Thursday Afternoon, October 22, 2015

Tribology Focus Topic
Room: 230B - Session TR+AS+NS+SS-ThA

Molecular Origins of Friction

Moderator: Nicolas Argibay, Sandia National Laboratories

2:20pm **TR+AS+NS+SS-ThA1 Atomic-Scale Mechanisms of Single Asperity Sliding**, ***Ashlie Martini***, *X. Hu*, University of California Merced, *M.V.P. Altoe*, Lawrence Berkeley National Laboratory **INVITED**

Isolating a single asperity to characterize its response to sliding is a heuristic approach to understanding the fundamental mechanisms that underlie friction and wear. A single asperity can be realized experimentally as the tip of an atomic force microscope cantilever. When the tip slides across a surface, friction is measured with atomic lattice-scale resolution and wear can be quantified in terms of nano- or even atom-scale volumes of material removed. However, challenges remain in interpreting these measurements because the observed friction and wear are due to processes that take place in the interface buried between the tip and the substrate on which it slides. Further, the nanometer scale of the contact implies that discrete atomic events in the interface may determine sliding behavior. Together, these observations suggest that the experiments could be complemented by atomistic models of the apex of the tip, near-contact substrate material and, of course, the interface itself. Although the simulations are limited to relatively small size and time scales, they have the potential to provide detailed information about mechanisms underlying phenomena that occur over short periods of time and small sliding distances. Specifically, in this research, we focus on the initial stages of friction and wear, and the processes that occur during the first tens of nanometers of sliding. The simulations are carefully designed such that they faithfully capture the corresponding experiments, including matching the materials, crystallography and geometry of the contacting bodies as observed through transmission electron microscope images of the tip and atomic force microscope images of the substrate taken at 10 nm intervals during the sliding process. The experiments offer an unprecedented view of wear occurring single atomic layers at a time, and the simulations provide detailed complementary information about the atomic-scale mechanisms underlying this process.

3:00pm **TR+AS+NS+SS-ThA3 Investigation of Epitaxy and Friction in Model Boundary Films**, ***Hongyu Gao***, University of California Merced, *W.T. Tysoe*, University of Wisconsin-Milwaukee, *A. Martini*, University of California Merced

Sliding friction of boundary films is investigated using ultrahigh vacuum (UHV) tribometer measurements of model alkali halide films on metals with complementary molecular dynamics (MD) simulations. We focus on a model system consisting of thin potassium chloride (KCl) films on an iron (Fe) substrate. The interaction potential between KCl and Fe is tuned using activation energy obtained from temperature programmed desorption (TPD) data and structures inferred from low-energy electron diffraction (LEED) measurements. The simulation is then used to explore the effect of film thickness and pressure on the formation of an epitaxial KCl film. The nature of this film and its near surface structure is then correlated with sliding friction behavior.

3:20pm **TR+AS+NS+SS-ThA4 Temperature Dependence of Atomic-scale Friction on Two-dimensional Materials**, ***Zhijiang Ye***, University of California Merced, *X.Z. Liu*, *K. Hasz*, *R.W. Carpick*, University of Pennsylvania, *A. Martini*, University of California Merced

Temperature plays an essential, yet complex role in determining atomic-scale friction. Recent studies of the temperature dependence of atomic-scale friction have reported different trends that suggest distinct and possibly contradictory underlying mechanisms. Specifically, friction is usually found to decrease with increasing temperature (due to thermolubricity), but this behavior is not always observed (attributed to adsorbates or meniscus effects). To understand the origins of these trends, we use molecular dynamics (MD) simulations and parallel replica dynamics (PRD) to study the temperature dependence of atomic friction on two-dimensional (2-D) materials, such as molybdenum disulfide. The MD simulations are designed to be closely-matched with corresponding atomic force microscope (AFM) measurements [1, 2]. Using the simulations and experiments, we explore how friction varies with temperature and how that variation is affected by other parameters, including sliding velocity, material, and environment. These studies provide new insights into how temperature affects friction on 2-D materials, and into the origins of atomic-scale friction generally.

References:

1. Xin-Z. Liu, Zhijiang Ye, Yalin Dong, Philip Egberts, Robert W. Carpick, and Ashlie Martini. Dynamics of Atomic Stick-Slip Friction Examined with Atomic Force Microscopy and Atomistic Simulations at Overlapping Speeds, *Phys. Rev. Lett.***114**, 146102 (2015).

2. Qunyang Li, Yalin Dong, Danny Perez, Ashlie Martini, and Robert W. Carpick. Speed dependence of atomic stick-slip friction in optimally matched experiments and molecular dynamics simulations. *Physical Rev. Lett*. **106**, 126101 (2011).

4:20pm **TR+AS+NS+SS-ThA7 Single Molecule Experiments to Explore Friction and Adhesion**, ***Rémy Pawlak***, *S. Kawai*, *A. Baratoff*, *T. Meier*, University of Basel, Switzerland, *W. Ouyang*, Tsinghua University, China, *T. Glatzel*, University of Basel, Switzerland, *E. Gnecco*, IMDEA-Nanociencia - Universidad Autónoma de Madrid, Spain, *A. Filippov*, Donetsk Institute of Physics and Engineering, Ukraine, *M. Urbakh*, Tel Aviv University, Israel, *E. Meyer*, University of Basel, Switzerland **INVITED**

Controlled manipulation processes of single-molecules with an atomic force microscope (AFM) provide valuable information about their interactions with surfaces, leading to fundamental insights into adhesion and friction properties. To understand such phenomena at such scale, tuning-fork based AFM operated at low temperature is an appropriate tool since complex manipulations of single-molecules can be readily performed and detected via advanced force spectroscopic techniques **[1]** . With such approach however, the measured frequency shifts are related to normal force gradients, and thus the interpretation of friction phenomena is not fully straightforward. To overcome this issue, we developed analytical models to simulate the experimental AFM data which allow us to determine adhesive energy and nanoscale friction. In this presentation, a first example will be given by the vertical pulling of long polymeric chains on Au(111), where their detachment leads to oscillations of the normal and lateral forces **[2]** . As in Frenkel-Kontorova (FK) models of friction, the polymer is represented by a chain of units connected by springs of stiffness k , each one interacting with a 2D periodic substrate potential. Force and gradient variations are dominated by the sequential detachment of each molecular units if k *i* s large enough to cause superlubric sliding. A second example will show vertical and lateral manipulations over a Cu(111) surface of a single porphyrin molecule attached to the AFM tip apex. In the frequency shift traces, atomic sawtooth modulations are systematically observed while sliding over the surface and are related to the internal degree of freedom of the molecular structure **[3]** .

References:

[1] R. Pawlak, S. Kawai, T. Glatzel, E. Meyer. *Single Molecule Force Spectroscopy* (ncAFM, *vol.3*, Springer, Japan 2015).

[2] S. Kawai et al., Quantifying the atomic-level mechanics of single long physisorbed molecular chains, *Proc. Nat. Acad. Sci.*, **111**, 3968–3972 (2014)

[3] R. Pawlak *et al* . *Intramolecular response of a single porphyrin molecule during AFM manipulations.* Submitted.

5:00pm **TR+AS+NS+SS-ThA9 Effects of Humidity on the Adhesion and Friction of Carbon-Based Materials**, ***Judith Harrison***, *M. Fallet*, *K.E. Ryan*, United States Naval Academy, *T. Knippenberg*, High Point University, *S.H. Kim*, *A. Al-Azizi*, Pennsylvania State University

Atomic-scale wear in nanoscale contacts is of particular importance for tip-based nanomanufacturing applications. As a result, wear resistant materials, such as diamond-like carbon (DLC), have been used to coat AFM tips to improve the lifespan and reliability of AFM probes and surfaces. Unfortunately, the tribological performance of these materials is known to depend on environmental conditions, such as humidity levels. We have performed macroscopic and atomic force microscopy friction experiments and molecular dynamics (MD) simulations aimed at examining adhesion and wear of DLC in humid environments.

Macro-scale friction tests showed friction and transfer film dependence on humid conditions. Low humidity suppresses transfer film formation while keeping the friction low. Intermediate humidity, however, does not reduce transfer film formation and increases the friction. The effect of humidity on friction was found to agree with the adhesion dependence on relative humidity as measured with atomic force microscopy.

Because it is difficult to elucidate atomic-scale mechanisms via experimental methods, molecular dynamics simulations have been employed to examine this behavior. Adhesion and sliding simulations of non-hydrogenated, ultrananocrystalline diamond (UNCD) and DLC surfaces with various levels of hydrogen in the presence of water using the qAIREBO and the ReaxFF potentials have been performed. Because both of

these potentials are able to model chemical reactions, the atomic-scale mechanisms responsible for adhesion and wear can be identified. Results obtained with both potentials will be compared to the experimental results.

5:20pm **TR+AS+NS+SS-ThA10 Single Asperity Tribochemical Wear of Silicon AFM Tips Sliding on Aluminum Oxide**, ***Erin Flater***, *S. Sorenson*, Luther College, *N. Ansari*, *A. Poda*, *W.R. Ashurst*, Auburn University, *B.P. Borovsky*, St. Olaf College

Understanding of tribological mechanisms at the submillimeter scale continues to be relevant since friction and wear limit the commercial viability of small-scale mechanical devices such as microelectromechanical systems (MEMS). For example, tribochemical processes play a significant role in many materials systems, including silicon oxide and aluminum oxide, which are relevant materials for MEMS devices. Our work focuses on understanding tribological processes at the interface of silicon AFM tips and amorphous aluminum oxide surfaces. We observe wear of silicon tips after repetitive sliding on the aluminum oxide surface, which occurs even at low contact pressures, implying that the wear process is chemical in nature. We quantify tip wear by intermittently interrupting the wear experiment to perform indirect *in-situ* tip imaging on a sharp-spiked sample. We use these tip images to quantify volume of material lost during scanning. Wear as a function of sliding distance is modeled using reaction rate theory and is compared to the Archard wear model. While some of our results appear to agree with an Archard model, these results may be more appropriately interpreted in light of the more fundamental reaction rate theory.

5:40pm **TR+AS+NS+SS-ThA11 Molecular Simulation of Indentation as a Probe of Scanning Probe Tip Mechanical Properties**, ***J. David Schall***, *K. Vummaneni*, Oakland University, *J.A. Harrison*, United States Naval Academy

Scanning probe tips should be robust, have low adhesion, and low wear to ensure repeatability and long tip life. As new tip materials are developed these properties must be quantified and compared to existing tip materials. In this study, molecular simulation is used to measure the elastic modulus and work of adhesion of a variety of tips against a common substrate material, in this case H-terminated diamond (111). The tip materials investigated include Si, SiC, amorphous SiC, diamond, diamond like carbon and ultra-nanocrystalline diamond (UNCD). SiC was recently proposed as a new high hardness, low wear tip material. In simulation the tip geometry can be controlled to enable direct comparisons between each tip material. Both dynamic simulations at 300K and quasi-static indentions using stepwise energy minimization with and with out adhesion between tip and substrate were used. Simulations of sliding friction and wear have also been conducted to investigate the correlation between tip materials properties and friction and wear.

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