Tribology Focus Topic
Room 101A - Session TR+AS+NS+SS-WeA

Nanoscale Wear: Applications to Nanometrology and Manufacturing

Moderators: Tevis Jacobs, University of Pittsburgh, Filippo Mangolini, University of Leeds, UK

2:20pm **TR+AS+NS+SS-WeA1 A Multi-Bond Model of Single-Asperity Wear at the Nano-Scale**, *Y. Shao,* Johns Hopkins University; *T.D.B. Jacobs,* University of Pittsburgh; ***Michael L. Falk***, Johns Hopkins University **INVITED**

Single-asperity wear experiments and simulations have identified different regimes of wear including Eyring- and Archard- like behaviors. A multi-bond dynamics model based on Filippov *et al.* [Phys. Rev. Lett. **92**, 135503 (2004)] captures both qualitatively distinct regimes of single-asperity wear under a unifying theoretical framework. In this model, the interfacial bond formation, wear-less rupture and transfer of atoms are governed by three competing thermally activated processes. The Eyring regime holds under the conditions of low load and low adhesive forces; few bonds form between the asperity and the surface and wear is a rare and rate-dependent event. As the normal stress increases the Eyring-like behavior of wear rate tends to break down. A nearly rate-independent regime holds under high load or high adhesive forces; bonds form readily and the resulting wear is limited by the sliding distance. In a restricted regime of normal load and sliding velocity, the dependence of wear rate on normal load is nearly linear and independent of sliding velocity, as described by the Archard equation. Detailed comparisons to experimental and molecular dynamics simulation investigations have illustrated both Eyring and Archard regimes and an intermediate cross-over between the two.

3:00pm **TR+AS+NS+SS-WeA3 Surface Chemical and Tribological Studies of Solid Lubricants for Space**, ***Jeffrey Lince,*** The Aerospace Corporation **INVITED**

Successful operation of satellites and launch vehicles requires using multiple moving mechanical assemblies (MMAs). The correct choice of lubricants and tribocoatings is critical for the operation of spacecraft MMAs. However, the space environment is challenging. Examples include vibration during launch, thermal cycling on orbit, and the need to work effectively for missions up to twenty years in duration without lubricant replenishment. Especially challenging is the need for tribomaterials to withstand the vacuum of space during lengthy missions. As such, they must exhibit low vapor pressures, since evaporation of lubricants can result in loss from and premature failure of devices, as well as contamination of sensitive spacecraft components. Although unique synthetic liquid lubricants are used heavily in spacecraft for a variety of applications, solid lubricants are used with many devices because of their low vapor pressure, lack of migration, relative insensitivity to temperature changes, and low contamination potential. Soft solid lubricants such as molybdenum disulfide (MoS_2) and polytetrafluoroethylene (PTFE) have been used traditionally. More recently, hard low friction coatings such as hydrogenated diamond-like carbon have shown promise for operation in vacuum with existing spacecraft lubricants, or even unlubricated operation in vacuum. In addition, increasing interest in low friction nanoparticles has highlighted their potential utility. Tribomaterials show performance in vacuum that differs from that in air. This issue is important for spacecraft hardware, because it is often prohibitive to test them in a space-like environment, including vacuum, before launch. In addition, degradation during long-term storage can occur, and real-time storage studies correlating surface chemical changes with tribological performance are lacking. In this talk, results will be presented from studies done at The Aerospace Corporation that elucidate the effects of vacuum and temperature extremes on the tribological performance of important spacecraft tribomaterials. Emphasis will be on correlating surface chemical and tribological properties.

4:20pm **TR+AS+NS+SS-WeA7 Molecular Control of Friction**, ***Roland Bennewitz***, INM - Leibniz Institute for New Materials, Germany; *J. Blass, BL. Bozna,* INM - Leibniz Institute for New Materials; *M. Albrecht, G. Wenz,* Saarland University **INVITED**

Molecular films on surfaces can be used to control friction if it is dominated by adhesive shear rather than surface deformation. The underlying molecular mechanisms can be explored by high-resolution friction force microscopy.

We have developed a molecular toolkit for the control of friction and adhesion by supramolecular interactions in aqueous environments. The contacting surfaces are functionalized by cyclodextrin molecules. The interaction is mediated by ditopic connector molecules with hydrophobic end groups which form inclusion complexes with the cyclodextrin molecules on opposing surfaces. Significant friction and adhesion has been measured in atomic force microscopy experiments for connector molecules with adamantane, ferrocene, and azobenzene end groups.

For adamantane connector molecules, adhesion is found to be strongly dependent on the pulling rate due to a transition from subsequent peeling of individual bonds for slow pulling to multivalency effects at fast pulling. In contrast, friction does not depend on the sliding velocity [1].

The use of azobenzene connector molecules allows for switching of adhesion and friction by light stimuli [2]. Switching of friction by electrochemical stimuli for ferrocene connector molecules is less effective due to molecular interactions which are specific to the connector molecules but do not change with the potential [3]. We will discuss differences in rupture and rebinding dynamics for the three connector molecules and their influence on the rate dependence of adhesion and friction.

Cyclodextrin molecules have also been included in stiff polymers whose end groups are attached to tips or surfaces. The polymer-functionalized surfaces exhibit interesting variations of shearing and peeling mechanisms.

1. Blass, J., et al., Dynamic effects in friction and adhesion through cooperative rupture and formation of supramolecular bonds. Nanoscale, 2015. 7(17): p. 7674-7681.

2. Blass, J., et al., Switching adhesion and friction by light using photosensitive guest-host interactions. Chemical Communications, 2015. 51(10): p. 1830-1833.

3. Bozna, B.L., et al., Friction Mediated by Redox-Active Supramolecular Connector Molecules. Langmuir, 2015. 31(39): p. 10708-10716.

5:00pm **TR+AS+NS+SS-WeA9 Plasticity Controlled Friction and Wear in Single-Asperity Contacts**, ***Izabela Szlufarska***, *L. Zhao, A. Li, C. Tangpatjaroen, D. Grierson,* University of Wisconsin - Madison **INVITED**

One of the critical challenges in designing materials with superior tribological properties is the current lack of understanding of the microstructural evolution that takes place in sliding contacts. Phenomena that contribute to such evolution are grain growth and refinement, evolution of dislocation networks, and interaction of dislocations with interfaces. In this talk I will discuss examples of how we use multi-scale simulations and atomic force microscopy (AFM) experiments to determine the role of microstructural evolution and plastic deformation in friction and wear. Specifically I will discuss: (i) Our developments of a continuum model that couples grain growth, plastic deformation, and mechanics. This model combines for the first time the phase field method, crystal plasticity, and finite element analysis of mechanical contacts, and parameters for this model are determined from atomistic simulations and experiments. The new model is capable of simulating deformation at strain rates comparable to those encountered in AFM experiments. (ii) Results from our molecular-level simulations on the effects of dopants on strength and wear resistance of nanostructured metal alloys. (iii) Discovery from our complementary AFM and nanoindentation experiments that, although a harder material (silicon carbide) is typically more wear resistant than a softer material (silicon), this trend can be reversed with smaller contact sizes. The contact pressure is the same in both sets of experiments, and both are carried out in the regime where a plastic zone is well-developed. We demonstrate that this surprising finding is due to a transition from abrasive to adhesive wear, which for the first time is observed in single-asperity contacts. Our results show that surface chemistry can have a significant effect on sub-surface plastic deformation.

5:40pm **TR+AS+NS+SS-WeA11 Applying Analytical Roughness Models to Real Surfaces: Reconstructing the Power Spectral Density from Surface Topography Measurements**, ***Tevis Jacobs***, *A. Gujrati, S.R. Khanal,* University of Pittsburgh; *T. Junge, L. Pastewka,* Karlsruhe Institute of Technology (KIT), Germany

Surface topography is a critical factor for optical, mechanical, and tribological properties of materials. Many studies report single scalar roughness parameters that contain information over just a limited range of wavelengths. Analytical models of roughness have shown in recent years that properties such as stiffness, adhesion, and friction depend on the nature of roughness across many length scales. The power spectral density (PSD) is the mathematical instrument that provides a description of surface roughness as a function of scale. A truly quantitative analysis of surface roughness in terms of the PSD is necessary to validate and apply these analytical roughness models. However, this is currently limited by: (A) inconsistencies in the way that the quantitative PSD is computed; (B) bandwidth-limits of conventional surface metrology; and (C) instrumental artifacts at the smallest scales. Here, we demonstrate these limitations – first, by comparing the various forms of the PSD, then by computing the PSDs both for simulated and experimental surfaces.

We show that experimentally-determined PSDs suffer three types of systematic error, each of which will hinder quantitative comparison to models. We demonstrate strategies for detection and mitigation of these artifacts, to ensure accurate and reliable PSDs. A novel web-based application has been created and made available for general use which computes accurate PSDs and assesses the limits of their reliability. This enables the application of analytical roughness models to calculate upper and lower bounds of surface properties.

Finally, we report on the roughness characterization of an ultrananocrystalline diamond (UNCD) surface over the range from Angstroms to centimeters. This range of characterization enables quantitative comparison with rough-surface adhesion models. By elucidating experimental barriers to accurate surface characterization, and by demonstrating solutions to these barriers, this work facilitates the application of analytical roughness models to real-world surfaces – both to predict and tailor surface properties.

6:00pm **TR+AS+NS+SS-WeA12 Universal Ageing Mechanism for Static and Sliding Friction of Metallic Nanoparticles***, M. Feldmann,* ***Dirk Dietzel****, A. Schirmeisen,* Institute of Applied Physics, Justus-Liebig-University Giessen, Germany

On the macroscale, the distinct difference between static and sliding friction can well be explained by the phenomenon of contact ageing, which is typically related to an increase of contact area with time within a multi asperity interface model. On the nanoscale, however, the role of contact ageing is less clear, especially when considering nanoscale asperities of constant size.

Recently, the role of contact ageing for nanoscale friction dynamics was analyzed for antimony nanoparticles sliding on HOPG. The antimony nanoparticles have been prepared by thermal evaporation on HOPG and comprise an ideal model system with atomically flat interfaces of constant size where friction can be described by the concept of structural superlubricity [1]. Friction of the particles was assessed by nanomanipulation techniques and it was found, that sliding friction can be described as a complex process of thermally activated contact ageing and bond breaking [2]. Further measurements have now revealed, that the particle movement follows an irregular stick slip pattern, where the slip events can be considered as recurring contact renewal, while the stick times can be interpreted as the age of the contact. By correlating the stick times with the lateral force values measured for contact breaking, we found that our system can well be described by logarithmic ageing [3], as it might be expected by assuming atom by atom relaxation processes at the interface.

To check whether ageing during sliding motion is fundamentally different from ageing under stationary conditions, we have performed additional "slide hold slide" measurements [4] and found that in both cases ageing can be described by exactly the same logarithmic function. This indicates, that the strength of the contact is determined by the ageing time but independent of the kinetic conditions. This means that static and sliding friction can be described by a universal ageing law where the age of the contact is the crucial parameter.

[1] D. Dietzel, M. Feldmann, H. Fuchs, U.D. Schwarz, A. Schirmeisen, Phys. Rev. Lett. 111, 235502 (2013)

[2] M. Feldmann, D. Dietzel, H. Fuchs, A. Schirmeisen, Phys. Rev. Lett. 112, 155503 (2014)

[3] M. Feldmann, D. Dietzel, A. Tekiel, J. Topple, P. Gruetter, A. Schirmeisen, Phys. Rev. Lett. 117, 025502 (2016)

[4] Q. Li, T.E. Tullis, D. Goldsby, R. W. Carpick, Nature 480, 233-236 (2011)

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