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Tip-based simulations of nanotribology of self-assembled monolayers MICHAEL CHANDROSS, CHRISTIAN D. LORENZ, MARK J. STEVENS, GARY S. GREST, Sandia National Laboratories — While nanotribological simulations are generally performed for two opposing parallel surfaces, the Atomic Force Microscopy (AFM) experiments to which they are often compared measure the interactions between a curved probe tip and a sample. The parallel plate geometry cannot capture many effects seen in experiments, including load-dependent contact areas and molecular transfer of material from the substrate to the tip. We present the results of true dynamical nanotribological simulations of alkylsilane self-assembled monolayers (SAMs) with realistic tip/substrate geometries. Tips matching experimental dimensions (up to ~ 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 AFM measurments. Conditions leading to tip fouling, and the effects on nanotribological measurements will also be discussed. Sandia is a multiprogram laboratory operated by Sandia Corp., a Lockheed Martin Company, for the United States Departme nt of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

Michael Chandross

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