Role of interface mixing on coherent heat conduction in periodic and aperiodic superlattices

Abstract

This project seeks to advance our understanding of the mechanics of heat propagation in nanoscale thermo-electronic devices. We utilize the molecular dynamics-based phonon wave-packet method to simulate how phonons transmit through materials featuring secondary periodicity, such as superlattices. A phonon, which quantifies the vibrations of atoms in solids, is the primary carrier of heat in most semiconductors and insulators. By enhancing our understanding of phonon transmission, we can facilitate the production of more efficient thermoelectric materials. Materials with improved energy conversion efficiency can tackle challenges in renewable energy, such as excessive waste heat in energy production and over-reliance on fossil fuel sources. Furthermore, efficient thermoelectric materials can expand the mission capabilities of NASA rovers and probes that utilize thermoelectricity for power generation.