

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Accelerated Molecular Dynamics Simulation of AFM Experiments Using the Bond-Boost Method WOO KYUN KIM, MICHAEL FALK, University of Michigan — We apply an accelerated molecular dynamics (MD) methodology to simulate the friction between a silicon tip and a silicon surface under perfect vacuum conditions. These simulations model recent Atomic Force Microscope (AFM) experiments which observed stick-slip motion and a lateral force showing dependences on temperature and sliding velocity. Our AFM models consist of crystalline silicon with an oxidized layer. We achieved the decrease in the simulated sliding velocity by several orders of magnitude compared with conventional MD simulations using the bond-boost method. This method is based on Voter's hyper molecular dynamics scheme accelerating the process between slip events. The decrease in the sliding velocity makes it possible to simulate systems closer to the regime of the actual experiments. We compare the simulation results with the experimental data to elucidate the atomic level processes during sliding. We studied the effects of atomic mass transfer between the tip and the substrate on friction. Moreover, the dependence of friction on temperature and sliding velocity has been quantified, and compared with the modified Tomlinson model.

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Date submitted: 24 Nov 2007

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