# Monday Morning, October 2, 2000

### Surface Science Room 210 - Session SS3-MoM

#### Surface Science Opportunities and New Applications Moderator: B.E. Koel, University of Southern California

#### 8:20am SS3-MoM1 Out of the Vacuum - Into the Liquid, M. Grunze<sup>1</sup>, University of Heidelberg, Germany INVITED

Motivated by the need to establish a knowledge base for microelectronics and heterogeneous catalysis, Surface Science matured as an interdisciplinary research area at the intersection of solid state physics and chemistry. The available experimental probes and theoretical concepts allow today to study surfaces and interfaces in unpreceded detail under vacuum or controlled gas atmospheres, but are less suitable to investigate surfaces in liquid environments. This challenge has been addressed by many members of the Surface Science community by directing their attention to the solid/liquid interface and to biological and biomaterial interfaces. In my presentation, I will discuss some recent examples of a successful transfer of traditional Surface Science concepts to the solid/liquid interface, and of new research areas at the intersection of physics, chemistry, and biology with impact on life science and medical procedures. The need for better experimental and theoretical tools to describe solid/liquid and biological interfaces will be discussed.

## 9:00am SS3-MoM3 Probing Interaction Potentials Between Surfaces in Water, J.G. Kushmerick, B.C. Bunker, Sandia National Laboratories

Adsorbed water layers are known to strongly mediate interactions between non-ionic surfaces. These so-called hydration forces control processes as diverse as protein folding and the undesired adhesion between hydrophobic surfaces in micromachine components. Until recently, most investigations of hydrophobic interactions have been performed using the surface forces apparatus and atomic force microscopy. The former technique is limited to investigations on extended mica surfaces, while the latter technique is limited to probing only the outer regions of forcedistance profiles due to "snap-to-contact" problems. The difficulties associated with making localized measurements of the hydration force have now been overcome using an interfacial force microscope (IFM), which allows force-distance profiles to be obtained at sub-nanometer resolution until the tip and surface are in intimate contact. Experiments have been performed in humid atmospheres and under water. Examples of IFM investigations of hydration interactions are provided for a range of hydrophobic-hydrophilic tip-substrate combinations prepared using functionalized self-assembled monolayers (SAMS). Investigations have also been performed on SAM coatings used to control stiction in micromachines and on polymeric coatings such as poly n-isopropyl acrylamide that can be switched between hydrophilic and hydrophobic states. Results on the polymers indicate that adhesive interactions can be modified by at least an order of magnitude by conformation changes associated with the adsorption and desorption of water. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-ACO4-94Al85000.

9:20am SS3-MoM4 Determination of Molecular Structure at Polymer Interfaces by Sum-Frequency Generation, K.A. Briggman, L.J. Richter, J.C. Stephenson, W.E. Wallace, National Institute of Standards and Technology The structure of polymer surfaces and interfaces can determine critical interfacial properties such as adhesion, molecular recognition and bonding in applications as diverse as optoelectronics and biomaterials. Linear vibrational spectroscopies (FTIR, ATIR, and Raman) are some of the most widely accepted and utilized diagnostics of bulk polymer systems but typically do not have sufficient specificity to probe interfaces. Vibrationally resolved sum-frequency generation (SFG), a non-linear optical technique, is uniquely interface specific as it is dipole forbidden in media with inversion symmetry. Additionally it has the ability to determine not only the alignment of molecular groups, but also their absolute orientation. We report vibrational SFG studies of the methylene and phenyl groups at the interfaces of thin, annealed polystyrene films. When applied to thin film systems, the contributions from multiple interfaces must be properly assigned. Multilayer systems are designed to separate the contribution of signals from the free surface and buried interface and to allow independent determinations of molecular orientation at each interface. The phenyl rings have polar order at the free surface and oriented away

from the film. The degree of order is significantly weaker at the buried interface. We will present a detailed analysis of the orientational distibution of the rings.

#### 9:40am SS3-MoM5 Nanocrystal Surface Melting -- A UHV X-ray Diffraction Study on n-Pb, K.F. Peters, Northwestern University, FRANCE; Y.-W. Chung, Northwestern University

Discovery of a nanocrystal surface phase transition is reported. The surface influence on the melting of nanoparticles has been debated since seminal concepts of surface melting and of a size-dependent melting temperature were given by Faraday and Thompson. On macroscopic Pb crystals, surface melting occurs on certain surface orientations yet not others. On highly curved surfaces of nanoparticles, 3 competing melting theories are based on liquid skin formation before melting, during melting, or never. Each theory also predicts a depression of the melting temperature Tm(D) as a function of crystallite diameter D. To measure the surface melting and melting temperature of Pb nanocrystals, we applied x-ray powder diffraction in situ in UHV.@footnote 1,2@ An array of Pb nanoparticle islands of 5-50 nm diameter was fabricated on a silica substrate by evaporation and annealing. The Pb 111/200 powder diffraction peaks were collected versus temperature. Narrowing of the diffraction peak revealed the melting of smaller particles at lower temperatures. Fourier analysis of the peak shape shows the evolution of the size distribution of 'crystallites' with increasing temperature. The size-dependent melting temperature was found to be Tm(D)=1-0.62/D, in close agreement with the Liquid Skin Melting Model. To measure directly the liquid skin growth on the crystallites, we rely on the undercooling of liquid particles without solidification. First the sample is heated to within 3K of the melting temperature of the largest particles in the sample (to melt the smaller particles). Upon slight cooling, we observed a reversible increase in the diffraction intensity and a narrowing of the diffraction peak shape. These changes in the crystallite volume and size are due to small changes in the liquid skin thickness (up to 0.5nm over a 20K temperature excursion for crystallites of 20 and 50nm diameter). @FootnoteText@ @footnote 1@Appl.Phys.Lett., 71 (16), 1997, 2391-2393. @footnote 2@Phys.Rev.B, 57, 21, 1998, 13430-13438.

10:00am SS3-MoM6 How to Study a High-Vapor Pressure Liquid under Ultrahigh Vacuum: Organic Chemistry at and near the Surface of Sulfuric Acid, J.T. Roberts, R. Michelsen, University of Minnesota

10:20am SS3-MOM7 Atomic Structure of Sulfide Natural Crystal Surfaces by Combined Photoelectron Imaging and Diffraction Methods, *E.M. Kneedler*, Surface/Interface Inc.; *X. Chen, S. Banerjee*, University of Wisconsin, Milwaukee; *E. Rotenberg*, Lawrence Berkeley National Laboratory; *B.P. Tonner*, University of Central Florida

Natural surfaces of minerals play an important role in the chemistry of the environment. Advances in the sophistication of surface structural techniques makes it possible to tackle an atomic structure determination of such surfaces with some degree of confidence. We have studied a number of sulfur bearing mineral surfaces using high resolution x-ray photoelectron diffraction, and x-ray photoemission microscopy. A model system with a large unit cell, Cu(100)-S, is a starting point for evaluating the accuracy of photoelectron diffraction methods on complex surfaces. Results are also presented for natural crystals of galena (PbS), pyrite (iron sulfide), and some preliminary results of chalcopyrite.

#### 10:40am SS3-MoM8 DNA Sequence Information Obtained by TOF-SIMS Analysis, K.F. Willey, W.L.B. White, T.J. Whitaker, Atom Sciences, Inc.

A high-speed DNA screening technology is currently being developed at Atom Sciences. Our approach utilizes gene chip technology, which has paved the way for widespread DNA diagnostics. Current technology utilizes DNA hybridization to complementary oligonucleotides of known sequence immobilized to a surface. Unknown DNA is typically labeled with radioisotopes, stable isotopes, or fluorescent tags in order to detect hybridization sites. This labeling is costly and can be an impediment to the widespread use of gene chips. We are developing a new technology that requires no labeling. In this technique, target DNA hybridizes to an array of known sequences of peptide nucleic acid (PNA) probes attached to a silicon substrate. The naturally occurring phosphate groups in DNA provide an ideal intrinsic label because PNA contains no phosphorous. PNA is an analog of DNA in which the sugar/phosphate backbone of DNA is replaced by a peptide backbone. Target DNA and PNA probes undergo hydrogen bonding of AT and GC base pairs (Watson-Crick rules). Diagnostic information is obtained by identifying DNA hybridization sites within the

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array using negative SIMS detection of phosphate fragments. The sensitivity of SIMS detection and use of PNA probes gives our technology distinct advantages over existing diagnostic techniques (e.g. fluorescence). The major drawback, however, is the cost of commercial SIMS instrumentation. Therefore, at Atom Sciences, we have developed an inexpensive TOF-SIMS instrument. We will discuss the advantages of using a DNA/PNA hybridization scheme and its application to identifying single base mismatches. We will also discuss the current SIMS instrument used for technology development and how it could be simplified for a clinical diagnostic setting.

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