Wednesday Morning, November 11, 2009

Tribology Focus Topic
Room: C4 - Session TR+NS-WeM

Nanomechanics and Nanotribology

Moderator: C.M. Mate, Hitachi San Jose Research Center

8:00am **TR+NS-WeM1 Nonlinear Contact Area Dependence of Sliding Friction for Metallic Nanoparticles**, ***D. Dietzel***, *T. Moenninghoff, A. Schirmeisen*, University of Münster, Germany

The existence of superlow friction under appropriate interface conditions is one of the most intriguing concepts in nanotribology. If an interface between two incommensurate surfaces is atomically clean, a state of virtually frictionless sliding is anticipated, often referred to as 'superlubricity' or 'structural lubricity'. But although superlubricity is a widely accepted theoretical concept, an unambiguous and direct verification has been difficult in the past. Theory predicts that the lattice mismatch at the interface causes a decrease of the potential barrier between stable states with increasing contact size that ultimately leads to vanishing friction. Therefore, analyzing the contact area dependence of superlubric friction might be a straightforward approach to confirm the frictional conditions.

Unfortunately, conventional friction force microscopy (FFM) has limitations inherent to the experimental configuration when it comes to contact area dependent measurements: Apart from the rather limited variety of material combinations, the fixed tip radius makes it especially difficult to analyze effects as a function of the contact area. In order to analyze the contact area dependence of interfacial friction, the friction between two objects in relative motion with a well-defined contact area should be measured instead of the friction between tip and surface. Therefore we have manipulated nanometer scale metallic particles on atomically flat surfaces by contact mode atomic force microscopy techniques and quantitative information on interfacial friction has been extracted from the lateral manipulation of these nanoparticles[1]. In previous experiments[2] we found two distinct frictional states during particle sliding of Sb-particles on HOPG substrate: Some particles show finite friction increasing linearly with interface area, thus reinforcing Amonton's law at the nanoscale, other particles assume a state of frictionless or 'superlubric' sliding.

In this contribution we show new measurements which were concentrated on the particles exhibiting vanishing friction. By optimizing our experimental sensitivity we succeeded for the first time to analyze the contact area dependence of friction force of these low friction particles. In contrast to the 'Amonton'-like particles, interfacial friction of the low friction particles showed strongly nonlinear contact area dependence. The experimental results are compared to theoretical considerations, which predict that the shear stress of sliding superlubric particles should decrease with increasing particle size.

[1]Dietzel et al., J. Appl. Phys.102, 084306 (2007).

[2]Dietzel et al., Phys. Rev. Lett. 101, 125505 (2008).

8:20am **TR+NS-WeM2 Why is Graphite so Slippery? Gathering Clues from Atomically Resolved Three-Dimensional Lateral Force Measurements**, ***M.Z. Baykara***, *T.C. Schwendemann, B.J. Albers, N. Pilet, E.I. Altman, U.D. Schwarz*, Yale University

Conventional lateral force experiments give insufficient insight into the fundamental reasons for graphite's outstanding qualities as a solid lubricant due to an averaging effect caused by the finite contact area of the tip with the sample. To overcome this limitation, we used a noncontact atomic force microscopy-based approach that enables use of atomically sharp tips. The new technique [1], performed using a home-built low temperature, ultrahigh vacuum atomic force microscope [2], allows the measurement of normal and lateral surface forces in a dense three-dimensional raster with picometer and piconewton resolution.

In this presentation, we analyze the height and lattice site dependence of lateral forces, their dependence on normal load, and the effect of tip shape in detail. The lateral forces are found to be heavily concentrated in the hollow sites of the graphite lattice, surrounded by a *matrix* of vanishingly small lateral forces. It will be argued that this astonishing localization may be a reason for graphite's excellent lubrication properties. In addition, the distance and load dependence of the lateral forces experienced along possible "escape routes" from the hollow sites, which would be followed by a slider that is dragged out of them, are studied. Surprisingly, the maximum lateral forces along these escape routes, which ultimately determine the static friction, are found to depend linearly on normal load, suggesting the validity of Amontons' law in the noncontact regime.

[1] B. J. Albers *et al.*, Nature Nanotechnology **4**, 307 (2009).

[2] B. J. Albers *et al.*, Rev. Sci Instrum. **79**, 033704 (2008).

8:40am **TR+NS-WeM3 Atomistic Simulations of Friction and Wear of Carbon-Based Materials**, ***I. Szlufarska***, *Y. Mo, M. Mishra*, University of Wisconsin, Madison **INVITED**

Controlling tribological properties requires understanding a bewildering array of interrelated mechanisms, including elastic instabilities, plastic deformation, fracture, and chemical reactions. Large scale atomistic simulations have been used to unravel some of these mechanisms. Tribological studies are typically divided into a wearless regime, where deformation is primarily elastic, and a wear regime where permanent deformation occurs. For wearless contacts, I will discuss the breakdown of continuum mechanics at the nanoscale and present our recent discovery of friction laws in dry nanoscale contacts. This discovery lays a foundation for unified friction laws across all length scales. In the wear regime I will focus on the origins of recently observed ductile wear in nominally brittle SiC. Although this ductile wear holds potential for greatly enhancing the ease of machining of high-performance ceramics, its origin is still an open question. I will evaluate potential mechanisms for ductile wear, including the possibility of transformation to more ductile phases, dislocation mediated plasticity, and nanoindentation-induced amorphization.

9:20am **TR+NS-WeM5 MD and AFM Studies of the Adhesion of Diamond, Silicon, and UNCD**, ***J.A. Harrison***, *P.L. Piotrowski, G.T. Gao*, United States Naval Academy, *R.J. Cannara*, National Institute of Standards and Technology, *R.W. Carpick*, University of Pennsylvania

For the past several years, we have used molecular dynamics (MD) simulations and classical reactive empirical bond-order (REBO and AIREBO) potentials to elucidate the atomic-scale mechanisms of friction and adhesion in solid lubricants. Recently, we have conducted complementary MD and atomic force microscopy (AFM) examinations of adhesion and atomic-scale friction for diamond, silicon, and nanocrystalline diamond interfaces. These materials are highly relevant to micro- and nano-electromechanical systems (M/NEMS), nanomanufacturing, and a host of other applications. The conditions of the simulations and the experiments were designed to correspond as closely as the methods allow. The effects of variables including diamond (or silicon) crystal orientation, hydrogen termination, temperature, and roughness on adhesion and friction can all be examined. In this talk, we will discuss our most recent results which highlight atomic mechanisms of friction and adhesion as well as the limits of continuum mechanics.

*JAH acknowledges support from The Air Force Office of Scientific Research (AFSOR) as part of the Extreme Friction MURI and from The Office of Naval Research. JAH & RWC also acknowledge support from AFOSR's Aerospace, Chemical, and Material Sciences Directorate.

9:40am **TR+NS-WeM6 Which Fractal Parameter Most Determines Adhesion?**, *D. Liu*, Worcester Polytechnic Institute, *J. Martin*, Analog Devices, Inc., ***N.A. Burnham***, Worcester Polytechnic Institute

The topography of a surface can be characterized by three fractal parameters: its surface roughness, its roughness exponent, and its lateral correlation length [1]. In 2001, T.S. Chow [2] predicted that a decrease in adhesion by orders of magnitude would follow from increasing the roughness exponent of a surface (i.e. by making it smoother), and that adhesion could also be lowered by decreasing its lateral correlation length (shorter wavelength). In 2007 [3], we published a simple analytical model, together with experimental data, that demonstrated the strong influence of surface roughness on adhesion. This year, using atomic force microscopy, experimental data were collected from MEMS sidewalls of varying topography but with the same chemical treatment in order to untangle which of the three fractal parameters is – or are – most important in determining adhesion. The data are inconsistent with Chow's predictions; his assumption was that only the asperities on the surface contribute to the adhesion. In contrast, our numerical simulations of the tip-sample adhesion for surfaces with varying fractal parameters include both the asperities and the bulk of the sample.

Together with the simulations, the previous and current experimental data support the conclusion that surface roughness is a significant predictor of adhesion, with the adhesion dropping by more than an order of magnitude for a roughness change from 1 to 10 nm. For the roughness exponent, the simulations follow the same trend as Chow's predictions, in that adhesion should decrease with increasing roughness exponent (smoother), but rather than predicting orders of magnitude change, the simulations reveal only a 20% decrease as the roughness exponent changes from 0 to 1. Here, the experimental data were more consistent with the simulation than Chow's predictions, although they were not conclusive. The scatter in the data was

large, and the range of the roughness exponent only varied from 0.85 to 0.99, for which the simulations predict a change in adhesion of approximately 10%. For the lateral correlation length, the experiment showed a wide range of adhesion values for smaller correlation lengths and low adhesion for larger correlation lengths (longer wavelengths); we are still investigating the theoretical basis of this observation. We hope to contribute to the understanding of adhesion so as to minimize stiction in MEMS.

References

1. A.-L. Barabasi and H.E. Stanley, Fractal concepts in surface growth (1995)

2. T.S. Chow, Phys. Rev. Lett. 86, 4592 (2001)

3. D. Liu, J. Martin, and N.A. Burnham, Appl. Phys. Lett. 91 043107 (2007)

10:40am **TR+NS-WeM9 Multiscale Modelling of the Indentation and Scratch Damage of Ultrathin Coatings on Architectural Glass**, ***S.J. Bull***, *A. Oila*, Newcastle University, UK

Although optical coatings are generally designed for their functional requirements it is often the mechanical properties of the system which limits performance. For instance, the major in-service failure mechanism of modern solar control coatings for architectural glass can be scratch damage. Many of these coatings are multilayer structures made from individual layers of less than 100nm thickness and different coating architectures are possible (i.e. different layer materials, thicknesses and stacking order). To assess their mechanical response, coated samples may be subjected to indentation and scratch tests; however, it is not always possible to predict the failure mechanisms of such coatings and modelling approaches have to be developed to understand the deformation mechanisms. This presentation will focus on the problems of measuring the plasticity and fracture properties of very thin coatings (<100nm) and the use of multi-scale modelling approaches to predict performance for coatings on glass.

11:00am **TR+NS-WeM10 Cognitive Molecular Engineering In Nanotribology - Intrinsic Friction Analysis**, *D.B. Knorr*, ***R.M. Overney***, University of Washington

In the new *Age of Molecular Engineering*, one of the objectives is to cognitively design molecules that if condensed, provide materials with anticipated properties. In regards of tribological systems, such as lubricants, the objective would be to offer chemists with molecular design parameters based on which molecules could be synthesized that dissipate energy in a targeted fashion. Thereby, the input would come either directly from experimental observations, or indirectly via computer simulations that are based on models that are relevant to the materials.

This is in contrast to the majority of current research efforts in tribology or nanotribology. State-of-the-art molecular models in tribology focus on generic periodic potentials that are thermally and mechanically inert. Experimental methods provide mostly only phenomenological parameters, such as the friction coefficient, or process descriptive parameters, such as the stick-slip phenomena. Such generic “black-box” approaches, fail to address frictional energy dissipation that are linked to material intrinsic molecular or submolecular modes of relaxation, and hence, do not provide the necessary input for a cognitive molecular design strategy for an effective tribological system.

This talk will highlight the importance of material intrinsic relaxation modes for frictional dissipation involving organic systems. Phenomenological friction analysis data, i.e., friction coefficients from friction-load curves, will be contrasted with spectroscopic data from an intrinsic friction analysis (IFA), involving a time-temperature superposition analysis of friction-velocity isotherms. Both data analysis methodologies, involving lateral force microscopy, reveal an astonishing correspondence regarding the dissipated energy and the energy involved in activating intrinsic relaxation modes and cooperative phenomena. Specifically, we will address surface and sub-surface energy relaxations in amorphous macromolecular model system (e.g., polystyrene) and their relevance to frictional energy dissipation within well defined loading regimes. Depending on the coupling strength (cause for cooperativity) between molecular actuators involved (e.g., rotating side chains or translating polymer backbones) the dissipation in energy can carry a significant entropic energy contribution, accounting for up to 80% of the apparent Arrhenius activation energy. The IFA methodology discussed in this paper that provides direct insight into the enthalpic and entropic energy contributions of friction dissipation processes is shown to be well suited as an analysis tool towards cognitive molecular engineering in tribology.

11:20am **TR+NS-WeM11 Optimization of Tailored Multifunctional Nanocomposite Structures**, ***T. Shenk***, *R. Winter*, *K. Benjamin*, South Dakota School of Mines and Technology

Polymer nanocomposites provide unique solutions to industrial and scientific applications where weight must be minimized and functionality maximized. Researchers are interested in improving the ability to tailor a product to meet specific weight, thermal, optical, mechanical and electrical requirements. Historically functional composite structures have been realized through a top-down approach. With the advent of atomic level measurement tools and experimental techniques a bottom-up approach to the creation of multifunctional structures is receiving intense study. We are developing unique multifunctional structures using such a bottom-up approach with the intent of developing molecular simulations to guide such a process. Properties of polymeric nanocomposite structures are tailored and optimized through a fundamental understanding of intermolecular forces. While macroscopic models of bulk properties of polymer nanocomposites have been characterized, much less is known on the dynamics of their interfacial characteristics, which must be fully developed in order to be able to tailor fabrication of multifunctional nanocomposites using the bottom-up approach. Self assembly, targeted functionalization and spin coating are used to provide consistent means of creating multilayer multifunctional thin film composite strictires allowing for the investigation of multifunctional composites. We investigate the affects of sonication, high shear mixing, and surface modification on the ability to control dispersion to create and predict multifunctional layers of epoxy spin coated nanocomposites and control desired mechanical properties such as conductivity, optical transmission and absorption, loss and storage moduli and coefficient of thermal expansion. The Interfacial Force Microscope (IFM), coupled with the Biaxial Loading Instrument, which allows for refined and uncoupled control of mixed-mode characterization of interface adhesion, will be used to determine interfacial characteristics of these multi-functional composites.

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