Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Molecular dynamics simulation investigations of atomic-scale wear YUCHONG SHAO, MICHAEL FALK, Johns Hopkins University — Frictional running-in and material transfer in wear take place at the micro- and nanoscale but the fundamental physics remain poorly understood. Here we intend to investigate wear and running-in phenomena in silicon based materials, which are widely utilized in micro/nano electromechanical systems(MEMS/NEMS). We use an atomic force microscopy (AFM) model composed of a crystalline silicon tip and substrate coated with native oxide layers. Molecular dynamics simulation has been performed over a range of temperatures, external loads and slip rates. Results show that adhesive wear takes place across the interface in an atom-by-atom fashion which remodels the tip leading to a final steady state. We quantify the rate of material transfer as a function of the coverage of non-bridging oxygen (NBO) atoms, which has a pronounced change of the system's tribological and wear behaviors. A constitutive rate and state model is proposed to predict the evolution of frictional strength and wear. This work is supported by the National Science Foundation under Award No. 0926111.

Yuchong Shao
Johns Hopkins University

Date submitted: 08 Nov 2012 Electronic form version 1.4