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Tip-based simulations of nanotribology of self-assembled monolayers MICHAEL CHANDROSS, GARY S. GREST, MARK J. STEVENS, Sandia National Laboratories — Friction and adhesion simulations are generally performed with opposing flat-plate geometries, ignoring the effects of load-dependent contact areas arising from curved probe tips. While some previous tip/substrate simulations do exist, they tend to either use multi-timestep approximations or unrealistically sharp tips. We present the results of true dynamical nanotribological simulations of alkylsilane self-assembled monolayers (SAMs) with realistic tip/substrate geometries. Tips matching experimental dimensions ($\sim$ 30 nm radius of curvature) were cut out of an amorphous silica substrate (a-SiO_2) and either coated with SAMs or annealed for uncoated tips. The adhesion and friction of the tip in contact with a SAM-coated amorphous a-SiO_2 substrate were studied with massively parallel molecular dynamics simulations. The effects of load-dependent contact areas are compared to previous simulations with flat plate geometries, and to atomic force microscopy measurments. Sandia is a multiprogram laboratory operated by Sandia Corp., a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

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