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Thermal transport of III-V semiconductor materials and superlattices based on molecular dynamics with optimized Tersoff potentials[1]

SONG MEI, IRENA KNEZEVIC, Univ of Wisconsin, Madison — III-V compound semiconductor materials are widely used in optoelectronics devices. III-V superlattices (SLs) make the active core of quantum cascade lasers (QCLs). Achieving room-temperature (RT), high-power, and continuous-wave (CW) operation in QCLs hinges on the understanding and engineering of thermal transport in the layers and across the interfaces. Cations in III-V ternary alloys differ a lot in mass and this effect on thermal transport is hard to capture using the scattering rates deduced from common perturbation theories. Molecular dynamics (MD) simulations can explicitly take the mass difference into consideration and are suitable for calculating the bulk thermal conductivity of III-V ternary alloys. Furthermore, the morphology and anharmonic interactions at an interface are naturally captured in MD, leading to an accurate description of interfacial transport. We adopt the Tersoff-type potentials for III-V binaries and optimize them according to acoustic phonon dispersions in order to capture thermal properties. The optimized potential is then used to directly compute the thermal boundary resistance at a heterojunction interface, as well as the thermal conductivity in the SL as a whole.

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