Nanometer-scale Science and Technology
Room: L - Session NS+TR-TuM

Modeling Nanoscale Phenomena
Moderator: S.B. Sinnott, University of Florida

8:20am **NS+TR-TuM2 Tribological Behavior of Nanostructured Materials Predicted from Molecular Dynamics Simulations**, ***E. Bucholz***, *T. Liang, S.R. Phillpot, S.B. Sinnott*, University of Florida

Nanostructured materials such as fullerenes and nanotubes have been of much interest to tribologists since the discovery of C_{60}, buckminsterfullerene, in 1985. Characterized by weak van der Waals (vdW) forces that govern the interactions between these nanostructured materials, low friction coefficients are obtained through combinations of rolling, sliding, and rotating at the sliding interface. This presentation will report on the tribological properties of onion-like carbon (OLC) fullerenes with and without a residual diamond core as a solid lubricant between two sliding, diamond-like carbon (DLC) surfaces. The molecular dynamics (MD) simulations presented here utilize the reactive empirical bond order (REBO) potential for short range interaction coupled with the Lennard-Jones (LJ) potential for long range vdW interactions Within these simulations no discernable difference is predicted between the OLC fullerenes with a diamond core and those without. Further, the frictional behavior of these systems is highly dependent on the interactions that take place between the fullerenes and the DLC substrates. Without the formation of bonds with the substrates, the OLC fullerenes in the simulations are able to roll providing extremely low frictional forces, but as bonds begin to form, the OLC fullerenes begin to slide which causes a significant increase in the observed friction. The presentation will also report on the mechanical properties of molybdenum disulfide (MoS_2) nanotubes and their response when used as solid lubricants between two sliding Mo surfaces. Variations in number of nanotube layers, temperature, and compressive load are examined in order to characterize each system. The authors acknowledge the support of the National Science Foundation Grant No. CMMI-0742580.

8:40am **NS+TR-TuM3 High Pressure at Small Scales in Tribology and Piezoelectronics: Insights from First-Principle Molecular Dynamics**, ***M.H. Müser***, University of Western Ontario, Canada **INVITED**

At very small scales, many solids have the ability to sustain extremely large pressures before wearing off, i.e., up to a few GPa. Some materials, deposited on top of such hard solids, undergo chemical changes at these pressures, thereby changing their mechanical or electrical properties dramatically. In my talk, I will discuss how first-principle molecular dynamics can be used to analyze the mechanisms responsible for changes in the response functions of the deposited materials. Specific examples will be zinc phosphates (ZPs), in their function as anti-wear additives in commercial lubricants, and doped pnictogen solids (DPSs), when used in non-volatile electronic memory or in programmable switches. Molecular dynamics reveals when and why ZPs show "smart material" properties and anticipate the possibility for DPSs to be switched with nanoscale piezoelectronic actuators.

9:20am **NS+TR-TuM5 Optical Energy Density Inside Metallic Nano-Apertures**, ***P. Zhu***, *H. Craighead*, Cornell University

We use numerical methods and calculate the optical energy density inside a sub-micron sized hole surrounded by metallic cladding as light wave travels through it. Such information is important in the use of Zero-Mode-Waveguides (ZMWs) [1], where the diameter of the apertures is less than the wavelength of the light. In ZMWs, it has been postulated the evanescent wave inside the aperture defines the illumination volume, which is a function of the illumination wavelength and the aperture cut-off wavelength, which is in-turn a function of the aperture-diameter. Although the cut-off wavelength of a circular hole in an infinitely thin perfect conductor is a monotonically increasing function of the hole diameter [2], we see from our calculation result that, inside apertures surrounded by aluminum cladding, optical energy density increases until it reaches a peak as aperture diameter increases, and then levels off as aperture becomes more transmitting. This result suggests that, in order to achieve the best signal-to-noise ratio in fluorescent single-molecule experiments involving ZMWs, there is an optimal aperture diameter for each wavelength and application.

[1] Levene et al, "Zero-Mode Waveguides for Single-Molecule Analysis at High Concentrations, Science, Vol 299, 2003.

[2] Jackson, J. D., Classical Electrodynamics, 1998.

9:40am **NS+TR-TuM6 Field Amplification in Surface-Enhanced Raman Scattering**, *E.J. Adles*, ***S. Franzen***, *D.E. Aspnes*, North Carolina State University

Surface-enhanced Raman scattering (SERS) is experiencing renewed popularity as a result of the present interest in nanostructures and reported observations of SERS from single molecules. However, the detailed reasons for enhancements, which have been reported to be as much as 10^{14}, remain unclear. We address the issue from a fundamental perspective that has provided insight into the physics of second-harmonic generation and other nonlinear-optical processes, considering metallic spherical inclusions for simplicity. One obvious result, although it contradicts many statements in the literature, is that resonant-plasmonic enhancement of both incident and emitted waves by the same sphere is impossible, since the sphere cannot simultaneously exhibit plasmonic resonances at the frequencies w_o and w_R of the driving and Raman fields, respectively. The presence of an adjacent inclusion nominally resonant at the other frequency does not resolve the issue due to coupling by the longitudinal (Coulomb) interaction. However, under certain circumstances amplification can occur at a second frequency by means of a resonance activated by a renormalization of the effective mass of the bonding electrons of the molecule due to their longitudinal interactions with the sphere. Local configurations in deposited thin films where this could occur would likely be extremely rare, but cannot be ruled out completely.

Authors Index

Bold page numbers indicate the presenter