Abstract Submitted for the MAR06 Meeting of The American Physical Society

Interfacial thermal transport at Liquid-Liquid and Biomolecular Interfaces PAWEL KEBLINSKI, NATALIA SHENOGINA, HARSHIT PATEL, SHEKHAR GARDE, Renssealer Polytechnic Institute — Systems with nanoscopic features contain a high density of interfaces. Thermal transport in such systems can be governed by the resistance to heat transfer of the interface. Although soft interfaces, such as those between immiscible liquids or between a biomolecule and solvent, are ubiquitous, few studies of thermal transport at such interfaces have been reported. Here we characterize the interfacial conductance, i.e., the inverse of the interfacial resistance, of soft interfaces as a function of molecular architecture, chemistry, and the strength of cross-interfacial intermolecular interactions through detailed molecular dynamics simulations. The conductance of various interfaces studied here, for example, water-organic liquid, water-surfactant, surfactant-organic liquid, is relatively high (in the range of 65-370 MW/m2/K) compared to that for solid-liquid interfaces (10 MW/m2/ K). Interestingly, the dependence of interfacial conductance on the chemistry and molecular architecture cannot be explained solely in terms of either bulk property mismatch or the strength of intermolecular attraction between the two phases. We will also discuss vibrational mode dependent thermal coupling at biomolecule-water interfaces.

> Pawel Keblinski Rensselaer Polytechnic Institute

Date submitted: 02 Dec 2005

Electronic form version 1.4