Thermal transport in III-V semiconductor materials and superlattices based on molecular dynamics with optimized tersoff potentials

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III–V compound semiconductor materials are widely used in high-speed electronic and optoelectronics devices. III–V superlattices (SLs) make the active core of quantum cascade lasers (QCLs). Despite the wide popularity of III–V materials and III–V SLs, phonon transport in such materials and nanostructures, especially those involving ternary alloys, is still poorly understood.

The dominant scattering mechanism in III–V ternary alloys is mass-difference scattering. In previous efforts to describe the thermal conductivity of bulk III-V ternary alloys, the virtual crystal approximation (VCA) together with the Klemens-Callaway model was often employed [1]. However, the cation masses in III–V ternary alloys can differ a great deal (e.g., m_{Al}=26.98 au, m_{In}=114.82 au). As a result, a simple first-order perturbation model like the VCA cannot accurately capture the influence that mass-difference scattering has on thermal conductivity in these systems. Molecular dynamics (MD) simulations treat atoms as classical particles following Newton's law of motion and explicitly consider the mass of each atom. Therefore, mass-difference scattering in III–V ternary alloys can be fully captured in MD simulations. In addition, all orders of the anharmonic phonon–phonon interactions are implicitly included in MD simulations, which is impossible in many other models.

To simulate III–V ternary alloys using MD, we adopt Tersoff-type nearest-neighbor potentials for III–V binaries [2]. Most reported potentials are parameterized to best capture the mechanical properties of these materials [3]-[5]. We further optimize these potentials to achieve agreement with acoustic-phonon dispersions, which ensures they are better suited for the calculation of thermal properties. We use equilibrium MD (EMD) simulations together with the Green-Kubo method to calculate the thermal conductivity of both binary crystals and ternary alloys. In ternary alloys, we simulate multiple random alloy structures and take the average to obtain the bulk thermal conductivity.

Furthermore, to study III–V SLs, the morphology of the interfaces can naturally be explicitly captured in MD, leading to an accurate description of interfacial transport. Nonequlibrium MD (NEMD) can provide insight into thermal transport across interfaces, and we will employ it to calculate the anisotropic thermal conductivity tensor in III–V SLs.

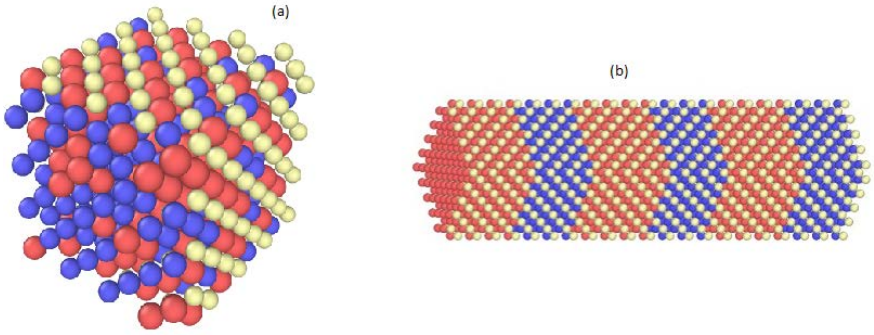

Figure 3. Sample simulation cells for (a) an InGaAs bulk alloy and (b) a InAs/GaAs superlattice. Red atoms represent Ga, blue atoms represent In, and yellow atoms represent As.

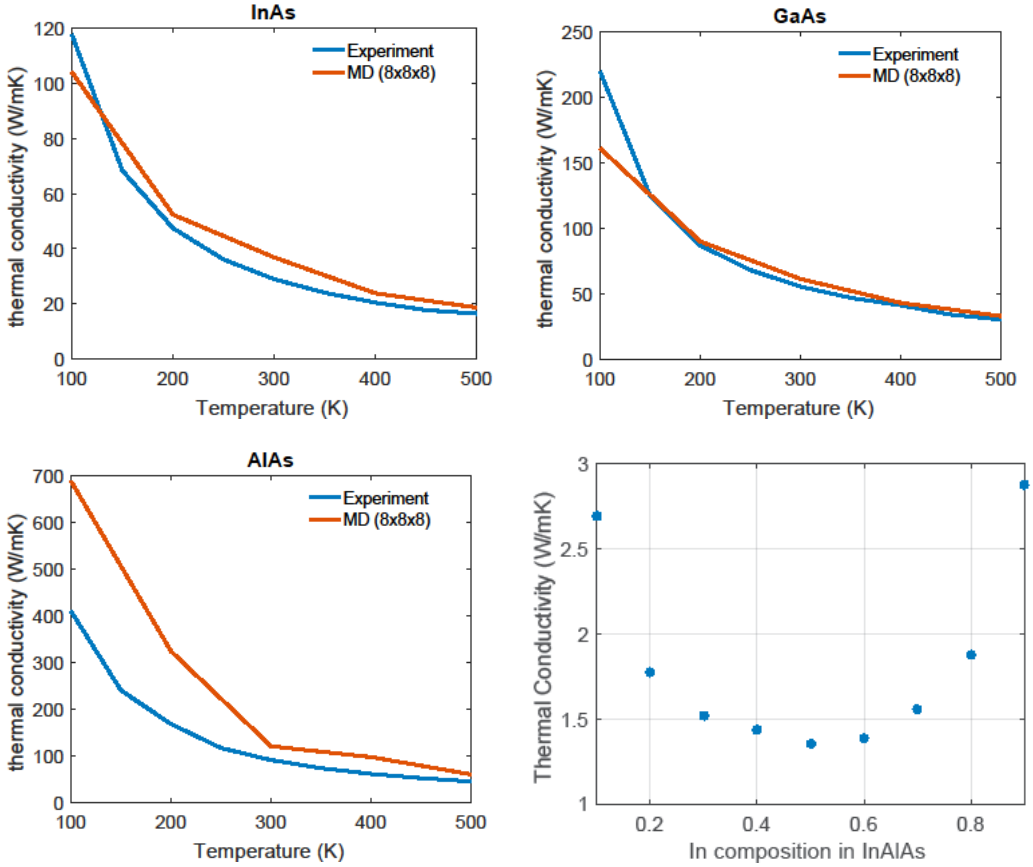

Figure 2 : Preliminary calculations of the thermal conductivity from EMD, for binary InAs (top left), GaAs (top right), and AlAs (bottom left) as a function of temperature (EMD is technically accurate only above the Debye temperature). (Bottom right) The room-temperature thermal conductivity versus In content in ternary InAlAs.

[1] B. Abeles, "Lattice Thermal Conductivity of Disordered Semiconductor Alloys at High Temperatures," Phys. Rev. 131, 1906 (1963).

[2] J. Tersoff, "Modeling solid-state chemistry: Interatomic potentials for multicomponent systems," Phys. Rev. B 39, 5566 (1989).

[3] M. Sayed, J.H. Jefferson, A.B. Walker, and A.G. Cullis, "Molecular dynamics simulations of implantation damage and recovery in semiconductors," Nucl. Instr. Meth. Phys. Res. B 102, 218 (1995).

[4] D. Powell, M. A. Migliorato, and A. G. Cullis, "Optimized Tersoff potential parameters for tetrahedrally bonded III-V semiconductors," Phys. Rev. B 75, 115202 (2007).

[5] T. Hammerschmidt, P. Kratzer, and M. Scheffler, "Analytic many-body potential for InAs/GaAs surfaces and nanostructures: Formation energy of InAs quantum dots," Phys. Rev. B 77, 235303 (2008).