Tribology Focus Topic
Room: 203 C - Session TR+AS-MoM

Bridging Scales and Characterization

Moderator: R.W. Carpick, University of Pennsylvania, L. Marks, Northwestern University

9:00am **TR+AS-MoM3 Friction in Full View**, ***L. Marks***, Northwestern University **INVITED**

Friction is a pervasive problem, by some estimates consuming about 5% of the GDP of the economies of the developed world, and a recent analysis has indicated that about one third of the fuel energy in automobiles goes to overcoming frictional losses. While the importance of minimizing friction can be traced back at least as far as the tomb of Tehuti-Hetep, circa 1880 B.C, where a man can be seen pouring a lubricant to assist moving a statue, there are still many unknowns in the field of tribology which encompasses friction as well as other critical processes such as wear and lubrication. For many of the phenomena in tribology there are still numerous unknowns, due in large part to what has been called the buried interface problem. The triboactive layer, is almost always hidden by the materials on both sides of it so the exact details of what is occurring are often hidden, only accessible by post-facto analyses and sometimes a matter for debate. While there have been several attempts to image the triboactive layer directly at the atomic scale dating from the original work by Gane and Bowden, progress has been slow. Over the last few years we have been developing both models from a materials science viewpoint via dislocations as well as in-situ techniques for imaging the buried interface. Related to this (perhaps not obviously) we have recently become involved in understanding the nanoscale tribology of hip replacements, including the perhaps surprising observation of a graphitic layer *in-vivo* that appears to play a major role in reducing implant failures.This talk will focus upon some of the recent results, ranging from more basic observation such as connecting wear fragment size and a new layer-by-layer wear mechanism to the standoff distance of interfacial dislocations through the formation of graphitic materials *in-vivo* as well as some direct observations of wear and sliding at the atomic scale.

9:40am **TR+AS-MoM5 Combining *In Situ* Nanotribology and Atomistic Simulations to Reveal the Strong Effect of Atomic-Scale Roughness on Nanoscale Adhesion**, ***T.D.B. Jacobs***, University of Pennsylvania, *K.E. Ryan*, *P.L. Keating*, United States Naval Academy, *D.S. Grierson*, systeMECH, LLC, *J.A. Lefever*, *K.T. Turner*, University of Pennsylvania, *J.A. Harrison*, United States Naval Academy, *R.W. Carpick*, University of Pennsylvania

As components in devices and microscopy applications shrink to nanometer length scales, adhesion forces play an increasingly dominant role in the physics of contact. In particular, tip-based approaches for data storage, nanomanufacturing, and nanoelectromechanical systems rely on accurate knowledge and control of adhesion between a sharp asperity and a surface. It is well known that surface roughness affects adhesion at macro- and microscopic scales. However, the atomic-scale roughness of nanoscale tips is rarely measured or accounted for. Here, we characterized the atomic-scale roughness of carbon-based probes, and measured the corresponding effect on adhesion using simulations and experimental techniques.

We have conducted contact and sliding experiments inside of a transmission electron microscope (TEM), using a modified *in situ* nanoindentation apparatus. Similar experiments were used recently to study wear of nanoscale silicon probes[1]. In the present work, nanoscale asperities composed of either diamond-like carbon (DLC) or ultrananocrystalline diamond (UNCD) were brought into contact and separated from a flat diamond substrate. The *in situ* nature of the testing allowed characterization of surface roughness with sub-nanometer resolution immediately before and after contact. Additionally, complementary adhesion simulations were conducted using molecular dynamics (MD) with conditions matched as closely as possible with the experiments (e.g., materials, asperity shape, environment). The RMS roughness for the experimental tips spanned 0.18 - 1.6 nm; for the simulated tips, the range was 0.03 nm (atomic corrugation) to 0.12 nm. Over the tested range of roughness, the measured work of adhesion was found to decrease by more than an order of magnitude as roughness increased, with a consistent trend observed between experimental and simulation results[2]. The dependence of adhesion upon roughness was accurately described by a simple analytical model.

This combination of simulation and novel *in situ* experimental methodologies allowed for an exploration of an unprecedented range of tip sizes and length scales for roughness, while also intrinsically verifying consistent behavior between the two approaches. These results demonstrate a high sensitivity of adhesion to interfacial roughness down to the atomic limit. Furthermore, they indicate that present approaches for extracting work of adhesion values from experimental measurements of adhesion forces contain significant uncertainty due to an unmeasured variable – atomic-scale roughness.

[1] T. D. B. Jacobs, R. W. Carpick, *Nature Nanotech.*, **8,** 108-112 (2013)

[2] T. D. B. Jacobs, *et al., Tribol. Lett.*, **50,** 81-93 (2013)

10:00am **TR+AS-MoM6 Nanotribological Properties of Positively and Negatively Charged Nanodiamonds as Additives to Solutions**, ***Z. Liu***, *S.D. Corely*, North Carolina State University, *O.A. Shenderova*, International Technology Center, *D. Brenner*, *J. Krim*, North Carolina State University

Nano-diamond (ND) particles are known to be beneficial for wear and friction reduction when used as additives in liquids,[1] but the fundamental origins of the improvement in tribological properties has not been established. In order to explore this issue, we have investigated the nanotribological properties of ND coated with self-assembled monolayers (SAM) as additives to solutions, employing gold/chrome coated quartz crystal microbalances (QCM). Measurements were performed with the QCM initially immersed in deionized water. ND particles with positively and negatively charged SAM end groups were then added to the water, while the frequency and amplitude of the QCM were monitored. Negative shifts in both the QCM frequency and amplitude were observed when ND with positively charged SAM end groups were added, while positive shifts in both the QCM frequency and amplitude were observed when ND with negatively charged ND end groups were added . The results are consistent with a lubricating effect for the negatively charged ND, but were only observed for sufficiently small negative ND particle size. Experiments on QCM surfaces with differing textures and roughness are in progress, to determine the separate contributing effects of surface roughness charge-water interactions.

Funding provided by NSF DMR.

1. Vadym N. Mochalin, Olga Shenderova, Dean Ho & Yury Gogotsi, Nature Nanotechnology 7, 11–23 (2012) doi:10.1038/nnano.2011.209

10:40am **TR+AS-MoM8 Atomic-scale Processes in Single Asperity Friction and Wear**, ***R.W. Carpick***, University of Pennsylvania **INVITED**

I will discuss recent atomic force microscopy studies of nanoscale single asperity contacts that reveal surprising new behavior and insights. First, the behavior of nanoscale contacts with truly 2-dimensional materials will be discussed. For nanoscale contacts to graphene, we find that the friction force exhibits a significant dependence on the number of 2-D layers[1]. Surprisingly, adhesion (the pull-off force) does not. However, studies as a function of scanning history reveal further complexities that arise from the combined effects of high flexibility and variable substrate interactions that occur at the limit of atomically-thin sheets. An even stronger effect occurs when graphene is fluorinated, where experiments and simulations both show that friction between nanoscale tips and fluorinated graphene (FGr) monolayers exceeds that for pristine graphene by an order of magnitude. The results can be interpreted in the context of the Prandtl-Tomlinson model of stick-slip friction.

I will then discuss new insights into the physics of nanoscale wear. A better understanding of wear would allow the development of rational strategies for controlling it at all length scales, and would help enable applications for which wear is a primary limitation such as micro-/nano-electromechanical systems (MEMS/NEMS). We have demonstrated the ability to characterize single-asperity wear with a high degree of precision by performing *in-situ* wear tests inside of a transmission electron microscope. For silicon probes slid against a flat diamond substrate, the shape evolution and volume loss due to wear are well described by kinetic model based on stress-assisted bond breaking mechanisms[2]. This allows new insights to be gained about the kinetics of atomic-scale wear[3].

[1] Lee, C., Li, Q., Kalb, W., Liu, X.-Z., Berger, H., Carpick, R.W. and Hone, J. "Frictional Characteristics of Atomically-Thin Sheets," Science, 328, 2010, 76-80.

[2] Jacobs, T.D. and Carpick, R.W. "Nanoscale Wear as a Stress-Assisted Chemical Reaction," Nature Nanotech., 8, 2013, 108-112.

[3] Jacobs, T.D., Gotsmann, B., Lantz, M.A. and Carpick, R.W. "On the Application of Transition State Theory to Atomic-Scale Wear," Tribol. Lett., 39, 2010, 257-271.

11:20am **TR+AS-MoM10 Examination of Adhesion and Friction of Hydrocarbon-based Materials: Elucidating Atomic-scale Wear Processes via Molecular Dynamics**, ***J.A. Harrison***, *K.E. Ryan, P.L. Keating*, United States Naval Academy, *J.D. Schall*, Oakland University, *K.T. Turner*, University of Pennsylvania, *D.S. Grierson*, systeMECH, LLC, *R.W. Carpick, V. Vahdat, T.D.B. Jacobs*, University of Pennsylvania

Molecular dynamics (MD) simulations are unique in their ability to elucidate atomic-scale phenomena because the positions, velocities, and forces of all atoms in the system are known as a function of time. We have performed complementary atomic force microscope (AFM) experiments and MD simulations aimed at examining adhesion, friction, and wear in diamond, ultrananocrystalline diamond (UNCD), and amorphous carbon (a-C:H) materials. Atomic-scale wear in nanoscale contacts is of particular importance for tip-based nanomanufacturing applications. In this paper, we examine the normal contact of a-C:H and UNCD axisymmetric tips with diamond, UNCD and a-C:H substrates. Adhesion and wear as a function of material, surface termination, impact point, and roughness were all examined. Results from the MD simulations were compared, and lend insight into, complementary AFM experiments. In addition, separate sets of MD simulations were performed using two different potential energy functions. The AIREBO potential is a bond-order potential that contains intermolecular interactions that was developed to model bond-breaking and bond-making processes. Results obtained using the AIREBO potential will be compared results obtained using the recently developed REBO+S potential. The REBO+S potential differs from the AIREBO potential in that alterations were made to the REBO potential cutoff distances, which alters the forces required to make and break bonds. Differences in adhesion and wear events obtained using the two different potentials with identical material pairs will be quantified. Supported by the National Science Foundation

11:40am **TR+AS-MoM11 Speed-Dependence of Atomic-Scale Friction**, *A. Martini*, ***Z. Ye***, University of California Merced, *Y. Dong*, Purdue University, *P. Egberts, XZ. Liu, R.W. Carpick*, University of Pennsylvania

Atomistic simulations and experimental atomic force microscopy measurements on a variety of different materials have shown that atomic-scale single asperity friction can be significantly affected by sliding speed. However, physical insights into how and why sliding speed affects friction are limited because the speeds accessible to most simulations are several orders of magnitude faster than those in the corresponding experiments. Typical simulations must be run at fast sliding speeds due to their necessarily short time scale, and accurate experimental nanoscale asperity friction measurements are limited to slow speeds because of difficulties in measuring high-speed forces with picoNewton resolution. Here we present friction results from molecular dynamics simulations where the sliding speeds are greatly reduced by using parallel replica dynamics. Parallel replica dynamics is an accelerated simulation technique that distributes simulation time across multiple processors and therefore adequately samples the various possible state-to-state pathways accessible to the system, as would a standard, single-processor simulation run for a very long time. This technique, accompanied by experiments where data is obtained using a novel high-speed data acquisition method, enables measurements and simulations to be quantitatively compared within the same physical regime; specifically, at the same sliding speed. Furthermore, the materials, load, contact size and orientation, system compliance, and temperature are identical within experimental uncertainty so as to minimize differences between experiments and simulations, allowing robust comparisons and interpretations. These coordinated studies enable us to understand the dependence of atomic-scale friction on sliding speed, and to determine the limits of validity of the Tomlinson-Prandtl model, a reduced-order model widely-used to describe atomic-scale sliding.

Authors Index

Bold page numbers indicate the presenter