

Abstract Submitted
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Accelerated Molecular Dynamics Simulation on Friction of Incommensurate Interfaces¹ WOO KYUN KIM, The University of Michigan, MICHAEL FALK, The Johns Hopkins University — We apply a molecular dynamics (MD) methodology to study the friction of incommensurate interfaces. While the traditional Tomlinson model assumes a single, repeatable transition, the sliding at the real incommensurate interface is comprised of a multitude of transition modes. This may account for recent Atomic Force Microscope (AFM) experimental results that indicate more complex temperature and velocity dependence of friction that deviate from the Tomlinson predictions. Conventional MD simulations are unable to simulate a wide range of sliding rates due to time scale limitations. In this study, we achieve decreases in the simulated sliding velocity by several orders of magnitude compared with conventional MD simulations using Voter's hyperdynamics scheme. This method uses a biased potential to reduce the barrier heights of the original potential to decrease the simulated time between slip events. The decrease in the sliding velocity makes it possible to see the atomic level processes during sliding speeds much closer to the experimental time scale. We carefully analyze the simulation results to elucidate the transition mechanisms.

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