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Phonon transmission across Si/Ge interface from first-principles by the Green's function method[1] ZHITING TIAN, KEIVAN ESFARJANI, GANG CHEN, MIT — Modeling phonon transmission as a function of phonon frequency and incidence angle is vital for multiscale modeling of heat transport in nanostructured materials. In this study, we calculate the phonon transmission in three-dimensions via Green's function method. It will be applied to silicon/germanium interface for which the force constants will be calculated from either the Stillinger-Weber semi-empirical potential, or from first-principles density functional methods. Both the perfect interface and the rough interface will be investigated. The transmission as a function of interface roughness will give us more guidance for surface engineering. Results between first-principles and the SW potential will be compared to see how reliable the predictions from SW potential are. The contribution of optical modes is illustrated by comparing the results will the prediction of the acoustic mismatch model (AMM) which is also harmonic and the long-wavelength limit of the general theory. It will now be possible to integrate the information on momentum and frequency-dependent transmission and the bulk mean free paths, both calculated from first-principles DFT, to accurately model heat transport in complex nanostructured materials.

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