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Correlations at Liquid/Solid Interfaces Relating Molecular Configurational Effects to the Kapitza Resistance[1] HIROKI KAIFU, SANDRA TROIAN, California Institute of Technology, 1200 E. California Blvd., MC 128-95, Pasadena, CA 91125 — Todays electronic systems for banking, medicine and transportation rely critically on ever more powerful integrated chips which can generate local power densities in excess of 100 W/cm^2 leading to catastrophic thermal failure. Such excess heat has become *the limiting factor* in information processing. Liquid cooling is therefore being used to mitigate this problem. Fundamental understanding of thermal resistance at liquid/solid (L/S) interfaces is therefore indispensable to future design. Interfacial thermal transport is normally quantified by the Kapitza resistance although its relation to phonon transport at L/S interfaces is still lacking. Computational studies have mostly focused on the effects of liquid wettability and contact density, whose enhancement favors formation of absorbed layers that lower the resistance. Using non-equilibrium molecular dynamic simulations of a monoatomic Lennard-Jones liquid confined between solid walls, we examine interface configuration effects by varying the intermolecular distance representing the L/S potential minimum. These studies reveal how configuration of the liquid and solid molecules at the interface in the absence of liquid flow controls the magnitude of the Kapitza resistance.

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