

Tuesday Afternoon, November 10, 2009

Tribology Focus Topic

Room: B2 - Session TR+SS-TuA

Surface Science for Tribology

Moderator: I. Szlufarska, University of Wisconsin, Madison

2:00pm **TR+SS-TuA1 Effect of the Surrounding Gas Pressure on Charge Separation Caused by Friction between Insulators**, T. Miura, E. Hosobuchi, S. Ueno, I. Arakawa, Gakushuin University, Japan

Friction between insulators induces charge separation at the interface. The surface electrification after sliding contact yields electric field in the gap near the contact and results in gas discharge if the friction is carried out in a gas ambience. This gas discharge reduces the charge that was once induced at the frictional interface. It has been believed that the initial charge separation was not affected by a surrounding gas and was determined solely by the frictional materials. We have investigated the charge separation rate before the gas discharge under various gas conditions and found that it linearly decreased with the logarithm of the pressure from 10 Pa to atmospheric pressure for Ne, Ar, and Kr.

The friction experiment was performed by means of pin-on-disk equipment. The pin was made of natural diamond and was gold coated. The disk was quartz or sapphire. The charge accumulated on the gold-coated pin was measured by an electrometer. The diameter of a contact area between the bare diamond tip and the disk was about 10 μm and the sliding velocity was 11 $\mu\text{m/s}$. The charge on the pin increased at a constant rate during sliding and fell to zero when the gas discharge occurred. The charge accumulation and the gas discharge were repeated during sliding friction in a gas ambience. The initial charge density at the interface of the sliding contact was calculated from the accumulation rate, the track width and the sliding velocity.

The charge density was typically the order of 1 mC/m^2 for sliding friction in a vacuum (10 Pa). It was found that the initial charge separation under atmospheric gas pressure is one order of magnitude smaller than that at 10 Pa. This reduction of the charge separation rate was observed for Ne, Ar, and Kr gas at almost the same efficiency. It is likely that the gas molecules penetrate into the frictional interface and interrupt or relax the charge separation. It should be necessary to investigate the surrounding gas effect on the initial charge separation in detail in order to reveal the origin of triboelectricity.

2:20pm **TR+SS-TuA2 In situ Tribology of Metal-Doped MoS₂: Interfacial Film Mechanics and Friction Behavior**, K.J. Wahl, Naval Research Laboratory, S.D. Dvorak, University of Maine, G.Y. Lee, I.L. Singer, Naval Research Laboratory

Tribological processes that influence friction and wear involve a complex combination of materials science, physics, chemistry, and rheology. Our understanding of these sliding contact phenomena is limited by the fact that all the action takes place in a buried interface. Most often the only evaluation of these interfaces is accomplished through *ex situ* means after separating the contacts. *In situ* approaches to studying friction and wear processes are challenging because most engineering surfaces are metals or ceramics that have no optical transparency at visible wavelengths. For this reason, most of what is known about interfacial processes occurring during sliding has been learned through optical probes of sliding interfaces.

We have used an *in situ* tribometer to perform reciprocating sliding tests of Pb-Mo-S and Ti-Mo-S solid lubricant coatings. Experiments were performed in dry and ambient air. The interfacial films formed during sliding were monitored with *in situ* Raman spectroscopy and optical microscopy through transparent counterfaces. The dominant velocity accommodation mode in both dry and humid conditions was interfacial sliding between the surface of the wear track and the outer surface of the transfer film on the counterbody. Humid air sliding resulted in a second velocity accommodation mode involving shear and/or extrusion of the transfer film. We will demonstrate and discuss how the interface properties – shear strength and transfer film mechanical properties – affect friction behavior of these solid lubricant coatings.

2:40pm **TR+SS-TuA3 Nanosecond X-Ray Pulses From Peeling Tape in Vacuum**, S. Putterman, J.V. Escobar, C.B. Camara, J. Hird, University of California, Los Angeles

INVITED

That the surface between two interacting bodies can be a source of visible light –triboluminescence– has been known for centuries. Observation of the emission of nanosecond long 100.mW pulses of X-Ray photons from

peeling tape indicates that tribological processes reach energy densities which are much greater than the few eV per molecule needed to generate visible photons. Analysis of the x-ray pulses indicates that they originate from micron scale regions near the vertex of peeling tape. Based upon this insight we are building a mechanically operated sub-millimeter x-ray source that can be used for medical imaging. The organized processes which transduce diffuse mechanical energy into x-ray pulses are not understood.

4:00pm **TR+SS-TuA7 Nanotribology at Cryogenic Temperatures**, S.S. Perry, X. Zhao, S.R. Phillpot, G. Sawyer, S.B. Sinnott, University of Florida
The temperature dependence of the kinetic friction between a silicon nitride probe tip and a number of crystalline surfaces has been evaluated through atomic force microscopy measurements performed under an ultrahigh vacuum environment over the temperature range 140-750 K. Surfaces interrogated include highly oriented pyrolytic graphite, molybdenum disulfide, and lead sulfide. A relatively weak dependence on temperature is observed in the friction measured between 300 K and 750 K. As temperature decreases below ambient temperatures, a sharp increase in friction is observed for all surfaces, however with variations in the temperature threshold. Collectively, these results obtained from fundamental interfaces are consistent with an activated mechanism of energy dissipation during sliding. An Arrhenius analysis of the temperature dependent friction over this range yields different effective activation energies, ranging from 0.1-0.4 eV for the thermally activated stick-slip motion of the probe tip on this surface. As temperature is reduced further, a distinct transition to a largely athermal behavior is detected and is shown to result from the onset of interfacial wear, entailing an alternative energy dissipation pathway.

4:20pm **TR+SS-TuA8 Molecular Dynamics Simulations of Nanoindentation of Si/SiO₂ Systems using the Charge Optimized Many-Body (COMB) Potential**, T.R. Shan, B. Devine, S.R. Phillpot, S.B. Sinnott, University of Florida

Oxides and carbides, such as SiO₂, Al₂O₃, HfO₂ and SiC, are widely used together with Si in many high-performance electronic devices, including metal-oxide-semiconductor (MOS) devices/junctions and gate stacks. 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. Since nanoindentation has been established as a primary tool for investigating the mechanical behavior of small volumes of materials, classical molecular dynamics simulation is used to examine the nanoindentation of Si/SiO₂ interfacial systems. 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 is used to model the structural evolution, mechanical response and charge transfer of Si/SiO₂ interfacial systems under the influence of a nanometer-scale indenter. The COMB potential allows for dynamic charge transfer between atoms and across interfaces, and does a good job in describing covalent and ionic bonding in these materials. Aspects of the Si/SiO₂ interface during nanoindentation, including dislocation formation and the mechanisms by which fracture occurs, will also be addressed. We gratefully acknowledge the support of the National Science Foundation through grant DMR-0426870.

4:40pm **TR+SS-TuA9 Influence of Molecular Structure and Alignment on Nanometer-Scale Tribology**, P. Barry, P. Chiu, S.R. Phillpot, S.B. Sinnott, University of Florida

We report on the effect of small, fluorocarbon molecules on self-mated, aligned polytetrafluoroethylene (PTFE)-PTFE tribology using atomistic molecular dynamics simulations. Three fluorocarbon molecular classes were considered: C₂F₆, C₄F₁₀ and C₈F₁₈ with the amount of lubricant between the classes kept constant. Further, the effects of a relatively thin lubricating layer and a relatively thick lubricating layer were compared. The simulations predicted that the systems with thicker lubricating layers exhibited a friction coefficient that was significantly lower than those a thinner lubricating layer. Correspondingly, substantially more molecular wear of the PTFE surfaces were predicted for the latter systems. Interestingly, unlubricated PTFE-PTFE self-mated systems demonstrated low friction coefficients and molecular wear when the chains were slid in a direction parallel to the chain alignment, and unlubricated, aligned polyethylene (PE)-PE systems exhibited comparable or lower friction coefficients. The simulations further predicted that unlubricated, aligned PE-PTFE systems had friction coefficient values in between those of the PE-PE systems and PTFE-PTFE systems in which the chains slid in directions that were perpendicular to the alignment of the chains.

Surprisingly, the highest friction coefficients in the PE-PTFE system occurred when the chains were slid in a direction parallel to the direction in which the chains were aligned. This result was attributed to the incommensurate nature of the sliding interface between the two different polymers. This work was carried out under the support of an AFOSR MURI.

5:00pm **TR+SS-TuA10 On the Mechanical Properties of Tungsten Disulfide Nanotubes**, *I. Kaplan-Ashiri, S.R. Cohen, K. Gartsman*, Weizmann Institute of Science, Israel, *G. Seifert*, Technische Universität, Germany, *H.D. Wagner, R. Tenne*, Weizmann Institute of Science, Israel

WS₂ forms multiwalled nanotubes which seem to be almost defect free and their structure can be precisely defined. Hence they can serve as good candidates for the study of nanomechanics.

Various mechanical tests were applied on individual WS₂ nanotubes to reveal their mechanical properties and behavior. First, nanotubes were axially compressed in atomic force microscope, and their Young's modulus was observed according to Euler's buckling point. An average value of 170GPa was obtained. A similar test which was conducted in the scanning electron microscope resulted in large elastic deformation of the nanotube. Here the Young's modulus was obtained from the post buckling equations, and found to be 150GPa. In a third experiment, the nanotubes were axially strained until fracture occurred. The Young's modulus was then observed according to Hooke's law and found to be 152GPa. These moduli values are in good agreement between themselves and also with density functional tight-binding (DFTB) calculations and the bulk material (150GPa).

Tensile strengths and strain values as high as 16GPa and 14% were observed as well. These values reveal that WS₂ nanotubes reached their theoretical strength, hence they are suspected to be defect free. The high strain value is unique to the tubular nanophase of WS₂ and is also in good agreement with molecular dynamics simulation of MoS₂ nanotubes. The nanotubes were deformed elastically until failure, in "sword in a sheath" mechanism and probably fractured in a brittle mode.

Clamped nanotubes were bent and the shear (sliding) modulus was obtained according to Timoshenko's bending equation and found to be 2GPa. This value is in good agreement with DFTB calculations (4GPa) for sliding of two adjacent layers of MoS₂.

Furthermore, a unique nonlinear elastic deformation was observed both in post buckling and in bending tests. This mode of deformation is associated with the tubular structure.

5:20pm **TR+SS-TuA11 Nanotribological Characterization of Various Skin Cream Ingredients using Atomic Force Microscopy**, *W. Tang, B. Bhushan*, The Ohio State University, *S. Ge*, China University of Mining and Technology

Skin cream is used to improve skin health and create a smooth, soft, pliable, and moist perception by altering the surface friction, adhesion, elastic modulus, and surface potential of the skin surface. As the industry continually searches for better cream formulations, it becomes increasingly necessary to study how different cream ingredients interact with skin surface on the nanoscale. In this paper, vaseline, glycerin, and lanolin oil, which are the widely used ingredients in moisture cream, as well as the common moisture cream, advanced moisture cream, and oil-free moisture cream, were studied using an atomic force microscope (AFM). The binding interaction between skin cream and skin surface is one of the important factors in determining cream thickness and consequently the proper performance of skin cream. Film thickness, adhesive force and effective Young's modulus of various cream treated skin was measured using the force calibration plot technique with the AFM. Skin goes through various daily activities with time and the durability properties are closely tied to product performance. The durability of various skin creams were studied by repeated cycling tests. The health and feel of skin are significantly affected by its surface charging and the surface potential of virgin skin, and various cream treated skin was measured to determine the effects of various skin cream using the Kelvin probe method with the AFM. Relevant mechanisms are discussed.

5:40pm **TR+SS-TuA12 An Imaging TOF-SIMS Study of the Tribochemical Interactions in Diamondlike Carbon Films**, *A. Erdemir, O. Eryilmaz*, Argonne National Laboratory

Diamondlike carbon (DLC) films combine many attractive properties which make them good prospect for a wide range of engineering applications. Depending on the sources of carbon (i.e., hydrocarbon gases or solid carbon or graphite targets) and the type of deposition method, some of the DLC films may contain large amounts of hydrogen in their structures and they are relatively soft. Those that are produced from solid carbon and/or graphite targets by arc-PVD and pulsed laser deposition are nearly hydrogen free but very hard. However, regardless of their chemical and/or

structural nature, all DLC films tend to be very sensitive toward the chemical composition of the test environments when tested for their friction and wear properties. In this study, we concentrate our attention on the friction and wear behaviors of both the hydrogenated and hydrogen-free DLC films in the presence of inert and reactive gaseous species like, argon, oxygen, hydrogen, and deuterium in test chambers. Using time-of-flight secondary electron mass spectrometry (TOF-SIMS), we explore the extent of tribochemical interactions that occurred during sliding tests. These studies have confirmed that the friction and wear behaviors of DLC films are indeed very closely controlled by the type and extent of tribochemical events that are triggered by the gaseous species in the surrounding atmosphere. In particular, hydrogen and deuterium in test environments seems to interact with the sliding surfaces of these films and thus have the greatest effect on friction and wear. Inert gases were detrimental for the friction and wear behaviors of hydrogen-free DLC, but beneficial to that of the highly hydrogenated DLC films. Based on the results from TOF-SIMS studies, we provide a mechanistic explanation for the tribochemistry of sliding surfaces and correlate these findings with the friction and wear behaviors of DLC films.

Authors Index

Bold page numbers indicate the presenter

— A —

Arakawa, I.: TR+SS-TuA1, 1

— B —

Barry, P.: TR+SS-TuA9, 1

Bhushan, B.: TR+SS-TuA11, 2

— C —

Camara, C.B.: TR+SS-TuA3, 1

Chiu, P.: TR+SS-TuA9, 1

Cohen, S.R.: TR+SS-TuA10, 2

— D —

Devine, B.: TR+SS-TuA8, 1

Dvorak, S.D.: TR+SS-TuA2, 1

— E —

Erdemir, A.: TR+SS-TuA12, **2**

Eryilmaz, O.: TR+SS-TuA12, 2

Escobar, J.V.: TR+SS-TuA3, 1

— G —

Gartsman, K.: TR+SS-TuA10, 2

Ge, S.: TR+SS-TuA11, 2

— H —

Hird, J.: TR+SS-TuA3, 1

Hosobuchi, E.: TR+SS-TuA1, 1

— K —

Kaplan-Ashiri, I.: TR+SS-TuA10, **2**

— L —

Lee, G.Y.: TR+SS-TuA2, 1

— M —

Miura, T.: TR+SS-TuA1, **1**

— P —

Perry, S.S.: TR+SS-TuA7, **1**

Phillpot, S.R.: TR+SS-TuA7, 1; TR+SS-TuA8, 1;

TR+SS-TuA9, 1

Putterman, S.: TR+SS-TuA3, **1**

— S —

Sawyer, G.: TR+SS-TuA7, 1

Seifert, G.: TR+SS-TuA10, 2

Shan, T.R.: TR+SS-TuA8, **1**

Singer, I.L.: TR+SS-TuA2, 1

Sinnott, S.B.: TR+SS-TuA7, 1; TR+SS-TuA8, 1;
TR+SS-TuA9, **1**

— T —

Tang, W.: TR+SS-TuA11, **2**

Tenne, R.: TR+SS-TuA10, 2

— U —

Ueno, S.: TR+SS-TuA1, 1

— W —

Wagner, H.D.: TR+SS-TuA10, 2

Wahl, K.J.: TR+SS-TuA2, **1**

— Z —

Zhao, X.: TR+SS-TuA7, 1