (2020).

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