Tribology Focus Topic
Room: 303 - Session TR+NS-ThM

Bridging Scales in Tribology

Moderator: J. David Schall, Oakland University

8:00am **TR+NS-ThM1 Temporal and Spatial Multiscale Simulations of Low-Velocity Frictional Sliding**, ***Woo-Kyun Kim***, University of Cincinnati **INVITED**

As the size of mechanical systems of technological interest such as micro electro-mechanical systems (MEMS) decreases, the need to develop experimental and theoretical tools to investigate micro/nanometer scale phenomena has been growing rapidly. Since its invention in 1986, the Atomic Force Microscope (AFM) has been a primary tool to study the atomic-scale friction and wear and atomistic simulation methods such as molecular dynamics (MD) have also been widely used because these simulations can provide direct access to atomic-scale mechanisms which cannot be observed experimentally. However, there is a great disparity in length and time scales between the simulated systems and the real experimental systems. One of the significant artifacts of these scale differences is that systems are loaded at by several orders of magnitudes larger rates in simulations than in experiments, which may completely distort the underlying mechanisms. Recently, a novel multiscale method, called hyper-QC, which can span both length and time scales simultaneously has been developed. Hyper-QC combines quasicontinuum (QC), a spatial multiscale method, and hyperdynamics, an accelerated MD scheme, in a single platform. In this talk, the hyper-QC simulation results of AFM experiments will be presented. Hyper-QC enables the reduction in the sliding rate by two or three orders of magnitudes from that of the conventional MD scheme as well as the reduced effective number of atoms that is achieved through the QC coarse-graining.

8:40am **TR+NS-ThM3 Crystal-Amorphous and Amorphous-Amorphous Transitions in Carbon under Tribological Load**, ***Lars Pastewka***, Karlsruhe Institute of Technology, Institute for Applied Materials IAM, Germany **INVITED**

Diamond and amorphous carbon (aC) are prototypical examples of wear resistant materials. Yet, these materials wear down, but little is known about the atomic scale processes that cause wear. Molecular dynamics is ideally suited to gain a deeper understanding of the underlying wear processes [1]. Such atomic-scale simulations reveal that both, mechanical and oxidative wear actions are active. Mechanical action transforms the material to a weaker state that is then easily oxidized. For diamond, we find a transition to an aC, while we find a high-density—low-density aC-aC transition for amorphous thin films. The velocity of the diamond/aC interface depends crucially on the diamond surface orientation with the highest speed found for (110) surfaces that are rubbed in the (001) direction, while the lowest interface speed was observed for the diamond (111) surface. High-density aC itself transforms even faster to a low density state that then succumbs to wear [2]. We relate the aC-aC transition to shear-banding in plasticity of amorphous materials, and argue that the formation of shear-bands is crucial for the wear resistance of carbon based hard coating. These findings are in perfect agreement with a 600 years old experimental knowledge of diamond polishers, and with recent experiments comparing wear in diamond and amorphous carbon thin films.

[1] L. Pastewka, S. Moser, P. Gumbsch, M. Moseler, Nat. Mater. 10, 34 (2011)

[2] T. Kunze, M. Posselt, S. Gemming, G. Seifert, A.R. Konicek, R.W. Carpick, L. Pastewka, M. Moseler, Tribol. Lett. 53, 119 (2014)

9:20am **TR+NS-ThM5 A Molecular Dynamics Investigation of the Atomic-Scale Wear of Carbon-Based Materials Upon Repetitive Contact**, ***Kathleen Ryan***, United States Naval Academy, *V. Vahdat*, University of Pennsylvania, *P.L. Keating*, United States Naval Academy, *Y. Jiang, K.T. Turner, R.W. Carpick*, University of Pennsylvania, *J.A. Harrison*, United States Naval Academy

Amplitude modulation atomic force microscopy (AM-AFM) involves hundreds of thousands of contacts between a tip and surface per second. Each contact can result in the formation and breakage of chemical bonds causing wear to the tip. Atomic-scale wear hinders the quality and reproducibility of structures created by tip-based nanomanufacturing processes. However, wear cannot be analyzed at the single-atom level using existing experimental methods. Continuum mechanics models can be used to estimate stresses, deformations, and the work of adhesion. However, these models can break down at the nanoscale as they rely upon assumptions about the tip shape and material properties, and ignore the discrete atomic structure of the materials. Molecular dynamics (MD) simulations allow the nanoscale behavior to be modeled by resolving the positions, velocities, and forces of all atoms in the system. Here, MD simulations are used to model the repeated contact of an axisymmetric, hydrogenated amorphous carbon (a-C:H) tip with a 3-dimensional ultrananocrystalline (3D UNCD) surface. Using a finite element method to select the smallest portion of the tip that should be modeled atomistically, the tip radius could be set at 15 nm, much larger than previous simulations of this type and in the range of experimental AFM tip sizes. Tip/surface material and tip shapes were also chosen to closely mimic those used in comparable experiments. The wear processes, including adhesive forces, material transfer, and changes to material hybridization are examined following multiple contact cycles. We observe discrete atomic bonding and transfer events, as opposed to plastic deformation or fracture of multi-atom clusters. This is consistent with interpretations of experimental wear behavior and adds significant new detail to the possible pathways for the wear process.

9:40am **TR+NS-ThM6 The Buried Interface: *In Situ* Methods for Tribology**, ***Brandon Krick***, Lehigh University, *K.G. Rowe, A.I. Bennett, D.W. Hahn, W.G. Sawyer*, University of Florida

Tribological phenomena occur at interfaces which are often difficult to directly observe or access. *In situ* techniques are rapidly emerging to probe surfaces buried at an interface, illuminating the physical, mechanical and chemical interactions between two surfaces in intimate contact. In this presentation, we discuss several *in* situ techniques, including optical microscopy of the real area of contact, thermal imaging of contact temperature, and Surface Plasmon Resonance of molecular transfer of a solid lubricant during sliding.

Utilizing an optical *in situ* microtribometer, we can explore the real area of contact and near contact surface topography of contacting surfaces; this technique has been used to visualize adhesive-elastic contact between a rigid sphere and a thin elastic foundation as well as randomly rough elastomer surface in contact with an infinitely stiff and flat (by comparison) surface. Similarly, an forward looking infrared (FLIR) microscope camera can reveal interface temperatures with microscopic resolutions. Finally, an *in situ* Surface Plasmon Resonance (SPR) tribometer is used to measure molecular-scale transfer of solid lubricants during sliding. For some systems, such as PTFE, transfer is detected as early as the first cycle of sliding, while minimal transfer is observed in other systems such as UHMWPE.

11:00am **TR+NS-ThM10 Contact and Friction Between Rough Adhesive Surfaces: From Atomic to Micrometer Scales**, ***Mark Robbins***, Johns Hopkins University, *L. Pastewka*, Fraunhofer Institute for Mechanics of Materials IWM, Germany **INVITED**

Experimental surfaces typically have roughness on a wide range of length scales. This roughness greatly reduces the fraction of the area that is in intimate molecular contact and thus can contribute to friction and adhesion. The talk will first describe recent numerical calculations of elastic contact between rough surfaces with nominally flat or spherical geometries on large scales. An efficient Greens function approach allows calculations for systems with roughness on nanometer to micrometer scales to be performed with atomic resolution in the contact. Results for a wide range of geometries can be collapsed using simple scaling relations that depend on the root mean squared surface slope, sphere radius, elastic modulus, and work of adhesion. The scaling relations explain why adhesive interactions have little effect unless the surfaces are extremely smooth or soft. The traditional Fuller-Tabor model for adhesion of rough surfaces is shown to be qualitatively inconsistent with the simulations. The effect of atomic scale plasticity on contact and adhesion is surprisingly small. The talk will conclude by considering how forces in the contact area give rise to friction at larger scales.

11:40am **TR+NS-ThM12 Scaling Properties of Measured Frictional Parameters in Microscale Contacts**, ***Brian P. Borovsky***, St. Olaf College

We present a study of the frictional properties of microscopic contacts (radius ~ 1 μm) in the high-speed regime (> 1 m/s) during the initiation of full slip. Energy dissipation, lateral contact stiffness, and amplitude of motion are measured for a transverse-shear quartz resonator in contact with a small spherical probe. Averaged values for the elastic and dissipative forces are derived as functions of shearing amplitude, at constant normal loads in the range from 10 μN to 8 mN. We observe a transition from partial to full slip at a threshold amplitude of motion, characterized by a maximum elastic force. Kinetic friction in the full-slip regime is observed to be about a factor of two smaller than this elastic force limit. Data from tests at

various normal loads can be collapsed onto common curves by normalizing the forces and amplitudes according their characteristic values. We discuss the observed scaling of these frictional parameters with the size of the contact and the extent of agreement with current theories of microslip.

12:00pm **TR+NS-ThM13 Scale Effects in Single-Asperity Friction**, ***Tristan Sharp***, Johns Hopkins University, *L. Pastewka*, Fraunhofer Institute for Mechanics of Materials IWM, Germany, *M.O. Robbins*, Johns Hopkins University

Simulations are used to examine the static friction in model single-asperity contacts between a rigid sphere and a flat elastic substrate. The sphere radius R and the contact radius a are varied from nanometers to micrometers. First the case of commensurate contact between identical aligned surfaces with repulsive interactions is considered. For small contacts all contacting atoms move coherently and the friction coefficient μ is independent of contact radius and load. In larger contacts, interfacial slip is mediated by localized dislocations. At first μ decreases with increasing contact radius: $\mu \sim (Ra_0)^{1/2}/a$, where a0 is the nearest-neighbor spacing. At even larger contact sizes, μ begins to drop more slowly. The results are in sharp contrast to Cattaneo-Mindlin continuum theory where μ is independent of contact size. Separate simulations are performed to connect the results to the dislocation-based models of contact-size effects due to Hurtado and Kim, and Gao, which assume adhesive interactions between surfaces and find $\mu \sim (a_0/a)^{1/2}$. The talk will conclude with discussions of the effect of changes in the relative alignment of crystalline axes.

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