Thursday Afternoon, November 7, 2002

Surface Science
Room: C-110 - Session SS-ThA

Tribology at Surfaces
Moderator: D.W. Brenner, North Carolina State University

2:00pm **SS-ThA1 QCM-STM Studies of the Nanoscale Dynamics of "Model-System" and "Real-World" Lubricants**, ***J. Krim***, North Carolina State University **INVITED**

In order to gain a fundamental understanding of friction, and the closely related phenomenon of lubrication, one must understand, at the molecular level, how the energy associated with the work to overcome friction is converted to heat.[1] Such knowledge is key to understanding the rate at which an interface will heat, and in addition how chemical reactions and other physical processes triggered by heat will be affected by friction. One of the simplest possible geometries in which friction can occur, and thus be studied, is that of a fluid or crystalline monolayer adsorbed on an atomically flat surface. This geometry is experimentally accessible to experiments with a Quartz Crystal Microbalance (QCM), to numerical simulation techniques, and to analytic theory. Measurements of the tribological properties of "model system" and "real world" lubricants have been performed for rare gases, octane and TCP adsorbed on lead, iron and/or copper surfaces in open geometries (with QCM) and also in confined geometries (by bringing a STM tip into tunneling contact with the QCM electrode). Lead substrates are of particular interest on account the recent observation of superconductivity-dependent sliding friction. Iron and copper substrates are of interest for a variety of practical applications. Interaction potentials for adsorbed rare gases are known to a high degree of accuracy, allowing highly reliable comparisons of theory to experiment. TCP is meanwhile a "real-world" lubricant known for its demonstrated anti-wear properties for macroscopic systems. Although this lubricant has been the subject of much research for over 40 years, the atomic-scale details of its lubrication mechanisms are far from being satisfactorily understood.

[1] "Surface science and the atomic-scale origins of friction: what once was old is new again.", J. Krim, Surf. Sci. 500, 741 (2002)

2:40pm **SS-ThA3 A Quantitative Study of the Mechanical and Adhesive Origin of Molecular-Level Friction**, ***J.E. Houston***, Sandia National Laboratories, *H.I. Kim*, Aerospace Corporation

In earlier work, we explored the origins of molecular-level friction using the interfacial force microscope and Au tips and substrates terminated by self-assembled monolayer films having various functional end groups. Here we continue that effort by applying contact-mechanics models to quantitatively analyze the mechanical properties of the films, their interfacial energies and the friction shear-stress values for each functional-group combination. Methyl end-group combinations represent only van der Waals bonding and purely mechanical friction, whereas carboxylic acid groups show significant hydrogen bonding. The results indicate that both the composite elastic modulus and the mechanical portion of the friction shear stress scale inversely with the total molecular length of the tip/substrate films. The adhesive energy shows an odd/even effect changing from inter-film for an even number of methylene units to purely intra-film bonding for odd-numbered films--the intra-film adhesion only appears in the lateral friction force. Very short methyl-terminated combinations indicate a significant non-contact component to the friction force. These results will be discussed in terms of the possible use of these films as molecular-level lubricants. Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin company, for the DOE under Contract DE-AC04-94AL85000.

3:00pm **SS-ThA4 Frictional Anisotropy at Crystalline Interfaces**, ***C.M. Mancinelli***, *A.J. Gellman*, Carnegie Mellon University, *J.S. Ko*, Merck & Co., Inc.

Fundamental tribological studies in an ultra-high vacuum environment have been performed to probe the effect of anisotropy on the friction between two single crystalline metal surfaces. The study of frictional anisotropy, or the effects of lattice orientation at crystal interfaces, has been conducted to address two main questions: whether slip between sliding surfaces occurs more easily along certain crystallographic directions, and whether the observed orientation effect on friction is a result of surface lattice commensurability. The results of a study of the frictional anisotropy between single crystalline Cu(100) surfaces will be presented. Tribological investigations were conducted on surfaces prepared to be either truly clean or modified by adsorption of molecular ethanol in the boundary lubrication regime. A detailed comparison will be made between these results and those previously obtained for the frictional anisotropy between single crystalline Ni(100) surfaces.

3:20pm **SS-ThA5 Nanopormorphism of C60 and Hydrocarbons on Metal Surfaces**, ***T.S. Coffey***, *M. Abdelmaksoud, J. Krim*, North Carolina State University

We report investigations of the validity of beliefs that nanoscale objects might have the same properties as macroscale objects, termed nanopormorphism. Since C60 molecules to rapidly rotate within their lattice position, tribologists envisioned nano-sized ball bearings. C60 is not an effective lubricant.[1] But differences in interfacial friction between rigid vs. rotating C60 remains an interesting topic. C60 forms close packed hexagonal films on both Ag(111) and Cu(111). However, on Ag(111), C60 spins in its lattice position, while it is rigid on Cu(111).[2] To determine if the spinning of C60 affects interfacial friction, we are employing QCM and AFM to compare the friction of methanol on C60/Ag(111) vs. methanol on C60/Cu(111). We examine whether the rolling nature of the C60 layer impacts the sliding friction as probed by QCM and AFM. Adsorbates at a surface can cause changes in the phonon dispersion curves, creating new modes that can be related to the sliding friction of the adsorbate. Among these new vibrational modes are three Frustrated Translational (FT) modes which probe the curvature of the molecule/surface potential along different spatial directions. For hydrocarbons adsorbed on many metals, the FT modes parallel to the surface (FTx, FTy) have energies much smaller than that perpendicular to the surface (FTz).[3] The stiffness or high "spring constant" of the FTz mode compared to the low "spring constant" of the FTx and FTy modes brings to mind molecular scale shock absorbers. We are using QCM to study octane and acetylene sliding on Cu(111) and Pb(111) to determine how energy and damping of the FTz mode affects sliding friction.

[1] T. Coffey et al., J. Phys. Condensed Matter, 13 (2001) 4991-4999.
[2] T. Sakurai et al., App. Surf. Sci., 87/88 (1995) 405.
[3] B.N.J. Persson and E. Tosatti, Eds, Physics of Sliding Friction, Ch. Woll, Kluwer Academic Publishers, Dorcdrecht, 1996.

4:00pm **SS-ThA7 Tribochemical Wear of Silicon Nitride on Oxide Surfaces Studied by Atomic Force Microscopy**, ***J.T. Dickinson***, *W. Maw, F. Stevens, S.C. Langford*, Washington State University

Nanometer scale tribochemical wear of silicon nitride AFM tips was characterized on a variety of substrates in aquous solutions using atomic force microscopy. Wear at this small scale contrasts markedly with the macroscopic wear of silicon nitride. For aquous mediated wear, a chemically active substrate (one with the appropriate surface metal-hydroxide bonds) is required. These results are generally consistent with wear due to the formation and breaking of chemical bonds between the tip and the substrate. The wear rates are shown to be nonlinear in the applied normal force. We propose that stress-induced intermediate states involving hydroxyl groups form on both the AFM tip and the substrate. Chemical reactions subsequently form transient bridging chemical bonds that are responsible for tip wear.

4:20pm **SS-ThA8 Adhesion Sensor: Non-Contact AFM for Quantitative Adhesion Measurements**, ***A. Schirmeisen***, *D. Weiner, H. Fuchs*, University of Muenster, Germany

The adhesion characteristics of metal coatings on Polycarbonate are of high technological interest. For example, Aluminum is used to coat plastic surfaces, with a wide range of applications. However, adhesion failure of metal coatings on polycarbonat is often observed. Methods such as flame annealing[1] or plasma treatment[2] are typically employed to improve adhesion characteristics. Yet little is known of the microscopic processes leading to the modified surface properties. We can quantify the adhesion properties of Al on differently treated polymers using dynamic AFM. Conventionally, adhesion tests are performed using a tape puller or similar device. The sample is usually destroyed after the test and no lateral resolution of the adhesion properties is achieved. In a novel approach using NC-AFM we can quantify the adhesion characteristics of the polymer-metal interface with nm-resolution. We measure frequency shift versus distance curves of a functionalised NC-AFM cantilever on the polymer surface. A specially designed UHV apparatus allows the in-situ preparation of tip and sample and the investigation of the interfacial force interactions with a UHV-AFM. The tip is functionalised by evaporation of a thin Al film on the cantilever. The adhesion properties of the polymer are modified by plasma treatment. Measurements of frequency shift versus tip-sample distance reveal the influence of the sample treatment on the adhesion properties. Following the approach of Durig,[3] we calculate force curves from the frequency shift data,[4] and extract quantitative values for the interfacial adhesion energy.

[1] A.P.Pijpers, R.J. Meier, J. Electron Spectr. 121 (2001) 299

[2] C. Seidel, H. Kopf, B.Gotsmann, T. Vieth, H. Fuchs, K. Reihs, Appl. Surf. Sci. 150 (1999) 19
[3] U. Durig, Appl. Phys. Lett. 75 (1999) 433
[4] Calculation based on programm from H. Holscher, CAESAR Institute, Germany.

4:40pm **SS-ThA9 The Frictional Behavior of a Hertzian Contact Analyzed using a New Contact Mechanical Model**, ***U.D. Schwarz***, Lawrence Berkeley National Laboratory, University of California

The study of the friction occurring at a Hertzian contact (i.e., the contact between a sphere and a flat surface or between two spheres) has always been a central issue in nanotribology, since realistic interfaces may be approximated by numerous individual Hertzian contacts that are within certain boundaries statistically distributed in all three dimensions. However, the theoretical description of the mechanical behavior of such contacts under load considering adhesion has been difficult in the past. Generally applicable models (i.e., models covering the "intermediate regime" between small, hard and large, soft contacts, as they might be most frequent in actual interfaces) required always numerical approaches. In this talk, I will present a new theory that covers the full parameter range for an adhesive Hertzian contact, but results in a simple equation describing the effective load acting on the surface that consists of adhesive and external contributions. The theory is based on a model interaction force that includes both short-range and long-range components. Comparison with numerical results obtained from the Maugis-Dugdale model as well as with experimental friction force microscopy data demonstrates the validity of the new approach.

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