Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Impact of adhesion on thermal boundary conductance at organic-metal interface[1] Y. JIN, C. SHAO, J. KIEFFER, K.P. PIPE, M. SHTEIN, University of Michigan, Ann Arbor — The thermal boundary conductance (TBC) at the interfaces between a small molecular organic semiconductor (copper phthalocyanine CuPc) and several metals (Al, Mg, Au, Ag) has been measured using the 3-omega method at room temperature. The TBC increases with the interfacial bonding strength of the two dissimilar materials. Our measurements of adhesion between the metal and organic films agree qualitatively with the distances between the metal surface and CuPc molecules measured by Stadtmüller et al. [1]. In contrast to the trend observed for organic-metal interfaces, the TBC of organic-organic interfaces (e.g. CuPc/C60) is insensitive to interface bonding due to the large overlap between materials' phonon density of states. Conventional acoustic and diffuse mismatch models fail to describe the observed trend in TBC. Modifying the acoustic mismatch model (AMM) with an effective spring constant describing interfacial bonding, an accurate trend is obtained. To better understand the influence of the molecular structure on TBC, we performed molecular dynamics simulations of interfacial heat transfer and interfacial bonding. These simulations reveal quantitative discrepancies in the simulated TBC relative to that predicted by the modified AMM model in the regime of poor interfacial adhesion, which we attribute to a greater contribution of anharmonicity. The bonding strength for vacuum deposited films is $\sim$2 GPa for CuPc/Ag and CuPc/Au, well within the regime in which anharmonic processes play an important role in interface thermal transport. [1] Stadtmüller et al. *PRB* 83 085416

[1]We acknowledge the financial support of this work by Air Force Office of Scientific Research MURI program. Grant No. FA9550-08-1-0340

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Date submitted: 21 Nov 2011 Electronic form version 1.4