Surface Science
Room 2004 - Session SS2+NS+TF-ThA

Tribology
Moderator: J. Krim, North Carolina State University

2:00pm SS2+NS+TF-ThA1 Investigation of the Tribology of Diamondlike Carbon and SAMs using Molecular Dynamics, *J. Harrison*, P. Mikulski, G. Gao, J. Schall, United States Naval Academy **INVITED**
Examination of the Tribology of DLC and SAMs using Molecular Dynamics@footnote 1@ The development of micron-sized devices, such as microelectromechanical devices, for terrestrial and space applications has prompted the need for protection of the surfaces of these devices. Amorphous carbon films, diamondlike carbon, and self-assembled monolayers (SAMs) are all possible candidates for the passivation and lubrication of these devices. The fundamental problem associated with controlling friction is a lack of understanding of the underlying atomic-scale processes that govern both friction and wear. Over the past several years, we have performed extensive molecular dynamics simulations using the REBO@footnote 2@ and the AIREBO@footnote 3@ potentials aimed at understanding the atomic-scale mechanisms of friction in hydrocarbon systems. We have examined the contact forces present at the interface of a nominally flat, DLC tip and model alkane SAMs during sliding. We have also examined the effects of tip roughness on the contact friction. In addition, we have done simulations that have analyzed the tribological, mechanical, and transport properties of amorphous carbon films and diamondlike carbon films with various compositions. Some of our recent results will be discussed. @FootnoteText@ @footnote 1@ This work was supported by The Air Force Office of Scientific Research under contracts F1ATA04295G001 and F1ATA04295G002 (The Extreme Friction MURI) and by The Office of Naval Research (N00014-06-WX-20205).@footnote 2@ D. W. Brenner, Shenderova, O. A., Harrison, J. A., Stuart, S. J., Ni, B., and Sinnott, S. B., J. Phys. C. 14, 783 (2002).@footnote 3@ S. J. Stuart, Tutein, A. B., and Harrison, J. A., J. Chem. Phys. 112, 6472 (2000). .

2:40pm SS2+NS+TF-ThA3 Interfacial Force Microscopy of Viscous Water on Hydrophilic Surfaces, *M.P. Goertz*, R.C. Major, X.-Y. Zhu, University of Minnesota; *J.E. Houston*, Sandia National Laboratories
The hydration of surfaces is important to many fields and its effect on system behavior has been studied for decades, yet the detailed origins of the forces involved are still under debate. We use interfacial force microscope (IFM) to measure the viscosity of water thin films with nanometer thickness on hydrophilic surfaces, including silica and carboxylic acid terminated alkanethiol self-assembled monolayers. We obtain the viscosity from this interfacial water from three different measurements: shear force measurement for a water meniscus formed between a tip and the hydrophilic surface under ambient conditions; shear force measurement for the interfaces under water; and repulsive, draining-force measurements of the two approaching interfaces immersed in water. In all three types of measurements, we obtain effective viscosities more than 10@super 6@ times greater than that of bulk water for interfacial separations on the nanometer scale. The experiments clearly show that the extent of the interphase layer and its level of viscosity depend sensitively on the strength of hydrophilic interaction, gradual degrading after the surfaces have been in water for a couple of hours. Thus, it is clear that a strong water/surface interaction gives rise to an increases in water-water bonding near the two surfaces and it is this increased level of bonding that is disturbed by the lateral tip motion resulting in the observed viscosity increase.

3:00pm SS2+NS+TF-ThA4 Design of Environmentally Friendly Lubrication Systems through Surface Grafting of Ultrahydrophilic High-density Polymer Brushes, *A. Takahara*, M. Kobayashi, Kyushu University, Japan; *K. Ishihara*, The University of Tokyo, Japan; *A. Suzuki, M. Kaido*, Toyota Motor Co., Ltd., Japan
The hydrophilic polymer brushes of poly(2,3-dihydroxypropyl methacrylate) (poly(2)) and poly(2-methacryloyloxyethyl phosphorylcholine) (poly(3)) were prepared by surface-initiated atom transfer radical polymerization of (2,2-dimethyl-1,3-dioxolan-4-yl)methyl methacrylate (1) and (3) on the initiator- immobilized silicon wafer. A large water contact angle hysteresis was observed for poly(2). Extremely low water contact angle and low contact angle hysteresis of poly(3) against water were observed. Neutron reflectivity measurements at water/poly(3) brush interface reveled that the poly(3) is highly stretched to the bulk

water phase. Frictional properties of the poly(2) and (3) brushes were characterized by sliding a glass ball probe on the polymer brush surfaces in various solvents under the load of 0.49 N at a sliding velocity of 90 mm/min. Friction coefficient of poly(3) brush was lower than that of poly(2) in water. This can be ascribed to the presence of phosphorylcholine in poly(3). Further low friction coefficient was observed, even in air, by sliding a poly(3) brush immobilized glass ball against poly(3)-immobilized silicon wafer.

3:20pm SS2+NS+TF-ThA5 Mechanical Properties of Alkanethiol Monolayers on Gold: A Force Spectroscopy Approach, *G. Oncins*, C. Vericat, F. Sanz, University of Barcelona, Spain
Since the discovery of the self-assembling process of alkanethiol molecules on gold, these monolayers have been a matter of increasing interest not only from the point of view of basic surface science, but also due to their many applications in nanotechnology.@footnote 1@ Their mechanical properties have been widely studied by several techniques, especially by scanning probe microscopy.@footnote 2@ The growth mechanism of these monolayers on gold in vacuum has been followed by in situ Scanning Tunnelling Microscopy (STM).@footnote 3@ Atomic Force Microscopy (AFM) has proved to be suitable to study the topography and mechanical properties of alkanethiol monolayers under compression.@footnote 4@ In this contribution, we used Force Spectroscopy to study the behavior of alkanethiol monolayers deposited on a (111) monocrystalline gold surface in an electrolyte aqueous solution. The analysis of the force curves shows that the tip indents the monolayer in a stepped way and that the force at which these stepped events have place depends on the compactness of the monolayer. Thanks to newly developed models to calculate the mechanical constants of monolayers on hard substrates,@footnote 5@ we were able to calculate the different values of Young's modulus for alkanethiol monolayers of different compactness and chain length. @FootnoteText@ @footnote 1@J. C. Love, L. A. Estroff, J. K. Kriebel, R. G. Nuzzo and G. M. Whitesides, Chem. Rev., 2005, 105, 1103.@footnote 2@R.W. Carpick, M. Salmeron, Chem. Rev., 1997, 97, 1163.@footnote 3@G.E. Poirier, Langmuir, 1999, 15, 1167.@footnote 4@E. Barrena, C. Ocal, M. Salmeron, J. Chem. Phys., 2000, 113(6), 2413.@footnote 5@E.K. Dimitriadis, F. Horkay, J. Maresca, B. Kachar, R.S. Chadwick, Biophys. J., 2002, 82(5), 2798.

3:40pm SS2+NS+TF-ThA6 Observations of Microslip in Realistic Microscopic Contacts with Combined Nanoindentation and Quartz Microbalance, *B. Borovsky*, St. Olaf College; *A. Booth*, Grinnell College
For emerging technologies such as micromachined devices, it is increasingly important to understand the frictional properties of microscale sliding contacts and how these may be optimized with ultrathin lubricant films. While high sliding speeds and multiple contact points characterize realistic systems of interest, most theoretical and experimental studies of small contacts do not access this physical regime. We have therefore used a combined indenter probe and quartz crystal microbalance (QCM) to study the contact between a sapphire sphere and a polycrystalline gold electrode undergoing transverse shear at speeds near 1 m/s. The contacts were lubricated with monolayer octadecanethiol films. We find that both the elastic and dissipative components of the interaction are best described by the microslip model for reciprocating interfaces. We directly observe a 60% reduction in the tangential stiffness as the interface undergoes a spontaneous transition from stuck to slipping. For a mostly-slipping interface, the frequency and bandwidth shifts of the QCM are proportional to each other and track changes in the contact radius, as derived from the normal contact stiffness. Furthermore, we observe shear loss tangents over 0.4, more than 100 times larger than expected for no-slip conditions. We will show that our results are consistent with force-equilibrium microslip theory@footnote 1,2@ by proposing a simplified dynamic model of hysteresis effects in microslip, based on the driven harmonic oscillator. Research supported by NSF, Research Corporation, and Hysitron, Inc. @FootnoteText@ @footnote 1@R. D. Mindlin, W. P. Mason, T. F. Osmer, and H. Deresiewicz, Proceedings of the First U. S. National Congress of Applied Mechanics, 1951, pp. 203-208.@footnote 2@K. L. Johnson, Contact Mechanics, Cambridge University Press, NY, 1985, pp. 216-230.

4:20pm SS2+NS+TF-ThA8 The Effect of Filling and Temperature on the Mechanical Responses of Carbon Nanotubes, *S.-J. Heo*, S.B. Sinnott, University of Florida
It is well known that carbon nanotubes (CNTs) have fascinating electrical, optical, chemical, and mechanical properties that differ from the properties of macroscale carbon materials such as graphite or diamond. As a result of these properties, CNTs are being considered as candidate materials for MicroElectoMechanical System (MEMS)/NanoElectroMechanical System

(NEMS) components. It is therefore worthwhile to study the mechanical behavior of CNTs to better understand how they might fit in with the mechanical property requirements of MEMS/NEMS. To facilitate this better understanding, we have explored two different mechanical responses of CNTs, to bending and compression, using classical molecular dynamics simulations. The second generation reactive bond order potential is used to model the short-range covalent interactions and a Lennard-Jones potential is used to model the long- range van der Waals interactions. In particular, we have modeled a three-point bend test to explore the mechanical responses of the single walls CNTs, single-walled CNTs filled with C60, double-walled CNTs, and triple-walled CNTs. A compression test has also been done on these same systems. Filling the single-walled CNTs, or increasing the number of inner shells in the case of multi-walled CNTs, is predicted to increase both the bending strength and the maximum buckling force. We have also investigated the effect of temperature on the mechanical responses of the CNTs. On the whole, higher temperatures are predicted to lower the bending strength of the CNTs. This work is supported by the National Science Foundation funded Network for Computational Nanotechnology (EEC-02288390).

4:40pm **SS2+NS+TF-ThA9 Assessing nanomechanical properties and nanoscratch resistance of Me-ZrN and ZrN thin films using Atomic Force Microscope**, *D.M. Mihut, J. Li, S.R. Kirkpatrick,* University of Nebraska-Lincoln*; S. Aouadi,* Southern Illinois University*; S.L. Rohde,* University of Nebraska-Lincoln

The present study aims at getting a better understanding of the correlation between nanomechanical properties (nanohardness (H), elastic modulus (E), H/E and H3/E2 ratio) and nanotribological properties (resulting from nanoscratch measurements) for three groups of Me-ZrN thin films (Inconel-ZrN, Cr-ZrN and Nb-ZrN) and ZrN thin films. Nanomechanical and nanotribological properties for Me-ZrN and ZrN thin films deposited by DC unbalanced magnetron sputtering were investigated using atomic force microscope (AFM) interfaced with a Hysitron Triboscope. The elastic recovery of thin films under a normal load applied during nanoindentation was evaluated and correlated with elastic recovery of thin films under a dynamic load applied during nanoscratch measurements and with other mechanical properties in order to predict the thin film composition that will better serve for wear resistant applications.

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