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Thermal Boundary Resistance Across Solid-Fluid Interface<sup>1</sup> SANGHAMITRA NEOGI, DAVIDE DONADIO, Max-Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz - Germany — The recent advances in the field of nanotechnology, specially the advent of nanostractures and nanocomposite materials, have prompted an increased interest in the study of thermal transport across interfaces. When heat flows across an interface, the local temperature presents a discontinuity which is related to the thermal boundary resistance (TBR), also known as the Kapitza resistance. The investigation of Kapitza resistance has important technological applications in the improvement of the thermal performances of composite materials. The current theoretical understanding of TBR is primarily based on the "acoustic mismatch theory" or the "diffusive mismatch model." Both these models consider only the bulk properties of the two materials, with no account being taken of the details of the material properties near the interface. Here, we investigate the thermal transport across a model solid-fluid interface using the technique of reverse non-equilibrium molecular dynamics simulations. The interaction potentials between the particles in our system are governed by the Lennard-Jones potential. We study the influence of pressure on the thermal boundary resistance for a range of mismatched interfaces and compare our results to the existing analytical models.

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