Nanophononics: dissipation and thermoelectric energy conversion in nanoscale devices

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Thermal dissipation in increasingly scaled MOS devices has prompted strong interest in both phonon emission and subsequent thermal transport in semiconductor nanostructures. New multi-gate devices designs further exacerbate thermal issues by further localizing heat dissipation. Simultaneously, dwindling energy resources have created renewed interests in thermoelectric (TE), or solid-state, energy conversion and refrigeration using semiconductor-based nanostructures, such as nanowires, nanoribbons, and superlattices. TE conversion is also an attractive approach for targeted cooling of local hotspots inside integrated circuits due to inherently no moving parts, ease of miniaturization and on-chip integration, and the nanostructures' enhanced TE conversion efficiency. In addition, thermoelectric power generation enables the reuse of waste heat in a variety of applications, from low-power and energy-efficient designs all the way up to internal combustion engines and solar cells. Beyond mere dissipation, nanoscale thermal effects can be used in a broad range of applications such as thermal rectification, sensing, and detection. In this talk, I will present techniques for numerical simulation and modeling of phonon transport in a broad range of nanostructures, focusing primarily on modeling extrinsic and disorder effects such as grain/sample boundaries, interfaces, edges, and alloy mass disorder. The talk revolves around numerically solving the phonon Boltzmann transport equation (pBTE), while the salient feature of the work is that it employs a full phonon dispersion combined with a momentum-dependent model of phonon boundary scattering.