Tribology Focus Topic
Room: 303 - Session TR-ThA

Tribology in Unique Environs
Moderator: Kathleen Ryan, United States Naval Academy

3:00pm **TR-ThA3 Molecular Mechanisms of Aqueous Boundary Lubrication by Mucinous Glycoproteins**, ***Stefan Zauscher***, Duke University **INVITED**

In this talk I will focus on lubricin and surface zone protein, secreted, cytoprotective glycoproteins, encoded by the gene PRG4, that are essential to maintaining joint function and long-term integrity of synovial joints by providing boundary lubrication, preventing cartilage-cartilage adhesion, and mediating adsorption of cells and proteins. Specifically I will report on our results from nanotribo-mechanical measurements on model surfaces and cartilage, combined with other surface specific, physicochemical measurements that shed new light on the mechanisms by which Prg4 provides lubrication and wear protection in diarthrodial joints. Furthermore, I will report on the interaction of PRG4 with collagenous model surfaces. taken together, our results suggest that the role of effective boundary lubricants in mediating friction in articular joints is largely one of wear protection of surface asperities, by maintaining the surfaces in a nonadhesive mode and causing shear dissipation in the biopolymeric boundary lubricant layer, even at the cost of attaining “high” coefficients of friction (COF ~ 0.15). Our results also contribute to the understanding of the conformation and physico-chemical function of mucinous glycoproteins on biological interfaces.

4:00pm **TR-ThA6 Unusual Friction and Wear Behavior of Graphene in Different Environments**, ***Ali Erdemir***, *D. Berman*, *A.V. Sumant*, Argonne National Laboratory **INVITED**

Graphene is a remarkable 2D material made of one-atom-thick carbon layer. Its unusual electrical, thermal, optical, and mechanical properties make it a promising material for numerous industrial applications. Recently, graphene was also shown to exhibit unusual tribological properties when used at sliding contact interfaces. In our laboratory, we have been exploring friction and wear behavior of graphene using nano-to-macro-scale tribological test systems and out of our research, we have discovered that a few layers of graphene on sliding surfaces can last tens of thousands of sliding cycles and the rubbing surfaces where graphene is applied to suffer very little or in some instances no wear. Friction was also dramatically reduced. We have found that graphene works equally well in humid or dry test environments; thus contrasting the very high environmental sensitivity of other solid lubricants like graphite or molybdenum disulfide. Our more recent studies have confirmed that even one layer of graphene put on a steel surface has a lifetime of more than 6000 cycles in hydrogen and the rubbing surfaces show no sign of wear. When 2 to 3 layers of large graphene sheets were applied, the lifetime increases to more than 30,000 cycles. Furthermore, under the right test conditions or against the right kind of counterfaces, graphene has the ability to literally vanish friction. This and other tribological observations point to a unique lubrication mechanism for graphene. In this talk, we will provide a comprehensive overview of recent experimental findings regarding the unusual friction and wear behavior of graphene and try to explain why it is so effective in drastically reducing friction and wear despite being only one atom thick.

4:40pm **TR-ThA8 Tribological Properties and Effects of Water on Carbon-Based Materials using Molecular Dynamics Simulations**, ***Marcel Fallet***, *K.E. Ryan*, United States Naval Academy, *M. Knippenberg*, High Point University, *P. Mikulski*, *J.A. Harrison*, United States Naval Academy

Tribological studies of C-based materials have come to the forefront of experimental and computational chemistry with applications for microfluidic devices and tip-based nano-manufacturing. The effects of humidity on friction and adhesion of some carbonaceous materials underscore the need to understand underlying mechanisms. Since it is difficult to determine atomic-scale behavior via experimental methods, molecular dynamics simulations have been employed to examine this behavior. Sliding simulations of non-hydrogenated, ultrananocrystalline diamond (UNCD) surfaces in the presence of water using the qAIREBO potential[1] have been performed. This reactive, bond-centric potential can model charge in C, H, and O systems. Hybridization changes, cross-sectional distributions of water, charge distributions, and other results will be presented to better understand the tribological impact of water in these systems.

5:00pm **TR-ThA9 An Atomistic Investigation of Tribological Performance of Solvated Nanodiamonds**, ***Farshad Saberi-Movahed***, *D. Brenner*, North Carolina State University, *O.A. Shenderova*, International Technology Center

Nanodiamonds synthesized by detonation of explosives have emerged as a promising additive to base lubricants to reduce wear and friction. Several mechanisms have been suggested for this observation, including creation of protective surface films, surface roughness reduction by abrasion and by filling in surface regions between asperities and by acting as spacers that roll and slide between contacting surfaces.

To better understand the details of these various mechanisms, and how these details relate to nanodiamond and surface structure and properties, we have been carrying out molecular dynamics of solvated nanodiamonds between sliding interfaces. Our initial simulations have focused on understanding the role of particle shape (round versus facetted) on viscosity of base fluid, the motion of the nanodiamond (sliding versus rolling), and correlation time of the nanodiamond motion as a function of pressure, and the interface sliding speed and separation. For example, we have observed that at higher nanodiamond volumetric ratio, the viscosity of water increased. It was also observed that the viscosity of the nanofluid decreased as the temperature increased. Simulation results for nanodiamonds with different surface functional groups, agglomerated nanodiamonds and nanodiamonds reacting with metal surfaces during sliding will be discussed, as well as studies using non-aqueous solvents.

This material is based upon work supported by the G8 Research Council through the National Science Foundation under Grant No. CMMI-1229889

5:20pm **TR-ThA10 Quantitative Analysis by AES and XRD and Tribologycal Properties of Multilayers and Nanocomposites Based on Titanium Nitride**, ***Arturo Talledo***, Universidad Nacional de Ingeniería, Peru, *J.A. Huaranga*, *J.L. Ampuero*, *J.J. Asmat*, *K. Paucar*, *C. Benndorf*, Universidad Nacional de Ingeniería, Perú

Multilayers and nanocomposites based on titanium nitride are widely investigated due to their high hardness and tribological properties. In this paper we report the production of coatings, on high speed steel, made by dc magnetron sputtering of multilayers TiN/VN, TiN/CrN and TiN/SiN as well as nanocomposites consistent in nanoparticles of SiN or CrN or VN embeded in matrixes of TiN. All these coatings were investigated by Auger Electron Spectroscopy and X-ray diffraction. Stoichiometry and structure were related to their respective Vickers hardness (measured by using Scanning Electron Microscopy), friction coefficient and abrasion wear measurements.

Authors Index

Bold page numbers indicate the presenter