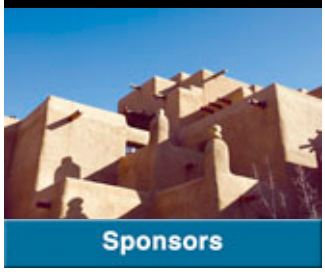
Materials Research Society
The Materials Gateway

ACNS - Day 3



DAY 3
Wednesday, May 14, 2008

CONTENTS

The 2008 American Conference on Neutron Science concluded on Wednesday. The final day of the conference was a busy one with a special prize lecture session with two talks in the morning and the recognition of Fellows of the society, a lunchtime lecture on the legacy of the Intense Pulse Neutron Source (IPNS), an afternoon special session on access to neutron facilities and education, as well as technical sessions including a poster session.

On Thursday, a tour of the Manuel Lujan Jr. Neutron Scattering Center at Los Alamos National Laboratory was conducted for interested conference attendees.

We hope you have enjoyed receiving and reading the Meeting Scene e-mails from Santa Fe. Please let us know if you have any comments or suggestions. Look for future Meeting Scene emails from the European MRS meeting in Strasbourg, France, from May 26-30.

Historic Santa Fe, New Mexico

2008 SUSTAINED RESEARCH PRIZE

Prof. Frank Bates (University of Minnesota) is the recipient of the 2008 Sustained Research Prize of the Neutron Scattering Society of America "for his pioneering SANS experiments that probe the structure and thermodynamics of polymeric fluids and block copolymers."


Frank Bates receiving the NSSA Sustained Research Prize and presenting his lecture.

In his talk titled "Small Angle Neutron Scattering: Enabling Scientific and Technological Advances in Polymer Science and Engineering" on Wednesday morning, Bates overviewed his involvement in polymers and neutron scattering over the past 17 years, and suggested that much of what we know about block copolymers comes from neutron scattering studies. He started chronologically with initial studies of copolymer melts under different processing conditions of deformation and flow. He described the development of an *in situ* shear cell for neutron studies by one of his students, Kurt Koppi, which was used to study shear-induced isotropic-to-lamellar transition in block copolymers, with lamellae orientation depending on processing conditions.

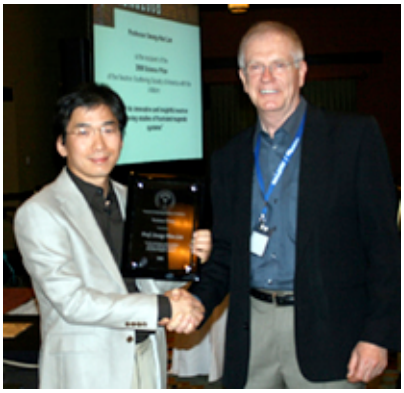
Bates then described his association with the Dow Chemical company in developing new copolymers. The prevalent view in the last decade was that we have run out of new commodity polymers. Bates described the development of PCHE (poly(cyclohexythylene)) from PS. This polymer is extremely brittle. The solution was the creation of a block copolymer of PCHE (molecules not entangled) and PE (molecules entangled). This material is ideal as an optical grade polymer with perfect refractive index matching between the two and is cheaper than currently used polycarbonate for optical applications. It was discovered that the pentablock copolymer (CECEC) is much tougher than the triblock version (CEC). *In-situ* SANS was crucial in understanding the structure and behavior of these polymers. Applications include injection molded lenses and optical compensator films in LCD screens. Processing is very easy, thus avoiding expensive films stretching methods used previously. He made a tantalizing mention of an important announcement in this area in the next two months.

Bates described more recent work on heptablock and undecablock copolymers and related SANS studies attempting to understand the structures and behaviors. He concluded his talk by

acknowledging a number of colleagues and collaborators he has worked with over the years. Bates did this by showing the various papers published and highlighting the names of his collaborators who were co-authors.

2008 SCIENCE PRIZE

Prof. Seung-Hun Lee (University of Virginia) is the recipient of the 2008 Science Prize of the Neutron Scattering Society of America "for his innovative and insightful neutron scattering studies of frustrated magnetic systems".



Seung-Hun Lee receiving the NSSA Science Prize and presenting his talk.

In his talk titled "Fun Times at NCNR (NIST Center for Neutron Research)", Lee discussed the fun times at NIST in terms of neutron studies on frustrated magnetic materials which he has been studying there. He started with a short introduction to magnetic spins and their interactions leading to cooperative phenomena. He explained ferromagnetic and antiferromagnetic states of magnetic materials, and systems with quantum fluctuations at absolute zero temperature, including the phase diagram. Then the question was posed – what is the most useful tool to study such kind of materials? A low energy probe, very flexible Q-resolution and also extreme sample environments are necessary. He showed the phase diagram (Q-space diagram) with different spectrometers on it, particularly focusing on SPINS and DCS. The author introduced SPINS at NCNR with its focusing analyzer system as a powerful tool in studying systems with short-range correlations.

Lee then gave an introduction to entanglement phenomena and showed how the low dimensionality suppresses magnetic long range order. He overviewed experiments on quantum spin-chains and geometrical frustrations, which lead to large degeneracy in ground spins even for classical spins. As an example, he showed typical frustrated lattices in complex compounds. Lee said that one question he gets asked in talks relates to practical uses of frustration. He answered stating that he did not know and did not care! In fact, a possible application is magnetic control of ferroelectric materials. Another example is the newly discovered family of Fe-As superconductors, wherein frustrated interactions can be observed. He also mentioned deferent low T behavior of pyrochlores and spinels ($Tb_2Ti_2O_7$, $Y_2Mn_2O_7$, etc.). He presented experimental results, in particular on the S=3/2 pyrochlore AFM, on 3D Spin-Peierls transition in ACr_2O_4 which was not yet completely understood, on emergent spin excitations in ACr_2O_4, where spin liquid

phase was observed. The most recent data was on crystal distortion in $ZnCr_2O_4$. In this compound, spin lattice coupling was found and the displacement of Cr atoms was observed which leads to crystal lattice phase transition. His also described Cr(S=3/2)-based spinels under an external magnetic field. A compound under study was $HgCr_2O_4$ wherein field-induced lattice distortion was investigated. The general conclusions of Lee's excellent talk concerned the hidden order found in spin liquid phases of quantum frustrated magnets, and novel phase transitions with and without applications of an external magnetic field.

RECOGNITION OF NSSA FELLOWS

Following the two prize lectures, NSSA President Roger Pynn recognized the following newly elected NSSA Fellows from 2007 and 2008 in the new NSSA Fellows program.

2007
Prof. Frank Bates (University of Minnesota)
Dr. Gian P. Felcher (Argonne National Laboratory)
Dr. Herbert A. Mook, Jr. (Oak Ridge National Laboratory)
Dr. John J. Rush (NIST Center for Neutron Research)
Prof. Thomas P. Russell (University of Massachusetts)
Dr. Constantine Stassis (Ames Laboratory)
Dr. J. Michael Rowe (NIST Center for Neutron Research)
Dr. John. M. Carpenter (Argonne National Laboratory)
Dr. John M. Tranquada (Brookhaven National Laboratory)

2008
Prof. Robert J. Birgeneau (University of California at Berkeley)
Dr. Larry Passell (Brookhaven National Laboratory)
Prof. Sunil Sinha (University of California at San Diego)
Prof. Julia R. Weertman (Northwestern University)
Prof. Sow-Hsin Chen (Massachusetts Institute of Technology)

Graduate student poster awards to Matthew E. Helgeson (Univ. Delaware) (l) and Katharine Page (Univ. California, Santa Barbara) (r)

LEGACY OF THE IPNS (INTENSE PULSE NEUTRON SOURCE)

The Intense Pulse Neutron Source (IPNS) at Argonne National Lab. was recently closed after many years of serving the neutron science community. Jerry Lander, one of the former Directors of the IPNS facility, gave an overview of the history of the IPNS and the lessons the neutron science community can learn from this going forward. He started with the CP-1, the first reactor to go critical in Chicago under the direction of the great Enrico Fermi. He mentioned the various machines and facilities that followed as neutron scattering and neutron science continued to make strides, and how these were related to the eventual setup of the IPNS. He also discussed the Brinkman report in the early 1980s that almost shut down IPNS just as it was beginning its amazing run. How this was overcome provides some lessons for the future. Some of these details as well as a history of the IPNS are available on the IPNS/Argonne National Lab. website.

Lander concluded by mentioning some of the lessons learned from the situation at IPNS and also what the neutron scattering community should keep in mind. In particular, he suggested that synchrotron radiation and neutrons are complementary for science. The neutron community should point out the difference between the two and show the limitations of synchrotron radiation sources, while at the same time strongly emphasizing the complementarity between the two. He ended by thanking the various people who were responsible for the success of the IPNS. Various

members in the audience pointed out Lander's own significant contributions to IPNS and the community.


TECHNICAL TALKS

IMAGINE - Neutron Laue Diffractometer at the High Flux Isotope Reactor (A3.1)
Flora Meilleur (North Carolina State Univ./Oak Ridge National Lab.) presented an overview of Laue diffraction at the ORNL SNS facility. IMAGINE is not a Laue diffractometer, rather it is a Quasi-Laue diffractometer. The author begun with an extensive explanation of the novelty of the instrument itself, and especially pointed out that the angular range of the new diffractometer will be 2*pi. A special goal is overcoming the problem of catching each neutron in the white spectrum coming onto the sample. The use of an image plate and specific geometrical solution can help in solving this issue. What kind of science can one do with this new instrument? Meilleur indicated several including supra-molecular crystallography, materials under extreme environments and protein structure studies. She made a comparison with the LADI-III instrument at ILL wherein data on Rubredoxin was collected during 14 hours whereas the instrument at the ORNL should be able to collect same data for only 1 hour. The next part of the talk was dedicated to a review of the facility where IMAGINE is going to be situated. She mentioned briefly some instrumental details of IMAGINE, i.e. tools for wavelength selection, realization of the dual mode: Laue and Tunable Quasi-Laue. Other interesting details mentioned were automated data collection which is realized through a user friendly interface, data processing and wavelength normalization procedure.

State of the SNS Backscattering Spectrometer, BASIS (A3.2)
Eugene Mamontov (SNS/ORNL) presented the current state of the backscattering spectrometer at the SNS named BASIS (backscattering Silicon Spectrometer). He started by presenting the main parameters of the installation, i.e. incident flight path, which is the longest path in the world, and the chopper system. The evacuated final flight path was introduced, specifying the analyzer and the detector systems along with the beam at the sample position specification. The FWHM was 3.5 muEV, at the same time the signal to ratio was better than 1000:1. According to the speaker, compared to other spectrometers such as the IN5 at ILL, BASIS appears to gain much in resolution and flexibility but loses, for example, at long wavelengths of neutrons where the intensity of these neutrons is very low. He made a comparison of different Si reflections (333, 311, 111) available at BASIS. Also mentioned were the data collection rates which were tested just recently. The author showed exciting numbers on counting even at 1/3rd the power of the source. At the end he reviewed the sample environments available (cryo-furnace, vacuum furnace, 5T magnet) and the user and experiments statistics.


The exhibit hallway at the Eldorado hotel

Nanoparticle-directed Self-assembly of Block-copolymers: Measurement of 3D Order (B2.3)
Kevin Yager of NIST discussed the self assembly of block-copolymers with incorporated nanoparticles into the polymer matrix. This field of study is particularly important because it allows for the construction of nanostructured materials with predictable properties on the nanometer scale. The author started from an explanation of the famous phase diagram of block-copolymers as a function of the length of the polymer chains. The crucial thing is to be able to measure the ordering of the polymer which can be partially done by many methods. In this study, the author used Si nanoparticles. The lamellar orientation of the PS-PMMA system was found to be oscillating as a function of thickness of the film. To quantify information about the orientation, Yager proposed using the 2D SANS technique wherein the sample was turned upon the different measurements. Thus, the 3D Q-space scattering picture was obtained. The next part of the talk was dedicated to the scattering model explanation in order to quantify the data obtained. An example of the 2D Qx-Qz map fit to the experimental SANS data was presented revealing good coincidence of the experimental results with calculations. Neutron reflectometry results were briefly discussed. The next steps in this study as pointed out by the speaker are measurements of GISANS spectra and reflectivity with off-specular scattering which will give complete 3D information on the polymer interfaces and internal structure of the film.

Internet access for attendees

Diphtheria Toxin Interaction with Model Lipid Membranes: Neutron Reflectometry Study (D2.2)
This study by Jaroslaw Majewski and coworkers of Los Alamos National Lab used a model lipid membrane, in the form of a monolayer at the liquid-air interface, to investigate membrane binding and penetration properties of the diphtheria toxin, a very potent bacterial toxin. The studies found differences in the structure of the membrane and bound toxin as a function of toxin concentration and pH. The results showed that high concentration of toxin is important to make the toxin dimerize once it is bound to the membrane. Changing the pH from 7 to 5 revealed a change in conformation of the protein from the closed to the open state. These studies will be very helpful in determining the membrane penetration mechanism of the diphtheria toxin which remains unknown.

Neutron Reflectometry Study of the Conformation of Membrane-Bound HIV Nef Protein (D2.3)
Michael Kent (Sandia National Labs.) described a study using a model lipid membrane, in the form of a monolayer at the liquid-air interface, to investigate the membrane binding and penetration properties of an important protein in HIV infection, Nef. Although much more work needs to be done, these studies show that neutron reflectivity has the ability to determine the conformation of membrane bound HIV proteins.

Botulinum Neurotoxin Assault on Lipid Membranes (D2.5)
Chad Miller (Los Alamos National Lab) described a study using a model lipid membrane, in the form of a monolayer at the liquid-air interface, to investigate the membrane binding and penetration properties of botulinum neurotoxin type A, possibly the most toxic substance known. The ability to study this toxin was enabled by the synthesis and purification of a double mutant which is non-toxic but has no significant structural differences from the wild type toxin. The studies found differences in the structure of the membrane and bound toxin as a function of toxin concentration and pH. The results showed that high concentration of toxin is important to make the toxin dimerize once it is bound to the membrane. It is thought that dimerization is necessary for translocation across the cellular membrane. The larges perturbations to the membrane were observed at low pH 5, consistent with the endocytosis pathway.

The New SANS Instrument at LENS (A3.3)
H. Kaiser of Indiana University described a new SANS instrument, one of four instruments to go into operation at the Low Energy Neutron Source (LENS) at Indiana University. This will be used to carry out new scientific studies and to develop innovative neutron optical devices for SANS instrumentation. However, this instrument also serves another purpose, as indicated by the session chair Laurence Passell. It is very difficult to get beam time at larger facilities such as the SNS in ORNL. Using the new SANS instrument at LENS is an excellent way for students and novices to get used to the technique and instrumentation without major time constraints so that when they go on to use the larger instruments and facilities, such users already have had some experience.

Poster Presentations

PDF Analysis of Ammonia Borane Nanocomposite in a Mesopouros Scaffold (PE3.7)
Hydrogen storage properties of NH_3BH_3 (AB) are greatly enhanced by nanocompositing AB in mesoporous silica, as described in the poster by H. Kim et al. (LANSCE, Los Alamos National Lab.). Despite such a substantial improvement, very little is known about this system. This is due to the failure of applying conventional structural analysis techniques such as crystallography or TEM. The atomic pair distribution function analysis (PDF) was employed on both neutron and x-ray data to investigate the structure of AB inside the pores. Preliminary results show the formation of nano-sized AB inside the pores, with structural correlations of more than 20 Å. Currently, several structural models are being tested, in order to gain an insight into the mechanism behind the improved hydrogen storage properties of this system.

Elastic Strain in Bulk Metallic Glasses: How to understand In-situ Diffraction Data (PG3.4)
Bulk metallic glasses were discovered more than 20 years ago. Despite extensive research efforts since then, mostly experimental, the structure of metallic glasses is still not well understood, according to this poster by A. Stoica et al. (NSSD, Oak Ridge National Lab.). Bulk metallic glasses exhibit impressive mechanical properties and processing capabilities that make them attractive for a variety of structural and functional applications Recent *in-situ* neutron and synchrotron diffraction experiments are described, and the insights thus gained on the local and medium-range ordering in these glassy alloys. This study offers a new perspective on the disordered structure in metallic glasses.

Hungary for European Spallation Source (ESS) (ESS-1)
The European Spallation Source (ESS) nuclear facility is expected to be the biggest neutron-scattering research center in the world. The giant project has been under development since 1991, and it counts 20 laboratories, universities and research organizations as partners. ESS will provide much more intensity than the present neutron sources, brighter neutrons beams, more than 40 neutron scattering instruments, and will enable scientists of all disciplines investigate materials in situ, in vivo, in real time and for real life applications. The ESS center will employ a total of 4,000 researchers over a 40-year period. The facility would become the world's most powerful neutron source available to researchers in fields such as materials science, nanotechnology, biosciences and engineering, offering a gain in effective performance between 10 and 100 over the existing neutron facilities. Three countries are competing to host the ESS: Sweden, Spain and Hungary. The presentation by L. Rosta et al. (ESS Hungary Company) depicted the advantages of having Hungary as the host country for ESS, and how the country meets the legal, administrative, economic, financial, safety and security requirements of the project.

Downtown Santa Fe

VISIT TO THE MANUEL LUJAN JR. NEUTRON SCATTERING CENTER

The last day of ACNS2008, Thursday, was reserved for a tour of the Manuel Lujan Jr. Neutron Scattering Center, the user facility at LANSCE, Los Alamos National Laboratory. 40 ACNS participants took part in the tour. The group left Santa Fe in the morning and was brought “up the hill” by Thomas Proffen (NPDF), Leilani Conradson (LANSCE user program coordinator) and Aundrea Espinosa (Lujan Center). Luke Daemen (FDS), Sven Vogel (HIPPO), Jim Rhyne (deputy leader for science @ Lujan Center) and Alan Hurd (group leader for the Lujan Center) served as tour guides for the two experimental halls and instruments at the Lujan Center. The Manuel Lujan

Jr. Neutron Scattering Center employs a pulsed spallation neutron source equipped with time-of-flight spectrometers for neutron scattering studies of condensed-matter. Instruments are located in two experimental rooms, ER1 and ER2 and are part of the Lujan Center complex. Visit their website lansce.lanl.gov/lujan/ for additional information.

Artwork at the Eldorado Hotel, venue of ACNS 2008

The Meeting Scene e-mail was compiled and edited by Dr. Gopal Rao, Web Science Editor, MRS, with contributions by Mikhail Zhernenkov, Alice I. Acatrinei and Chad Miller, of Los Alamos National Lab.

Comments and feedback are welcome.

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