Boltzmann model for lattice thermal conductivity in nanostructures

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The common approach to account for the phonon scattering by boundaries in Boltzmann models is to introduce a relaxation time whose expression is given by Casimir theory, modified with specularity factors. Such an approach is physically reasonable when the other phonon scattering mechanisms can be ignored. In the case where interplay between the various phonon scattering processes is present, the widely used Casimir theory turns out to be physically inappropriate to describe the overall phonon scattering rate in the crystal, and a more general theory for the phonon scattering rate becomes essential to predict the lattice thermal conductivity. This theory would be of utmost importance to predict the lattice thermal conductivity in nanosized materials because in such materials the phonon-boundary scattering mechanism coexists with other phonon processes over a wide temperature range. Furthermore, in the case of nanosized materials (where surface to volume ratio is not negligible), interaction takes place between the surface phonons and the volume phonons. This may lead to a significant modification in the phonon scattering rate. Indeed, such a surface effect should be described by a fundamental treatment rather than simple specularity factors.

In this contribution we tackle all these issues and present an accurate Boltzmann model for the lattice thermal conductivity in nanosized materials. In order to generate expressions for the rates at which phonons are scattered by the boundaries of a finite crystal in the presence of intrinsic scattering and alloy scattering mechanisms, we solve Boltzmann equation for phonons in a finite crystal with taking into account the physical nature of the phonon processes and the spatial dependence of the phonon distribution function. We derive the phonon eigenfrequencies of the nanostructures that are key determinants of the lattice thermal conductivity from elasticity theories to account for the size effect and the Brillouin zone folding. We account for the effects of surfaces by considering the contribution of surface phonons to the lattice thermal conductivity. The reliability of the developed model is demonstrated clearly with reference to reported experimental data regarding the effects of the size and composition on the lattice thermal conductivity of SiGe nanostructures.