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Calculation of modal contributions to thermal transport across Si/Ge and $In_{0.53}Ga_{0.47}As$/InP interfaces KIARASH GORDIZ, ASEGUN HENRY, Georgia Institute of Technology — Reliable and quantitative calculation of the conductance of different phonons across an interface can have a significant impact on the applications where thermal interface resistance is limiting and can aid in the rational design of thermal interface materials. A new formalism for extracting the modal contributions to thermal interface conductance with full inclusion of temperature dependent anharmonicity and all of the atom level topography is presented. Application of the formalism to Si/Ge and $In_{0.53}Ga_{0.47}As$/InP interfaces reveals fundamental information on the nature of the vibrational modes involved in heat transfer and the interactions/correlations among them. Four distinct classes of vibrational modes are detected for the two interfaces. For Si/Ge interface, the density of states for these vibrational classes are completely mixed, while surprisingly for $In_{0.53}Ga_{0.47}As$/InP interface they are completely segregated. For Si/Ge interface, interfacial modes, located around 12THz, contribute near 20% to the total conductance, while for $In_{0.53}Ga_{0.47}As$/InP interface, low frequency extended modes contribute more than 50% to the total conductance, which is even larger than the maximum predicted contribution by phonon gas model. Temperature dependent anharmonicity analysis shows that increasing temperature decreases the contribution by extended modes and increases the contribution by partially extended modes. In both of the interfaces, Interfacial modes exhibit the maximum per mode contribution.

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