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How intermixing and anharmonicity enhances interfacial thermal conductance?[1] CARLOS POLANCO, JINGJIE ZHANG, NAM LE, ROUZBEH RASTGARKAFSHGARKOLAEI, PAMELA NORRIS, AVIK GHOSH, Univ of Virginia — The thermal conductance at an interface, whether ballistic or diffusive, can be expressed as a product of the number of conducting channels (M) and their average transmission (T). The common expectation is that interfacial defects reduce T and thus hurt the conductance. This is however at odds with recent simulations showing that a thin intermixing layer can in fact enhance the conductance. We argue that such an enhancement occurs when the increase in number of modes outweighs the reduction in their average transmission. The new channels open as a result of (a) the random interfacial structure that relaxes the conservation rules for the transverse momentum and promotes transitions between formerly symmetry disallowed channels; and (b) inelastic scattering through phonon-phonon interactions that allow modes beyond the contact cut-off frequency to contribute to transport. We use these results to build a back of the envelope model for interfacial conductance that depends on the mixing distribution, the anharmonic strength, the phonon polarization and wavelength. Non-Equilibrium Green's Function (NEGF) as well as Molecular Dynamics (MD) simulations on Si/mixed layer/Ge, as well as simpler FCC crystals support our results.

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