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Molecular Dynamics Simulations of Nanotribology with Accurate Probe Tip Models MICHAEL CHANDROSS, Sandia National Laboratories, CHRISTIAN LORENZ, Iowa State University, GARY GREST, Sandia National Laboratories — Results for extensive dynamical nanotribological simulations of amorphous silica tips in contact with alkylsilane self-assembled monolayers (SAMs) will be presented. The radius of curvature of the tips match experimental dimensions. Comparison with contact mechanics models indicate that the standard JKR and DMT models do not give the correct dependence of contact area on applied force. The dependence of the tribological response on the chain length of the SAM has been determined. For short chains and for long chains at low loads the SAM presents a disordered sliding surface to the tip and the chain length is irrelevant. This result is in agreement with our previous simulations for SAMs in contact with a flat surface. For longer chains at higher loads the tip penetrates the monolayer and the friction is dominated by a plowing mechanism. 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.

Michael Chandross
Sandia National Laboratories

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