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Interface Conductance Modal Analysis KIARASH GORDIZ, ASEGUN HENRY, Georgia Institute of Technology — Reliably and quantitatively calculating the conductance of phonons across an interface between two materials has been one of the major unresolved questions in thermal transport physics for the last century. Theories have been presented in this regard, but their predictive power is limited. A new formalism to extract the modal contributions to thermal interface conductance with full inclusion of temperature dependent anharmonicity and all of the atom level topography is presented. The results indicate that when two materials are joined a new set of vibrational modes are required to correctly describe the transport across the interface. The new set of vibrational modes is inconsistent with the physical picture described by phonon gas model (PGM), because some of the most important modes are localized and non-propagating and therefore do not have a well-defined velocity nor do they impinge on the interface. Among these new modes, certain classifications emerge, as most modes extend at least partially into the other material. Localized interfacial modes are also present and exhibit a high conductance contribution on a per mode basis by strongly coupling to other types of vibrational modes. We apply our formalism to different interfaces and present thermal interface conductance accumulation functions, two-dimensional cross-correlation matrices, and a quantitative determination of the contributions arising from inelastic effects. The provided new perspective on interface thermal transport can open new gates towards deeper understanding of phonon-phonon and electron-phonon interactions around interfaces.

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