

Wednesday Morning, October 20, 2010

Tribology Focus Topic

Room: Tesuque - Session TR+MN+NS+SS-WeM

Influence of Atmosphere, Temperature, and Materials on Friction

Moderator: J.D. Schall, Oakland University

8:00am TR+MN+NS+SS-WeM1 'Demystifying' Gas Phase Lubrication: Tribochemistry, Third Bodies and Competition, I.L. Singer, Naval Research Laboratory **INVITED**

Gas phase lubrication, also called vapor phase lubrication, refers to processes in which the gas surrounding a sliding (or rolling) contact contributes to lubrication [1]. It has wide ranging applications from internal combustion engines to MEMS. Some gases simply condense on surfaces, others decompose and deposit lubricating films on the surface, e.g. hydrocarbon films decompose and deposit graphite. Some can be made to react on the surface, as do various monomers that tribopolymerize and form lubricious third bodies at the contact. Alternatively, gases can react with the surface to form films; the most ubiquitous example is the oxide film formed on metals, which prevents (on earth, but not in outer space) surfaces from weld upon contact. Reaction films have been studied extensively by surface scientists; less well understood are tribofilms, films formed by rubbing action. Another important component to the lubrication process is film removal, which can occur during sliding or rolling; the competition between film formation and film removal always needs to be considered. In some cases, gas lubrication provides low friction and low wear; in other cases, it can increase friction and wear. In this talk, I will review gas phase lubrication processes and present several gas phase lubrication studies that still mystify me.

[1] For overview, see http://nsfarchive.org/wiki/index.php?title=Gas_Phase_Lubrication

8:40am TR+MN+NS+SS-WeM3 Understanding Vapor Phase Lubrication Mechanism of Alcohol for MEMS and Other Materials, S.H. Kim, Pennsylvania State University

Microelectromechanical systems (MEMS) are usually fabricated from silicon-based materials which have poor tribological properties such as high friction, high adhesion, and low wear-resistance. We have recently demonstrated unprecedented success of MEML lubrication using alcohol vapor. The main difference of alcohol vapor phase lubrication (VPL) from other coating-based approaches is that it allows continuous replenishment of lubricant molecules from the vapor phase, rather than relying on one-time loaded coating layers. In our previous studies, we have observed tribochemically-formed polymeric species. Then, an interesting question is if the polymeric species is responsible for effective lubrication or not. This talk addresses the origin of tribochemical reaction products and the lubrication mechanism for alcohol VPL for silicon oxide surfaces. In summary, the tribochemical polymerization appears to be associated with the substrate wear process occurring due to insufficient adsorbate supply or high mechanical load. The tribochemical reactions do not seem to be the primary lubrication mechanism for vapor phase lubrication of SiO₂ surfaces with alcohol, although they may lubricate the substrate momentarily upon failure of the alcohol vapor delivery to the sliding contact.

9:00am TR+MN+NS+SS-WeM4 Mechanistic Aspects of Vapor Phase Lubrication of Silicon, M.T. Dugger, J.A. Ohlhausen, S.M. Dirk, Sandia National Laboratories

The lubrication of silicon surfaces with alcohol vapors has recently been demonstrated [D.B. Asay, et. al, Langmuir 24 (2007) p.155]. With a sufficient concentration of pentanol vapor present, sliding of a silica ball on an oxidized silicon wafer can proceed with no measurable wear. The initial results of time-of-flight secondary ion mass spectrometry (ToF-SIMS) analysis of wear surfaces revealed a reaction product having thickness on the order of a monolayer, and with an ion spectrum that included fragments having molecular weights of 200 or more that occurred only inside the wear tracks. The parent alcohol molecule (pentanol) has molecular weight of 88 amu, suggesting that reactions of adsorbed alcohols on the wearing surfaces allowed polymerization of the alcohols to form higher molecular weight species. In addition to pin-on-disk studies, lubrication of silicon surfaces with pentanol vapors has also been demonstrated using MicroElectroMechanical Systems (MEMS) devices. Extraordinary increases in the operating life of MEMS devices have been observed with vapor phase lubrication. Devices with thermal actuators as well as electrostatic actuators have been successfully operated, demonstrating that the heated surfaces of the thermal actuators do not form prohibitively large

amounts of reaction product from the alcohol vapor. The same reaction product between pentanol and the silicon surface observed in pin-on-disk tests has also been found on MEMS contacting surfaces using ToF-SIMS analysis.

Recent investigations of the reaction mechanisms of the alcohol molecules with the oxidized silicon surfaces have shown that wearless sliding requires a concentration of the alcohol vapor that is dependent upon the contact stress during sliding, with higher stress requiring a greater concentration of alcohol. Different vapor precursors including those with acid functionality, olefins, and methyl termination also produce polymeric reaction products, and can lubricate the silica surfaces. Doping the operating environment with oxygen was found to quench the formation of the polymeric reaction product, and demonstrates that polymer formation is not necessary for wearless sliding.

9:20am TR+MN+NS+SS-WeM5 Tribological Study of Octadecylphosphonic Acid Self-Assembled Monolayers Across Velocity Regimes, O. Matthews, S. Barkley, Luther College, C. Bouxsein, M. Deram, N. Eigenfeld, St. Olaf College, A. Poda, W.R. Ashurst, Auburn University, B. Borovsky, St. Olaf College, E. Flater, Luther College

Microelectromechanical systems (MEMS) are critically-limited by interfacial phenomena such as friction and adhesion. The most common method of reducing friction between MEMS surfaces is the use of molecularly-thin self-assembled monolayer (SAM) coatings. Typically silicon MEMS have been coated with silane-based SAMs, such as octadecyltrichlorosilane (OTS), and have resulted in some modest improvement in device performance and lifetime. Continued progress in the development of MEMS may require new materials systems to be implemented. Through a collaborative effort, we investigate the frictional properties of octadecylphosphonic acid monolayers deposited on aluminum oxide surfaces across speed regimes. Measurements using an atomic force microscope (AFM) and a nanoindenter-quartz crystal microbalance are performed each with a microsphere-terminated probe. This allows for a comparative study with similar contact sizes, pressures, surface roughness, and interfacial chemistry. Speeds between the different instruments range from microns per second to meters per second. Preliminary AFM friction vs. load and friction vs. velocity measurements are presented, with the goal of investigating phosphonate SAM/ metal oxide systems as alternative MEMS materials.

9:40am TR+MN+NS+SS-WeM6 Triboelectrification and Triboplasma Generation and its Application for Surface Modification, S.V. Singh, P.K. Michelsen, Y. Kusano, Technical University of Denmark

Triboplasma gas discharges are often induced by triboelectrification around a sliding contact. Only an empirical classification is available for triboelectrification, whereas a detailed physical mechanism behind it is still unknown. Laboratory triboplasmas are mostly characterized by using optical diagnostics, and the optical emissions are reported to be observed mostly in ultraviolet region, corresponding to nitrogen emission lines. These measurements do not directly address triboelectrification. Here we present the evidence of electrostatic charging at the sliding contact and gas break down between the contacts through electrical measurements. Furthermore, the applicability of triboplasma for surface modification on polymeric materials was studied. Two capacitive probes were used for the investigation of a triboelectrification and triboplasma generated in a pin-on-rotating disk apparatus. These probes were mounted above the disk and on the pin, respectively. Measurements show a clear evidence of tribocharging, charge decay and triboplasma generation. Several combination of sliding contact materials with tendency to gain opposite charging and different sliding speeds, as high as 1000 rotation per minute, were carefully chosen. In addition, influence of different gas environment and pressure were investigated. Triboplasma induced surface modifications were characterized by water contact angle and X-ray photoelectron spectroscopy measurements.

10:40am TR+MN+NS+SS-WeM9 Friction at Cryogenic Temperatures, S.S. Perry, University of Florida **INVITED**

There are a number of applications where operation over a wide temperature range is required for device success. These extreme conditions are often the motivation for variable temperature studies in tribology; however, a paucity of relevant tribology data exists for temperatures below 273 K.

In the range from 300 K to 100 K the friction coefficient of various solid lubricants has recently been shown to increase with decreasing temperature. Molecular scale measurements employing an atomic force microscope over a temperature range from 140 K to 750 K at a vacuum level of 2×10^{-10} torr

have identified a temperature activated behavior of the friction and friction coefficient for the solid lubricants graphite and molybdenum disulfide. These molecular scale experiments were performed under conditions for which interfacial sliding was confirmed, interfacial wear was absent, and the role of adsorbed contaminants could be dismissed.

The potential influence of interfacial wear as well as the mechanism underlying the measured temperature dependence will be discussed.

11:20am **TR+MN+NS+SS-WeM11 *In-Situ* Scanning Auger Analysis of a Tribological Wear Scar in UHV Conditions**, *B.P. Miller, O.J. Furlong, W.T. Tysoe*, University of Wisconsin-Milwaukee

Lubrication of sliding copper-copper interfaces for use in brushes in electrical motors provides a particular challenge. Not only is a reduction in friction and wear required, but also allowing for high conductivity through the contact. Therefore, a self-limiting tribofilm is essential. The following explores the surface chemistry and tribology of dimethyl disulfide (DMDS) on copper surfaces to establish whether it is sufficiently reactive to potentially form a tribofilm near room temperature as required for lubrication of the sliding copper-copper contact in an electric motor. The surface chemistry and decomposition pathways of DMDS on copper surfaces are analyzed using temperature-programmed desorption (TPD), reflection-absorption infrared spectroscopy (RAIRS) and X-ray photoelectron spectroscopy (XPS). It is shown that DMDS reacts to form methyl thiolate species on the copper surface at room temperature. After heating to about 430K, methane and C₂ hydrocarbons desorb leaving molecular sulfur adsorbed onto the surface. A UHV tribometer chamber was equipped with a scanning electron gun having a ~100 micron diameter spot size. DMDS was dosed in the gas phase while performing friction measurements so that *in-situ* elemental analysis of the wear scar could be made. An increase in the sulfur signal is witnessed inside compared to outside of the tribological wear scar. A depth profile Auger analysis of the sample showed selective diffusion of sulfur into the bulk only inside the wear scar attributed to tribologically induced effects. This novel method of analysis can give important insights into the fundamentals of tribological systems.

11:40am **TR+MN+NS+SS-WeM12 First Principles Calculations and Atomistic Simulations of Tribology at Sliding Molybdenum Disulfide Surfaces**, *T. Liang, S.R. Phillpot, S.B. Sinnott*, University of Florida

Molybdenum disulfide is the most commonly used solid lubricant coating in aerospace applications. In this work, we carry out first principles density functional theory (DFT) calculations of the potential energy surface between two MoS₂ surfaces and examine the influence of oxidation on the results. In addition, we present the results of a recently developed empirical many-body potential for Mo and S systems and examine nano-scale friction between sliding MoS₂ surfaces using classical molecular dynamics (MD) simulations. In particular, MD simulations of interfacial sliding at various loads, temperatures and sliding directions are carried out. The loads and friction forces are extracted to calculate the friction coefficient of the MoS₂ as a function of temperature, and the results are compared to experimental pin-on-disk measurements of MoS₂ coatings and atomic force microscopy measurements on single crystal MoS₂ surfaces. The results from both the DFT calculations and the MD simulations help us to better understand the origins of lubricity on MoS₂.

Wednesday Afternoon, October 20, 2010

Tribology Focus Topic

Room: Tesuque - Session TR+NS+SS-WeA

Mechanical & Chemical Effects on Friction and Wear

Moderator: S.S. Perry, University of Florida

2:00pm **TR+NS+SS-WeA1 Quantitative Assessment of Sample Stiffness and Sliding Friction from Force Curves in Atomic Force Microscopy**, J.R. Pratt, G.A. Shaw, NIST, L. Kumanchik, University of Florida, N.A. Burnham, Worcester Polytechnic Institute

It has long been recognized that the angular deflection of an atomic force microscope (AFM) cantilever under "normal" loading conditions can be profoundly influenced by the friction between the tip and the surface. It is shown here that a remarkably quantifiable hysteresis occurs in the slope of loading curves whenever the normal flexural stiffness of the AFM cantilever is *greater* than that of the sample. This situation arises naturally in cantilever-on-cantilever calibration, but also when trying to measure the stiffness of nanomechanical devices or test structures, or when probing any type of surface or structure that is much more compliant along the surface normal than in transverse directions. Expressions and techniques for evaluating the coefficient of sliding friction between the cantilever tip and sample from normal force curves, as well as relations for determining the stiffness of a mechanically compliant specimen are presented. The model is experimentally supported by the results of cantilever-on-cantilever spring constant calibrations. The cantilever spring constants determined here agree with the values determined using the NIST electrostatic force balance within the limits of the largest uncertainty component, which had a relative value of less than 2.5%. This points the way for quantitative testing of micromechanical and nanomechanical components, more accurate calibration of AFM force, and provides nanotribologists access to information about contact friction from normal force curves [1].

1. J. Appl. Physics **107**, 044305 (2010), doi:10.1063/1.3284957

2:20pm **TR+NS+SS-WeA2 Nanotribological Properties of Polyzwitterionic Brushes**, Z. Zhang, A.J. Morse, S.P. Armes, University of Sheffield, UK, A.L. Lewis, Biocompatibles UK Ltd., UK, G.J. Leggett, University of Sheffield, UK

2:40pm **TR+NS+SS-WeA3 Atomic-scale Processes in Friction and Wear: From Diamond to Graphene**, R.W. Carpick, University of Pennsylvania **INVITED**

Nanoscale friction and wear are primary limitations for small-scale devices such as atomic force microscopy (AFM) probes and micro- or nano-electronic mechanical systems with contacting surfaces, and is also relevant to understanding friction and wear in larger-scale contacts. We first present studies that quantify the nanoscale volume loss in sliding wear using AFM and periodic *ex-situ* transmission electron microscopy (TEM) imaging. Novel carbon-based AFM tip materials, including ultrananocrystalline diamond and diamondlike carbon, exhibit superior wear resistance compared to conventional materials (silicon and silicon nitride)¹⁻³. We then present results from wear tests performed inside of the TEM using modified *in-situ* indentation techniques. This permits real-time visualization of the contact geometry and shape evolution of a single asperity with sliding over a countersurface. This allows us to measure wear with a higher degree of precision than previously possible. Insights comparing the wear resistance of carbon-based and Si-based materials, particularly in the context of atom-by-atom wear processes, will be discussed⁴. Finally, we will discuss how nanoscale friction in graphene and other atomically-thin sheets is governed by the high flexibility intrinsic to the atomic scale⁵.

1. *Prevention of nanoscale wear in atomic force microscopy through the use of monolithic ultrananocrystalline diamond probes*. J. Liu, D.S. Grierson, J. Notbohm, S. Li, S.D. O'Connor, K.T. Turner, R.W. Carpick, P. Jaroenapibal, A.V. Sumant, J.A. Carlisle, N. Neelakantan & N. Moldovan, **Small**, in press (2010).

2. *Ultra-low nanoscale wear through atom-by-atom attrition in silicon-containing diamond-like-carbon*. H. Bhaskaran, B. Gotsmann, A. Sebastian, U. Drechsler, M. Lantz, M. Despont, P. Jaroenapibal, R.W. Carpick, Y. Chen & K. Sridharan, **Nature Nanotechnology** **5**, 181-185 (2010).

3. *Wear resistant diamond nanoprobe tips with integrated silicon heater for tip-based nanomanufacturing*. P.C. Fletcher, J.R. Felts, Z. Dai, T.D. Jacobs, H. Zeng, W. Lee, P.E. Sheehan, J.A. Carlisle, R.W. Carpick & W.P. King, **ACS Nano**, accepted (2010).

4. *On the application of transition state theory to atomic-scale wear*. T.D. Jacobs, B. Gotsmann, M.A. Lantz & R.W. Carpick, **Tribol. Lett.**, accepted (2010).

5. *Frictional characteristics of atomically-thin sheets*. C. Lee, Q. Li, W. Kalb, X.-Z. Liu, H. Berger, R.W. Carpick & J. Hone, **Science** **328**, 76-80 (2010).

4:00pm **TR+NS+SS-WeA7 Lubricin Reduces Microscale Cartilage Wear**, J.M. Coles, D.P. Chang, Duke University, L. Zhang, G.D. Jay, Brown University / Rhode Island Hospital, F. Guilak, S. Zauscher, Duke University

Articular cartilage is the load bearing surface of mammalian joints. Relatively little wear occurs in cartilage and the tissue is able to sustain millions of loading cycles despite limited regenerative capacity. Though many studies of cartilage friction and lubrication have been performed, often with a stated goal of understanding cartilage wear prevention, very few have measured wear directly and none have directly assessed the effects of synovial fluid constituents in mediating wear. Here we show that the synovial fluid glycoprotein lubricin reduces microscale cartilage wear *in vitro*. We used colloidal probe microscopy to induce wear and use the change in the average height of the surface as a measure of worn volume. The height change in locations worn in the presence of lubricin was significantly less than in those worn in the control solution. These data indicate that lubricin is important for cartilage preservation physiologically and may have implications for treating or preventing joint disease.

4:20pm **TR+NS+SS-WeA8 Friction of Metallic Nanoparticles: The Influence of Particle Morphology, Orientation and Air Exposure**, D. Dietzel, T. Moeninghoff, C. Herding, M. Feldmann, H. Fuchs, Westfaelische Wilhelms-Universitaet Muenster, Germany, C. Ritter, U.D. Schwarz, Yale University, A. Schirmeisen, Westfaelische Wilhelms-Universitaet Muenster, Germany

The contact area dependence of the interfacial friction experienced during the translation of the antimony is studied under different conditions using the tip of an atomic force microscope as a manipulation tool [1]. In vacuum a dual behavior in the friction-area curves is found had been found earlier, characterized by the observation that some particles exhibit friction below the detection limit while other similarly sized particles showed constant shear stress values [2]. New investigations with improved sensitivity confirm the reproducibility of this effect and that neither the particle's morphology nor their relative orientation towards the substrate lattice change this behavior. In contrast, we find that a temporary exposure to ambient air can lead to a drastic increase in the particle's friction.

[1] A. Schirmeisen and U. D. Schwarz, *ChemPhysChem* **10** (2009) 2358

[2] D. Dietzel et al., *Physical Review Letters* **101** (2008) 125505

4:40pm **TR+NS+SS-WeA9 Modeling Materials in Contact using Molecular Simulation**, J.D. Schall, R.V. Petrach, Oakland University **INVITED**

Molecular dynamics (MD) simulation has become an extremely powerful tool for materials science research due to the wealth of atomic level information it provides. In this talk an overview of the MD simulation method will be given. Then a number of applications where MD simulations have been applied to study materials in contact will be discussed. Topics will include the tribology of amorphous carbon films in the presence of hydrogen, and recent work involving the indentation of free-standing graphene sheets. In simulation of the tribology of amorphous carbon, chemical reactions between opposing films were monitored and used to elucidate the mechanisms for enhanced friction and wear properties and to discover the mechanisms of transfer layer formation. These simulations illustrate the need for surface passivation of amorphous carbon films in applications where low friction is desired. We have also investigated the role of silicon on the properties of these films using a parametrization of Brenner's second generation reactive empirical bond order potential for Si-C-H interactions. Recent results of the simulation of indentation of free-standing graphene films will be shared.

5:20pm **TR+NS+SS-WeA11 Modeling Tribochemistry of DLC vs DLC in the Presence of Water**, J.A. Harrison, P.T. Mikulski, M.T. Knippenberg, United States Naval Academy

Because the structure and properties of diamond-like carbon (DLC) can vary depending upon deposition conditions, the tribological response of DLC (and diamond) is very sensitive to environmental conditions. For instance, the presence of water vapor has been shown to negatively impact the friction performance of hydrogenated DLCs but to improve the

performance of nanocrystalline and ultrananocrystalline DLCs. Tribochemical reactions of the water with the DLC are thought to be at the heart of this long-standing puzzle.

With that in mind, we have been working to develop a potential energy function that is capable of modeling DLC in the presence of water. To be realistic, such a potential energy function should be able to model tribochemical reactions that may occur as a result of the sliding. In addition, because H, C, and O have very different electronegativities, the potential energy function must be capable of modeling charges and fluctuating charges that arise from electronegativity differences in a realistic way. This talk will outline our efforts at potential development and present some preliminary results of DLC friction in the presence of water.

**Supported by The Air Force Office of Scientific Research.

5:40pm **TR+NS+SS-WeA12 Effects of Impact and Sliding Forces on Failure Behavior of a DLC Coating.** *J.F. Su, L. Wang, X. Nie*, University of Windsor, Canada

The wear and tribological properties of diamond-like carbon (DLC) coatings have been investigated and well documented under various laboratorial and industrial conditions. However, investigations into failure behavior of the coatings when subjected to cyclic impact-sliding loads are scarce. In this study, an inclined ball-on-plate impact-sliding tests were used to evaluate the fatigue cracking and peeling failure behavior of a DLC (a-C:H) coating and a TiN coating as comparison. By adjusting the impact velocity of a steel impacting ball that is connected to and driven by air cylinder, various dynamic impact loads can be obtained. The impact load vs. time curves were recorded and showed three stages, i.e., impact loading stage, vibration stage and quasi-static sliding stage for each impact-sliding cycle. Four loading combinations of impact/static forces (50N/100N, 100N/100N, 50N/200N and 100N/200N) were used in the tests. The test results showed that the DLC coating performed better than the TiN coating under the impact forces but worse under the sliding stages where the quasi-static force was applied by the air cylinder.

Thursday Afternoon Poster Sessions

Tribology Focus Topic

Room: Southwest Exhibit Hall - Session TR-ThP

Tribology Focus Session Poster Session

TR-ThP1 A Study of Sliding Friction Across Velocity Regimes for Alternative MEMS-type Interfaces using Proximal Probes and Quartz Microbalance. S. Barkley, Luther College, C. Bouxsein, M. Deram, N. Eigenfeld, St. Olaf College, L. Matthews, Luther College, A. Poda, W.R. Ashurst, Auburn University, E. Flater, Luther College, B. Borovsky, St. Olaf College

As mechanical devices have shrunk to microscopic sizes, the need for a more fundamental understanding of friction and other surface phenomena has become urgent. While the emerging technology of microelectromechanical systems (MEMS) shows promise as the mechanical counterpart to integrated circuits, progress remains slow as structural materials and lubricant strategies continue to be developed. We report on the results of a collaborative effort to study the frictional properties of organic monolayers on metal oxide surfaces. Both a nanoindenter-quartz crystal microbalance (NI-QCM) and an atomic force microscope (AFM) in lateral force mode have been used to perform tribological experiments at sliding velocities spanning the range from microns per second to meters per second. Our initial studies have employed octadecylphosphonic acid self-assembled monolayers chemisorbed onto aluminum oxide components with realistic contact roughness, sizes, and pressures. These interfacial systems have the potential to offer an alternative to silicon-based device fabrication. We present the development of custom microsphere probes for the NI-QCM and AFM systems, as well as the fabrication and characterization of the phosphonate monolayers. We discuss preliminary data from frictional studies across velocity regimes.

TR-ThP2 Deposition and Characterization of TiAlN/WN Multilayer Thin Films Deposited by dc Magnetron Sputtering. O. Jimenez-Aleman, J. Garcia, Universidad de Guadalajara, Mexico, L. Huerta, Universidad Nacional Autonoma de Mexico, M. Flores, Universidad de Guadalajara, Mexico

TiAlN/WN multilayer thin films with a range of different compositions and number of layers were deposited by PVD magnetron sputtering onto a variety of metallic substrates in a mixture of Ar/N₂ atmospheres. The utilisation of different nitride-formers elements and nitrogen (as a reactive gas) allows the deposition of alternative coatings with improved properties (e.g. wear and corrosion resistance) to those observed in individual commercial nitrides. The structure and morphology of the coatings were studied by means of X-ray Diffraction and Scanning Electron Microscopy. The elemental compositions and the surface chemistry (to gain precise information on the bonding environment) of these coatings were obtained by XPS. Microhardness and scratch tests were used to evaluate the mechanical properties and the adhesion of TiAlN/WN thin films respectively. The corrosion resistance was studied by potentiodynamic polarisation experiments in saline solutions of 0.5 M. The tribological properties were studied through reciprocating sliding against ceramic counterparts and different loads. In this paper we report the results relating to the influence of deposition conditions such as deposition temperature, period size and nitrogen content on coating properties. The improvement of corrosion and wear resistance by the utilisation of a multilayered TiAlN/WN arrangement is also presented and discussed.

TR-ThP3 Tribocorrosion Behavior of TiAlN and TiAlN/TiAl Multilayers. M. Flores, E. Rodríguez, O. Jiménez, J. García, Universidad de Guadalajara, Mexico, L. Huerta, Universidad Nacional Autonoma de Mexico

In the present work we investigate the tribocorrosion behavior of TiAlN, TiAlN/TiAl and TiAlN/TiAl/Pt coatings deposited on 316L stainless steel by magnetron sputtering. The period size of the multilayers was from 250nm to 1350 nm. The friction and wear tests were performed on a ball-on-flat tribometer and conducted in dry (unlubricated) conditions at room temperature. The loads used were 1 to 10 N, the oscillating frequencies were 1-5 Hz. The corrosion was studied using open circuit potential (OCP) measurements and potentiodynamic polarization in ringier solutions. Tribocorrosion tests were performed using a ball-on-flat tribometer where the sliding contact is fully immersed in a Ringer's solution. The potentiodynamic polarizations and OCP measurements were performed during, and after sliding test. The structure and composition of multilayers were studied by means of XRD and XPS techniques respectively. The surface topography and worn surface were studied by means of optical microscopy and profilometry. The results indicate that coefficient of friction

(COF) of TiAlN coatings decreased when metal layers are introduced and the corrosion resistance of TiAlN/TiAl coatings is improved when Pt layers are introduced. The synergy effect of the tribocorrosion tests is reported.

TR-ThP4 A Reactive, Fluctuating-Charge Potential for Carbon, Hydrogen, and Oxygen. M.T. Knippenberg, P.T. Mikulski, J.A. Harrison, United States Naval Academy

A classical bond-order potential energy function that incorporates fluctuating charges and reactions for carbon-, hydrogen-, and oxygen-containing molecules is presented. The model treats atomic charges as separate degrees of freedom that can be integrated over the course of the simulation, with charge fluctuations arising from the difference in electronegativity in bonds between atoms. Using the bond order that is already calculated, fluctuating charges are equilibrated during the course of the simulation. To test the validity of the potential, the dipole moments of oxygen-containing molecules are examined. Additional tests compare surface energies and structure of oxygen-containing diamond films.

TR-ThP5 Radial Compression Studies of Tungsten Disulfide Nanotubes. E. Kalfon-Cohen, O. Goldbart, R. Schreiber, Weizmann Institute of Science, Israel, D. Barlam, Ben Gurion University, Israel, T. Lorenz, G. Seifert, Technical University Dresden, Germany, S.R. Cohen, Weizmann Institute of Science, Israel

Understanding the mechanical properties of nanotubes is of significant practical and fundamental interest. Multiwalled nanotubes and nanoparticles of metal dichalcogenides such as WS₂ express unique mechanical and tribological characteristics.[1] The structure of WS₂ nanotubes consists of layers of covalently bound trigonal bipyramidal WS₂. The interaction between the layers is a van der Waals interaction between adjacent sulfur sheets. One of the intriguing aspects of these structures is the response of these layers under mechanical stress. Whereas some of the elastic constants of these unique structures have been addressed by experimental and theoretical work, the radial compression mode has not yet been studied. Relatively few studies of radial modulus of multiwalled carbon nanotubes have been made, and these also do not explicitly include the multilayered aspect of the structures. Here, we report an experimental and modeling study of this mode in the WS₂ nanotubes.

Three independent atomic force microscope (AFM) experiments were employed to measure the nanomechanical response, using both large (R=200 nm) and small (R=3-15 nm) probe tips. Two different analytical models were applied to analyze the results.[2] For a large AFM tip, a Hertzian model presuming an elliptical contact was applied. A shell continuum model is applied in the case of the sharper AFM tips. This model treats the nanotube wall as a thin, curved membrane. The results indicate that the derived modulus varies with nanotube diameter and compression depth

The modulus values derived from the analytical models were used as initial input for finite element analysis (FEA). The FEA model described the nanotubes as alternating high stiffness (representing the covalent shells) and low stiffness (representing the vdW gap) layers for the outer two shells, with a homogeneous inner core. This model was fit with the experimental results over the initial linear elastic region of the first few nm of deformation. Values obtained varied for different nanotube diameters, and compression depths, showing the importance of the inter-layer contact. In addition, first-principles calculations using density functional theory tight binding give qualitative agreement with a reversible collapse of the nanotubes, seen at larger deformations.

[1] L. Rapoport, et al, *Nature* **387**, 791-93 (1997); I. Kaplan-Ashiri et al, *Proc. Natl. Acad. Sci. USA*, **103**, 523 (2006); I. Kaplan-Ashiri et al, *J. Phys. Chem C*, **111** 8432-8436 (2007)

[2] W. Shen, et al, *Phys. Rev. Lett.* **84**, 3634 (2000); M. Minary-Jolandan et al., *J. Appl. Phys.* **103**, 073516 (2008).

TR-ThP6 Tribocorrosion Behavior of nc-TiN/a-Si₃N₄ Nanocomposite Deposited on Metallic Substrates for Biomedical Applications. J. García, M. Flores, E. Rodríguez, O. Jiménez, Universidad de Guadalajara, Mexico

The tribocorrosion property of a nc-TiN/a-Si₃N₄ nanocomposite deposited using DC and RF codeposition reactive magnetron sputtering technique on SS316L nitrated and Titanium Ti6Al4V alloy against ceramic and metallic balls was studied in comparison with substrate materials using a reciprocating tribotester in distilled water, 1% NaCl water solution and artificial saliva solution. The effects of load and reciprocating sliding speed on the tribocorrosion properties of the nanocomposite were investigated. The structure and composition of coatings were studied by means of XRD and XPS techniques respectively. Under the experimental conditions of the

present study, the nc-TiN/a-Si₃N₄ nanocomposite showed excellent resistance against corrosion and lower wear rate compared with SS316L nitrated and Titanium substrates. Profilometer analysis shows that on both materials most of overall tribocorrosion damage is due to mechanical wear. The tests suggest that nc-TiN/a-Si₃N₄ nanocomposite is a promising biomaterial for applications where reciprocating conditions occur.

TR-ThP8 A Tribological Study on Plasma Electrolytic Oxidation Process of Al319, H. Eiliat, X. Nie, University of Windsor, Canada

In this study, a plasma electrolytic oxidation process is used in order to produce a layer of oxide on aluminum silicon alloy 316. A pulsed dc power mode with frequencies up to 2000 Hz is selected with current density variations from 0.06 to 1.4 A/cm². Surface morphology (roughness), microstructure (grain size) and other properties of the plasma induced layer such as hardness and toughness are studied. Various coating conditions are compared based on treatment time, wear scar and coefficient of friction. These are critical coating properties for automotive engine block applications. The study is concluded by selecting the best coating condition with the optimized thickness.

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Coles, J.M.: TR+NS+SS-WeA7, 3

— D —

Deram, M.: TR+MN+NS+SS-WeM5, 1; TR-ThP1, 5
Dietzel, D.: TR+NS+SS-WeA8, 3
Dirk, S.M.: TR+MN+NS+SS-WeM4, 1
Dugger, M.T.: TR+MN+NS+SS-WeM4, 1

— E —

Eigenfeld, N.: TR+MN+NS+SS-WeM5, 1; TR-ThP1, 5
Eiliat, H.: TR-ThP8, 6

— F —

Feldmann, M.: TR+NS+SS-WeA8, 3
Flater, E.: TR+MN+NS+SS-WeM5, 1; TR-ThP1, 5
Flores, M.: TR-ThP2, 5; TR-ThP3, 5; TR-ThP6, 5
Fuchs, H.: TR+NS+SS-WeA8, 3
Furlong, O.J.: TR+MN+NS+SS-WeM11, 2

— G —

García, J.: TR-ThP2, 5
García, J.: TR-ThP3, 5; TR-ThP6, 5
Goldbart, O.: TR-ThP5, 5
Guilak, F.: TR+NS+SS-WeA7, 3

— H —

Harrison, J.A.: TR+NS+SS-WeA11, 3; TR-ThP4, 5
Herding, C.: TR+NS+SS-WeA8, 3
Huerta, L.: TR-ThP2, 5; TR-ThP3, 5

— J —

Jay, G.D.: TR+NS+SS-WeA7, 3
Jiménez, O.: TR-ThP3, 5; TR-ThP6, 5
Jimenez-Aleman, O.: TR-ThP2, 5

— K —

Kalfon-Cohen, E.: TR-ThP5, 5
Kim, S.H.: TR+MN+NS+SS-WeM3, 1
Knippenberg, M.T.: TR+NS+SS-WeA11, 3; TR-ThP4, 5
Kumanchik, L.: TR+NS+SS-WeA1, 3
Kusano, Y.: TR+MN+NS+SS-WeM6, 1

— L —

Leggett, G.J.: TR+NS+SS-WeA2, 3
Lewis, A.L.: TR+NS+SS-WeA2, 3
Liang, T.: TR+MN+NS+SS-WeM12, 2
Lorenz, T.: TR-ThP5, 5

— M —

Matthews, L.: TR-ThP1, 5
Matthews, O.: TR+MN+NS+SS-WeM5, 1
Michelsen, P.K.: TR+MN+NS+SS-WeM6, 1
Mikulski, P.T.: TR+NS+SS-WeA11, 3; TR-ThP4, 5
Miller, B.P.: TR+MN+NS+SS-WeM11, 2
Moeninghoff, T.: TR+NS+SS-WeA8, 3
Morse, A.J.: TR+NS+SS-WeA2, 3

— N —

Nie, X.: TR+NS+SS-WeA12, 4; TR-ThP8, 6

— O —

Ohlhausen, J.A.: TR+MN+NS+SS-WeM4, 1

— P —

Perry, S.S.: TR+MN+NS+SS-WeM9, 1
Petrach, R.V.: TR+NS+SS-WeA9, 3
Phillpot, S.R.: TR+MN+NS+SS-WeM12, 2
Poda, A.: TR+MN+NS+SS-WeM5, 1; TR-ThP1, 5
Pratt, J.R.: TR+NS+SS-WeA1, 3

— R —

Ritter, C.: TR+NS+SS-WeA8, 3
Rodríguez, E.: TR-ThP3, 5; TR-ThP6, 5

— S —

Schall, J.D.: TR+NS+SS-WeA9, 3
Schirmeisen, A.: TR+NS+SS-WeA8, 3
Schreiber, R.: TR-ThP5, 5
Schwarz, U.D.: TR+NS+SS-WeA8, 3
Seifert, G.: TR-ThP5, 5
Shaw, G.A.: TR+NS+SS-WeA1, 3
Singer, I.L.: TR+MN+NS+SS-WeM1, 1
Singh, S.V.: TR+MN+NS+SS-WeM6, 1
Sinnott, S.B.: TR+MN+NS+SS-WeM12, 2
Su, J.F.: TR+NS+SS-WeA12, 4

— T —

Tysoe, W.T.: TR+MN+NS+SS-WeM11, 2

— W —

Wang, L.: TR+NS+SS-WeA12, 4

— Z —

Zauscher, S.: TR+NS+SS-WeA7, 3
Zhang, L.: TR+NS+SS-WeA7, 3
Zhang, Z.: TR+NS+SS-WeA2, 3