Thursday Morning, November 3, 2011

Tribology Focus Topic
Room: 111 - Session TR+AS+SS-ThM

Atomic-scale Characterization of Tribological Interfaces

Moderator: S. Perry, University of Florida

8:00am **TR+AS+SS-ThM1 Electrochemical Control of Atomic Friction**, ***F. Hausen***, INM - Leibniz Institute for New Materials, Germany, *A. Labuda,* McGill University, Canada, *N.N. Gosvami, R. Bennewitz*, INM - Leibniz Institute for New Materials, Germany

Electrochemical methods allow for fast and reversible modification of metal surfaces through deposition and dissolution of metal films, adsorption and desorption of anions, as well as oxidation and reduction. The surface composition and structure undergo dramatic changes in these processes, which should cause significant changes in the friction on the surface.

We present friction force measurements at the nanometer scale on Au(111) and Au(100) single crystal electrodes performed by means of friction force microscopy in various electrolytes. The resolution of atomic stick-slip events in an electrochemical cell is improved by the development of a dedicated instrument [1]. A significant difference in friction is found for the bare electrodes compared to the modified surfaces. Friction is extremely weak and exhibits almost no load dependence on clean Au(111) surfaces. Upon electrochemical oxidation of the surface, significant friction with linear load dependence is observed. This process is reversible and allows switching repeatedly between high and low friction [2]. In the regime of anion adsorption our results indicate a frictional response with threshold behaviour. The threshold depends on both applied normal load and the electrochemical potential [3].

After deposition of copper on gold by underpotential deposition in perchloric acid, the atomic stick-slip changes into a periodicity which indicates frictional response of CuCl with a linear load dependence. In chloride-free sulphuric acid a different behaviour is found, indicating competing effects of ion adsorption on friction forces at small scales.

[1] A. Labuda et al., Rev. Sci. Instruments 81, 083701 (2010)

[2] A. Labuda et al., Langmuir (2011, available online)

[3] F. Hausen et al., Electrochimica Acta (2011, in print)

8:20am **TR+AS+SS-ThM2 Surface Alterations Effects on Ice Adhesion Strength**, ***C. Ellis-Terrell***, *M. Miller,* Southwest Research Institute, *M. Zou,* University of Arkansas at Fayetteville, *R. Wei,* Southwest Research Institute, *S. Beckford,* University of Arkansas at Fayetteville, *G. Hatton*, Shell Global Solutions, Inc.

Ice adhesion is a serious problem in areas such as the oil, gas, and automotive industry, telecommunications and power line transmission. There is a significant amount of research directed towards designing a coating to reduce ice accumulation. This study focuses on measuring the effects of surface roughness and surface energy on ice adhesion strength. Surface texturing ranged from high to low surface roughness. A sandblasting technique was applied to the aluminum surface creating a high surface roughness. Surface energy changes were created by depositing a silicon doped hydrocarbon film, using plasma enhanced vapor deposition. A custom built apparatus was employed to specifically measure the adhesion force of an ice droplet. The results illustrate that the smoother as-received surfaces have lower ice adhesion strength than the rougher sandblasted surfaces.

8:40am **TR+AS+SS-ThM3 Atomistic Simulations of Nanoindentation and Nanoscratching of SiO_2/Si and HfO_2/Si Systems using COMB Potentials**, ***T.-R. Shan***, *X. Sun, S.R. Phillpot, S.B. Sinnott*, University of Florida

Oxides such as SiO_2, Al_2O_3 and HfO_2, are typically used together with Si in many high-performance electronic devices, including metal-oxide-semiconductor (MOS) devices/junctions and micro- and nano-electromechanical systems (MEMS/NEMS). The lack of precise control over mechanical properties can lead to the degradation of these materials. It is therefore critical to understand the nanometer-scale mechanical properties of materials or complex systems being considered for use in electronic devices. Nanoindentation and nanoscratching are important methods for investigating the mechanical behavior of small volumes of materials, such as thin film systems. Here, classical molecular dynamics simulations are used to examine the responses to nanoindentation and nanoscratching of thin films of SiO_2 and HfO_2 on silicon substrates. The goal is to determine the influence of thin film types and the structure of thin film and substrate interface on the responses. Because these systems consist of heterogeneous interface with significant changes in bonding as one crosses from one side of the interface to the other, the empirical charge optimized many-body (COMB) potential as implemented in large-scale atomic/molecular massively parallel simulator (LAMMPS) program is used to model the structural evolution, mechanical response and charge transfer in these systems in response to a nanometer-scale spherical indenter. Aspects of the SiO_2/Si and HfO_2/Si interfaces during nanoindentation and nanoscratching, including the mechanisms by which fracture and plasticity occurs, will also be addressed. We gratefully acknowledge the support of the National Science Foundation through grant numbers DMR-0426870 and DMR-1005779).

9:00am **TR+AS+SS-ThM4 Accelerated Molecular Dynamics Simulations of Nanoscale Friction**, *W.K. Kim,* University of Minnesota, ***M.L. Falk***, Johns Hopkins University **INVITED**

Accelerated molecular dynamics simulations are implemented to model the sliding process of atomic force microscope experiments and to lower the sliding speeds below those in a conventional MD simulation. In this study the hyperdynamics method, originally devised to extend MD time scales for non-driven systems, is applied to the frictional sliding system. This technique is combined with a parallel algorithm that simultaneously simulates the system over a range of slider positions so that the overall acceleration rate is approximately the number of processors multiplied by the boost factor from the hyperdynamics method. The new methodologies are tested using two-dimensional and three-dimensional Lennard-Jones AFM models. The methodology is then applied to simulated sliding between an oxidized silicon tip and surface achieving a range of six decades of velocity and reproducing the experimentally observed velocity dependence of the friction force. In doing so we learn something new about this system and about friction between amorphous surfaces in general. Unlike in the crystalline case, as increasing force is applied to the amorphous tip intermediate states arise. These intermediate states serve as critical transition pathways. The emergence of such states leads to the emergence of a plateau in sliding velocity at lower sliding speeds and higher temperatures. A simple theory based on these observations successfully describes both the experimental and the simulated data.

9:40am **TR+AS+SS-ThM6 Molecular Dynamics Simulations of Contact between Carbon-Based Materials: Isolating the Effects of Experimental Variables**, ***J.A. Harrison***, *K.E. Ryan, P.L. Keating,* US Naval Academy, *D.S. Grierson, J. Liu, K.T. Turner,* University of Wisconsin Madison, *R.W. Carpick*, University of Pennsylvania

The behavior of nanoscale contacts is complex and often cannot be understood through continuum mechanics alone. Here, parallel molecular dynamics (MD) simulations using the AIREBO potential for hydrocarbons to model indentation and friction, are used to investigate nanoscale contacts of carbon-based materials, such as diamond, DLC, and ultrananocrystalline diamond (UNCD). Specifically, the contact of carbon-based AFM probes is simulated to understand the effects of experimental parameters, including tip geometry and material selection, on the adhesion between the tip and sample. Results from the MD simulations will be compared to and discussed within the context of the complementary atomic force microscope experiments and finite element simulations. The tribological response of carbon-based materials is very sensitive to environmental conditions. For example, the presence of water has been shown to negatively impact the friction performance of hydrogenated DLCs but to improve the performance of nanocrystalline and ultrananocrystaline diamond. We have been working to develop a potential energy function that is capable of modeling carbon-based materials in the presence of water. This talk will also outline our current efforts at potential development.

10:40am **TR+AS+SS-ThM9 Modeling the Pressure Dependence of Shear Strength in Sliding, Boundary-Layer Friction**, ***M. Garvey***, *M. Weinert, W.T. Tysoe*, University of Wisconsin-Milwaukee

The pressure dependence of the shear strength of model alkali halide lubricant systems has been investigated at the density functional theory level. This is compared to the experimental dependence given by $S = S_0 + \alpha P$, where P is the contact pressure, S_0 is the zero-pressure shear-strength and α is the coefficient of pressure dependence. Sliding potentials were calculated and shear is found to occur between the film and the sliding interface. The heights of the potentials were calculated as a function of compression, allowing the lateral force to be calculated as a function of

pressure. The calculated values of S_0 and α are in good agreement with experimental data.

11:00am **TR+AS+SS-ThM10 Lubrication Mechanisms of MoS_2 Fullerene-Like Nanoparticles: Coupling Computer and Experimental Works**, ***E.W. Bucholz***, University of Florida, *I. Lahouij, F. Dassenoy,* Ecole Centrale de Lyon, France, *S.B. Sinnott,* University of Florida, *J.M. Martin*, Ecole Centrale de Lyon, France

Inorganic fullerene (IF)-like MoS_2 nanoparticles have been shown to be good lubricating and anti-wear additives when dispersed in a base oil. This improved tribological performance appears to be a result of the size and structure of the nanoparticles along with the test conditions. Possible lubrication mechanisms include pure rolling to sliding to the exfoliation of lamellar MoS_2 sheets inside the contact. *In situ* transmission electron microscopy (TEM) experiments have been used to manipulate individual MoS_2 nanoparticles and investigate their responses to compression and friction under different conditions. However, the very small scale of the MoS_2 nanoparticles makes distinguishing the properties which affect the lubrication mechanism exceedingly difficult; thus, a computational approach is used to more fully understand the most important mechanisms. Therefore, classical molecular dynamics (MD) simulations of individual nested MoS_2 nanoparticles are performed where they are subjected to compression and shear forces between sulfur-terminated molybdenum surfaces. Two specific nanoparticle configurations are considered, with both structures containing three layers. The first configuration is a curved, ellipsoidal MoS_2 nanoparticle structure with a major and minor diameter of approximately 8.9 and 6.6nm, respectively. The second nanoparticle configuration is an octahedron with grain boundaries that are approximately 6.2 nm in length. MD simulations of these structures indicate the role of curved and faceted morphologies as well as grain boundaries on the rolling/sliding behavior and nanosheet exfoliation of the particles. The results are used to interpret the experimental TEM findings and predict the dominant mechanisms associated with enhanced lubrication through the addition of these particles to base oils. This work is supported by the Office of Naval Research .

11:20am **TR+AS+SS-ThM11 Shape-Independent Lateral Force Calibration**, *E.V. Anderson,* ***N.A. Burnham***, Worcester Polytechnic Institute

The primary problem with lateral force microscopy (LFM) has been the difficulty in calibrating the cantilever and tip in order to obtain quantitative friction data. Two recent review articles and several research articles have expressed this difficulty and the need for a simple, universally-accepted method [1,2]. The available procedures have numerous limitations. Some require specialized samples or setups. Others are difficult to perform. A number are indirect, or only suitable for certain cantilevers. Several risk damage to the tip or sample, or both, and might require the geometry of the cantilever, which can be hard to measure. We present a procedure that alleviates these problems [3]. The linear relationship between the detected voltage and lateral force is exploited to obtain the slope (calibration factor) and intercept that convert voltage to lateral force. The method is independent of sample shape, probe shape, and scan parameters (load force, gain, and scan rate). The accuracy was investigated on an order-of-magnitude level and was within 50% of torsional spring constants obtained from geometry, and the precision was under 10%. Small scan areas were also found to produce accurate calibration factors and could help to limit tip-sample wear. Quantification of nano-Newton friction forces might now become routine.

1. M. L. B. Palacio, B. Bhushan, *Crit. Rev. Solid State Mater. Sci.* **2010**, *35*, 73-104.

2. M. Munz, *J. Phys. D: Appl. Phys.* **2010**, *43*, 063001.

3. E.V. Anderson, S. Chakraborty, T. Esformes, D. Eggiman, C. DeGraf, K. M. Stevens, D. Liu, and N.A. Burnham, "Shape-Independent Lateral Force Calibration," submitted April 2011.

11:40am **TR+AS+SS-ThM12 Atomic Stick-Slip Friction Studied by Optimally-Matched Accelerated MD Simulations and AFM Experiments**, ***Y. Dong***, Purdue University, *Q. Li, R.W. Carpick,* University of Pennsylvania, *A. Martini*, Purdue University

Atomic-scale stick-slip friction of platinum on gold (111) surface is quantitatively studied both experimentally and through optimally-matched accelerated molecular dynamics (MD). In order to make a direct comparison between simulation and experiment, many other factors are matched as closely as possible, such as misalignment, size effect of the tip, cantilever compliance, normal load and so on. The Parallel Replica Dynamic Method (ParRep) is used to accelerate the simulation so scan velocities can be decreased to scales approaching those used in atomic force microscope experiments. A logarithm dependence of friction on scanning velocity is observed both in Atomic Force Microscope (AFM) and MD reveals that at low speed the atomic friction lies in thermal activation regime. A further comparison shows that AFM and MD provide consistent energetics, which supports that MD can be used to interpret AFM results; but attempt frequencies differ by orders of magnitude, which is attributed to the inertia discrepancy.

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