\documentstyle[11pt,apsab]{article}
\nofiles
\MeetingID{MAR06}
%\DateSubmitted{20051130}
\LogNumber{MAR06-2005-006290}
\SubmittingMemberSurname{Chandross}
\SubmittingMemberGivenName{Michael}
%\SubmittingMemberID{60007719,USA}
\SubmittingMemberEmail{mechand@sandia.gov}
\PresentationType{oral}
\SortCategory{07.8.4}{}{}{}
\received{30
Nov 2005}
\begin{document}
\Title{Tip-based simulations of nanotribology of
self-assembled
monolayers}
\AuthorSurname{Chandross}
\AuthorGivenName{Michael}
%\AuthorEmail{mechand@sandia.gov}
\AuthorSurname{Lorenz}
\AuthorGivenName{Christian
D.}
%\AuthorEmail{cdloren@sandia.gov}
\AuthorSurname{Stevens}
\AuthorGivenName{Mark
J.}
%\AuthorEmail{msteve@sandia.gov}
\AuthorSurname{Grest}
\AuthorGivenName{Gary
S.}
%\AuthorEmail{gsgrest@sandia.gov}
\AuthorAffil{Sandia National
Laboratories}
\CategoryType{C}
\begin{abstract}
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 $\sim$~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
AFM measurments. Conditions leading to tip fouling, and the

SAND2005-7604C

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.
\end{abstract}
\end{document}