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Non-equilibrium Molecular Dynamics Study of the Thermal Resistance at the Interface Between Two Materials JOHN LYVER IV, ESTELA BLAISTEN-BAROJAS, Computational Materials Science Center, George Mason University, Fairfax, VA 22030 — Two different crystalline systems comprised of atoms interacting through Lennard-Jones (LJ) potentials were set in contact. The thermal conduction through such solid-solid interface was studied as a function of temperature and relative materials parameters, where the species differ in mass, hard-core atomic diameter and well depth. The computational setup simulated a solid sample with two different materials separated at a central interface. A non-equilibrium Molecular Dynamics approach was taken to calculate the Kapitza thermal resistance across the interface and its dependence on the two species and LJ parameters. It is found that the Kapitza resistance decreases as a function of temperature for mostly all combinations of the two materials LJ parameters.

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