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Interface Conductance Modal Analysis ASEGUN HENRY, Georgia Institute of Technology — A formalism termed the interface conductance modal analysis (ICMA) method will be presented, which allows for calculations of the modal contributions to thermal interface conductance within the context of molecular dynamics (MD) simulations, which inherently include anharmonicity to full order. The eigen modes of vibration are calculated from harmonic lattice dynamics (LD) calculations, however the generality of ICMA formalism also allows for incorporation of anharmonic LD results into the calculations. The formalism itself is based on a modal decomposition of the heat flow across an interface, which is then substituted into expressions for the conductance either based on equilibrium or nonequilibrium MD. Several example cases will be covered and the interesting insights that emerge from the ICMA analyses will be discussed in detail. The ICMA method enables more in-depth study of various effects such as temperature, anharmonicity, interdiffusion, roughness, imperfections, dislocations, stress, changes in crystal structure through a single unified model, as it can essentially treat any material or object where the atoms vibrate around equilibrium sites (e.g., ordered or disordered solids and molecules).

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