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Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.
Nanotribology of MEMS Anti-Friction Coatings

The colorful image appeared on the cover of the *JOM*. It is a close-up of a simulation in which an uncoated silicon dioxide probe tip (radius of curvature 10 nm) is brought into contact with a self-assembled monolayer (SAM)-coated surface. These new simulations will more closely mimic atomic-force and interfacial-force microscopy (IFM) experiments and will improve understanding of the effects of load-dependent contact area on the nanotribology of SAM. See: “Nanotribology of Anti-Friction Coatings in MEMS”, Michael Chandross, Christian D. Lorenz, Gary S. Grest (Dept. 1114), Mark J. Stevens, and Edmund B. Webb III, *JOM* 57, pp.55-61 (2005)
Time sequence of the molecular dynamics simulated evolution of a water film placed on top of self-assembled monolayers (not shown) with two 25Å holes. Water de-bonds physi-absorbed alkylsilane SAMs after 2 ns. Simulations predict that water quickly penetrates larger holes and removes ("debonds") the SAM.

POCs: Gary Grest and Mike Chandross
The SNL-developed Interfacial Force Microscope for Nanotribology Investigations
(Jack Houston & William Smith – 1114)

IFM Advantages

Quantitative

**Mechanically Stable**: measures entire force profile

**Zero Compliance**: no energy stored during measurement

Measure both normal and lateral (friction) forces

A 2D Interferometer Sensor → the Ultra-Sensitive Interfacial Force Microscope (J Houston & W Smith – 1114)

Current IFM Sensor

- RF bridge deflection detection and capacitive electrostatic force feedback balances torque due to both normal and lateral probe forces.
- Non-compliant sensor overcomes limitations of displacement sensors used, e.g., in AFM
- RF bridge scheme sets lower limit on sensor size and ultimate sensitivity to ~10 nN
- Strictly a research instrument

Next Generation Sensor

- Enables, for example
  - Molecular-level studies of adhesion, friction and nano-mechanical properties
  - Advanced “adaptive” imaging techniques

- New interferometer sensor design will achieve 50-fold increase in sensitivity and is virtually insensitive to sensor size permitting even greater sensitivity
- Totally independent normal and lateral force detection (first of its kind in scanning-probe field)
- Fully computer controlled operation
A sequential nucleation and growth process has been developed to construct complex nanostructured films step-by-step from aqueous solutions. This method can be applied to a wide range of materials, and can be combined with top-down techniques to create spatially resolved micropatterns. The cover figure shows images of oriented nanowires, nanoneedles, nanotubes, nanoplates and stacked columns, wagon-wheels, hierarchical films based on wagon-wheels, hierarchically ordered mesophase silicate, and micropatterned flower-like structures. Nanostructured films with controlled architectures are desirable for many applications in optics, electronics, biology, medicine, and energy/chemical conversions. See: “Sequential Nucleation and Growth of Complex Nanostructured Films”, T. L. Sounart, J. Liu, J. A. Voigt, J. W. P. Hsu (Dept 1114), E. D. Spoerke, Z. Tian, Y. B. Jiang, *Advanced Functional Materials* 16, pp. 335-344 (2006)
Nanorod alignment, density, dimensions depend on humidity, substrate roughness. Polymer infiltration into dense nanorod arrays results in incomplete filling/contact and interruption of conjugation (POC: Julia Hsu)
Selective ZnO Nanorod Growth on Multigrain (Polycrystalline) Ag Foil

ZnO nanorods selectively grow on <111> oriented Ag grains, with their <0001> axis perpendicular to the substrate. The nanorods preferentially grow at the edges of the upper terraces, with the same in-plane orientation (6-fold degenerate) indicating definite alignment between ZnO and Ag lattices despite the large lattice mismatch (> 10%). POC: Julia Hsu
ZnO Nanorod “Shoreline”

False colored scanning electron microscopy image on zinc oxide (ZnO) nanorods grown on multi-grain silver foil. Silver foil grains with different crystal orientations display distinctly different morphology. The ZnO density depends on the orientation of the silver grain. The image was generated from the work of Julia Hsu, Jerry Floro, and Bonnie McKenzie.
Novel Nanoparticle Synthesis

TEM Micrograph of (a) a silver-gold alloy nanoparticle radiolytically synthesized from solution using Co-60 gamma irradiation from the Sandia Gamma Irradiation (GIF) Facility, and (b) a GIF radiolysis synthesized gold nanoprism – POC: Tina Nenoff
Zeolite materials are useful for a number of industrial applications, such as catalytic cracking or hydroisomerization of hydrocarbon molecules as well as ion exchange in purification applications. Zeolites can also be useful for separations processes since their pore dimensions (0.74 nm in this case) are of the same size regime as the kinetic diameter of many small molecules of interest. POC – Tina Nenoff
Na$_{16}$Nb$_{12.8}$Ti$_{3.2}$O$_{44.8}$(OH)$_{3.2}$•8H$_2$O SOMS

SOMS - Sandia Octahedral Molecular Sieves, a patented novel material family for ionic selectivity and radioactive waste clean up. A view down the b-axis revealing 1D channels. The randomly distributed Ti/Nb atoms are shown in purple, while the Na atoms are shown in green. Channel water molecules excluded for ease of viewing.

POC: Tina Nenoff
Desalination using nanopores, CO$_2$ capture, biomimetic catalysis

Kevin Leung, Surface & Interface Sciences Department, SNL

Combined DFT, AIMD, and force field studies of electrolyte permeation in nanopores

DFT shows Na+/Cl- exhibits large, O(2-3) eV binding energies inside carbon nanotube array that are completely neglected in force fields calculations. Results are pertinent to desalination & supercapacitor research.

ion in (6,6) CNT:
Na$^+$: -2.8 eV
Cl$^-$: -1.7 eV
Leung & Marsman, JCP (in press)

intrinsic attraction for Na$^+$ due to surface dipoles in hydroxylated silica nanopores

AIMD (ab initio molecular dynamics) simulations of CO$_2$+OH$^-$ -> HCO$_3^-$ in liquid water

DFT+U simulation of transition metal porphyrins on electrodes and in water
Leung et al., JACS 128:3659 (2006)

CO$_2$ $\rightarrow$ HCO$_3^-$

vacuum: no barrier
in water: large barrier (~0.5 eV)
nanopore: small barrier?
Other Interesting 1114 Images

LEEM and FIM images are accessible through the “Visit our Labs” Surface Imaging Laboratory link maintained by Gary Kellogg