

Final Report

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Title: International Conference on Surface X-ray and Neutron Scattering (SXNS-11)

SXNS-11 Conference chair: Michael J. Bedzyk, NU

SXNS-11 Conference co-chairs: Paul Fenter, Argonne National Laboratory (ANL), Jin Wang, ANL, John Ankner, Oak Ridge National Laboratory (ORNL)

### **Publications that resulted from SXNS-11:**

The accomplishments of the SXNS-11 conference as reported by P. Fenter, G. B. Stephenson (ANL), H. You (ANL), M. Bedzyk, J. Ankner, J. Daillant (CEA France), J. Kortright (LBNL), P. Miceli (U Missouri), and S. Satija (NIST) were published in *Synchrotron Radiation News (SRN)*, Vol. 23, No. 6, (2010). The text that follows this paragraph is primarily taken from this SRN Meeting Report. A total of 20 refereed papers from the SXNS-11 conference are now in press for publication in a special issue of the *Journal of Applied Physics* with editors; M. L. Schlossman (UI-Chicago), M. Bedzyk, J. Lang (ANL) and P. F. Lyman (UW-Milwaukee).

### **Detailed Summary of Accomplishments:**

The 11<sup>th</sup> International Surface X-ray and Neutron Scattering (SXNS) Conference was held on July 13-17, 2010, on the Northwestern University (NU) campus, in Evanston Illinois (<http://www.sxns11.northwestern.edu/>) and hosted by the NU Materials Research Science and Engineering Center. This biennial conference brought together a community of 164 attendees from 16 countries. There were 41 graduate student and more than 14 postdoctoral fellow participants. The field now makes use of a broad range of new experimental capabilities that have been made possible through the development of increasingly brilliant X-ray and neutron sources around the world, including third generation synchrotron sources, neutron reactor and spallation sources, as well as the recent development of X-ray lasers.

SXNS-11 was opened by conference Chair, Michael Bedzyk (Northwestern Univ.), and the attendees were greeted by representatives of the conference sponsors (Dean Julio Ottino and Vice President of Research Jay Walsh, from Northwestern, and Director Eric Isaacs of Argonne National Laboratory), who emphasized the importance of the conference subject matter for the two sponsoring institutions, as well as towards solving the important energy-related problems that we face. The meeting was organized loosely into thematic sessions.

The opening session was chaired by Helmut Dosch (DESY, Germany) who challenged the attendees to think broadly, beyond the issues of near-equilibrium properties of ordered systems, towards grand challenges concerning disordered materials and energy transfer in systems in non-equilibrium conditions. The session began with a plenary presentation by Sunil Sinha (UC-San Diego) who presented his recent work on the incorporation and exploitation of partial coherence. The session, otherwise organized around **Magnetism**, emphasized the use of polarized neutron reflectivity/scattering, although also emphasizing the complementarity of X-ray reflectivity as well as conventional magnetization measurements in complex structure determination. In

particular Suzanne te Velthuis (ANL) described her work to understand magnetism in complex oxide hetero-structures. The application of soft x-ray magnetic reflectivity to study ultrathin films was also described.

The session on **Soft Interfaces** covered a wide variety of topics from the adsorption of proteins, polymer thin films and self-assembly of proteins and nanoparticles at interfaces. The presentation showcased the power of reflectivity, grazing-incidence diffraction (GID) and x-ray photon correlation spectroscopy (XPCS) to study soft matter interfaces. Giovanna Fragneto (Institute Laue-Langevin, France) emphasized the role of deuteration in studying the structure of proteins at interfaces by neutron reflectivity. The question of how cholesterol distributes in lipid membrane layers was discussed by Andrey Ivankin (Illinois Institute of Technology). Particularly relevant was the combination of X-ray reflectivity and GIXD studies, which gave detailed information for the distribution of cholesterol for both in-plane and out-of-plane directions in lipid membranes.

The ordering of nanoparticles was another common theme that illustrated the power of surface scattering for in-depth structural studies of nanoparticle assemblies near interfaces. Masa Fukuto (Brookhaven) combined XR and GIXS to study the binding of protein streptavidin to biotin bearing lipid monolayers and its 2D crystallization. Kinetics and self-assembly of gold nanoparticles were the subject of an elegant GISAX study presented by Zhang Jiang (ANL). The relatively young age of the speakers in this session bodes well for the growth of the study of “soft interfaces” in the future.

A session on **Coherence and Ultrafast** science began the second day. The advent of fully coherent and femtosecond-pulse x-ray sources such as LCLS and XFEL is an exciting recent development for this area. These x-ray sources push the peak brilliance of available sources by orders of magnitudes compared to the current 3<sup>rd</sup> generation x-ray sources, enabling coherent x-ray scattering from interfaces and nanoscale objects.

Topics included surface reconstruction, nanoparticles and nanorods, membranes, and thin films. Highlights of the session were the powerful applications of coherent x-ray scattering techniques enabling those sciences. Michael Pierce (ANL) used monolayer-sensitive x-ray photon correlation spectroscopy using coherent x-ray scattering to reveal the dynamics of reconstructed surfaces of gold or platinum that appear to be static without coherent x-ray beams. Ana Diaz (Paul Scherrer Institute, Switzerland), reviewed the use of lens-less imaging techniques and demonstrated applications of an iterative oversampling technique to image nanostructures grown on Si substrates, including the shapes and the lattice strains of the buried interfaces.

The Thursday afternoon session on **Liquid-Solid Interfaces** focused on the challenging, and sometimes controversial, questions: What is the nature of the interface between and hydrophobic solid and water? What is the structure of an aqueous electrolyte within a few Angstroms of a solid surface? How do membranes interact with a surface? Very often, small differences in interaction potentials, unimportant in the bulk, dramatically affect interfacial structures, in particular for aqueous systems where complex solvation and hydration forces come into play.

Andrew Nelson (Australian Nuclear Science and Technology Organization) demonstrated that traces of water alter the surface organization of ionic liquids in a complex way by combining neutron and x-ray reflectivity, and emphasized how such insights are critical to surface electrochemistry. Understanding the interfacial behavior of aqueous ionic solutions requires

elemental sensitivity, Sang Soo Lee (ANL) showed how resonant anomalous reflectivity reveals very detailed descriptions of the surface species. Olaf Magnussen (Kiel University, Germany) reported time dependent studies of electro-deposition using grazing incidence diffraction enabling the full description of the nucleation and growth of islands in seconds.

The session on **Growth and Processing** exemplified the unique capabilities of x-ray scattering methods for in situ surface science studies. X-rays penetrate harsh environments, do not obscure film deposition/processing, and provide unique information through in-situ observations. Knowing the subsurface structure, which eludes most surface-sensitive techniques, is often central to understanding how film materials grow and assemble.

Paul Fuoss (ANL) presented results on solid-oxide fuel cells (SOFC) and emphasized that high performance is required for their successful application, which is limited by the oxygen-supported current. He showed that in situ crystal truncation rod measurements during film growth could illuminate the relationship between the oxygen pressure during growth, Sr segregation, and the performance of SOFCs. Jon Tischler (ORNL) described the time-dependent coverage obtained from single shots of pulsed laser deposition by measuring x-ray reflection in real time. Scattering experiments are essential for establishing the fundamental physical behavior of solid state kinetics because they can determine correlation functions by accurately measuring statistical distributions. This was highlighted by Karl Ludwig (Boston University) who studied the nanoscale surface morphology of Si during low-energy ion bombardment through real-time surface diffuse scattering measurements that could be critically compared to theories of surface kinetics.

The Friday afternoon session on **Interfacial and Film Structures** highlighted studies of functional properties in hard- and soft-condensed matter systems with established reflectivity and diffraction approaches, coupled with advances in sources, detectors, and analysis, to elucidate structure/property relationships in realistic materials. Approaches that were revolutionary when first demonstrated are now used routinely to address questions that previously would have been considered too challenging.

Fast 2D detectors have significantly increased the efficiency of reciprocal space mapping. This was demonstrated in studies of surface reconstructions, epitaxial nanostructures, morphology of phase separation in block co-polymer films, and molecular semiconducting films. The use of anomalous or resonant scattering was highlighted in several studies. Anomalous phasing of crystal truncation rod data was shown by Roy Clarke (Univ. of Michigan) to reveal chemical segregation at the interface between epitaxial nanostructures and substrate. Soft x-ray resonant reflectivity was highlighted in studies of polymer film structure, where tuning to the carbon *K* edge yields contrast between different types of bonds. Markus Mezger (Lawrence Berkeley National Laboratory) highlighted a new twist on this approach by using the molecular resonant linear dichroism in soft X-ray reflectivity studies to probe depth-dependant orientational order of polymer chain segments that influence charge and mass transport in polymer films.

The Saturday morning session on **Interfacial Nano-Science** highlighted the power of surface x-ray scattering for in situ studies during heating, straining, and growth of nanostructures, using microdiffraction and imaging with time resolutions spanning from seconds to picoseconds. A major focus was semiconductor nanostructures and nanowires. A plenary presentation by Robert Feidenhans'l (Univ. of Copenhagen, Denmark) reported time-resolved x-ray diffraction and optical reflectivity observations of three different acoustic oscillation modes in nanowires

excited by laser heating, on time scales from 10 ps to 100 ns. Several talks reported crystalline phase and strain measurements on both collections and individual wires, elucidating the growth processes. A second prominent theme was the atomic structure of liquid-solid interfaces present during nanowire growth or probed using nanostructures. Exciting results reported included the effects of reconstruction of the solid surface on supercooling, the effects of confinement on the structure of the liquid, and effects of stress and temperature on solid-liquid interfaces.

The final scientific session of the conference was on **Phase-Sensitive Approaches**. The recovery of phase information is a powerful opportunity in the application of scattering techniques to probing complex structures because, once recovered, phase information transforms scattering into imaging/microscopy tool. Over the past few years, the application of such phase sensitive approaches has exploded, from its initial use in X-ray standing waves (which is explicitly phase sensitive), and now includes the use of phase-recovery algorithms from data that are implicitly phase sensitive (e.g., CoBRA, Feinup algorithms) as well as those that are explicitly phase sensitive (resonant reflectivity). Jorg Zegenhagen (European Synchrotron Radiation Facility) reviewed the use of X-ray standing waves, and described recent novel applications of this technique including the ability to probe the spatial distribution of the conduction band in complex oxides. This session and the SXNS-11 meeting was brought to a close with the observation that the breadth of SXNS subject matter (soft vs. hard matter, chemistry vs. materials sciences and biology, etc.) was a strength for this community through the common “language” of scattering, allowing technical developments in one area to be quickly deployed elsewhere. This would allow this community to meet important scientific and technological challenges in the future.

There was also a strong scientific program represented in the posters, with 102 posters separated into two sessions. Three poster presentations that were recognized with Student Poster Awards: Jonathan Emery (Northwestern University) who studied epitaxial strained oxide layers on silicon surfaces; Rana Ashkar (Indiana University) who described spin-echo resolved grazing incidence scattering from periodic structures, and Yeling Dai (UC- San Diego) who reported on grazing incidence X-ray off-specular scattering studies of surfactant films.

The 12<sup>th</sup> SXNS Conference will be held in 2012 in Kolkata, India. The meeting will be hosted by the Saha Institute of Nuclear Physics. Milan Sanyal is the conference chair.