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Modal Contributions to Heat Conduction across Crystalline and Amorphous Si/Ge Interfaces KIARASH GORDIZ, ASEGUN HENRY, Georgia Institute of Technology — Until now, our entire understanding of interfacial heat transfer has been based on the phonon gas model and Landauer formalism. Based on this framework, it is difficult to offer any intuition on heat transfer between two solid materials if one side of the interface is an amorphous structure. Here, using the interface conductance modal analysis (ICMA) method, we investigate the modal contributions to thermal interface conductance (TIC) through crystalline (c) and amorphous (a) Si/Ge interfaces. It is revealed that around 15% of the conductance through the cSi/cGe interface arises from less than 0.1% of the modes of vibration in the structure that exist between 12-13THz and because of their large eigenvectors around the interface are classified as interfacial modes. Correlation maps show that these interfacial modes exhibit strong correlations with all the other modes. The physics behind this strong coupling ability is studied by calculating the mode-level harmonic and anharmonic energy distribution among all the atoms in the system. It is found that these interfacial modes are enabled by the large degree of anharmonicity near the interface, which is higher than the bulk and ultimately allows this small group of modes to couple to other modes of vibration. In addition, unlike the cSi/cGe, correlation maps for aSi/cGe, cSi/aGe, and aSi/aGe interfaces show that the majority of contributions to TIC arise from auto-correlations instead of cross-correlations. The provided analysis sheds light on the nature of localized vibrations at interfaces and can be enlightening for other investigations of localization.

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