

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

Theodore Maranets, Evan Doe, Yan Wang

Superlattices (SLs) can induce phonon coherence through the periodic layering of two or more materials, enabling tailored thermal transport properties. While most theoretical studies assume atomically sharp, perfect interfaces, real SLs often feature atomic interdiffusion spanning approximately a single atomic layer or more. Such interface mixing can significantly influence phonon coherence and transport behavior. In this study, we employ atomistic wave-packet simulations to systematically investigate the effects of interface mixing on coherent heat conduction. Our analysis identifies two competing mechanisms that govern phonon transport across mixed interfaces: (1) Interface mixing disrupts coherent mode-conversion effects arising from the interface arrangement. (2) The disorder enhances the potential for interference events, generating additional coherent phonon transport pathways. The second mechanism enhances the transmission of Bragg-reflected modes in periodic SLs and most phonons in aperiodic SLs, which otherwise lack coherent mode-conversion in perfect structures. Conversely, the first mechanism dominates in periodic SLs for non-Bragg-reflected modes, where transmission is already high due to substantial mode-conversion. These findings provide insights into the interplay between interface imperfections and phonon coherence.

Arxiv Link

<https://arxiv.org/abs/2501.17346>